# Formal verification of quantum algorithms using quantum Hoare logic

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- Quantum programming languages have been developing rapidly in recent years:

  $\mathcal{Q}$wire, LIQUi$|\rangle$, Q$\#$, OpenQASM, Cirq, ProjectQ, etc.

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Deductive verification can help: no need for simulation or traversing the state space.

# Classical vs. Quantum programming

| Classical | Quantum |
| --- | --- |
| Variable (bit) | Qubit |
| State (function) | Density matrix |
| Assignment | Unitary transformation |
| Conditional | Measurement |
| Assertion / predicate | Quantum predicate |
| Entailment of predicates | Löwner order |

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- A *mixed state* on $n$ qubits is given by a *density matrix* with dimension $2^n \times 2^n$.

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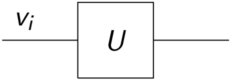
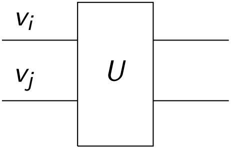
Unitary transformations may act on one or more variables:




$U$ acts on $V_i$




$U$ acts on $V_i \otimes V_j$

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Measurement using hermitian matrices $M_1, \ldots, M_n$ satisfying $\sum_i M_i^\dagger M_i = I_N$.

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Measurement returns a result between 1 and $n$, and can modify the state!

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- Evalution of $P$ on density state $\rho$ is given by $\mathrm{tr}(P\rho)$. (intuition: probability that $\rho$ satisfies $P$).
- Assertion $P$ entails assertion $Q$ if $P \leq_L Q$.

# Quantum Hoare logic (TOPLAS, 2011)

Syntax:

$$S ::= \textbf{skip} \mid \overline{q} = U[\overline{q}] \mid S_1; S_2 \mid \textbf{measure } M[\overline{q}] : \overline{S}$$
$$\mid \textbf{while } M[\overline{q}] = 1 \textbf{ do } S$$

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Semantics (mapping of density matrices):

$[\![\textbf{skip}]\!](\rho) = \rho.$
$[\![\overline{q} = U[\overline{q}]]\!](\rho) = U\rho U^\dagger.$
$[\![S_1; S_2]\!](\rho) = [\![S_2]\!]([\![S_1]\!](\rho)).$
$[\![\textbf{measure}\ M[\overline{q}] : \overline{S}]\!](\rho) = \sum_m [\![S_m]\!](M_m \rho M_m^\dagger).$
$[\![\textbf{while}\ M[\overline{q}] = 1\ \textbf{do}\ S]\!](\rho) = \sum_{k=0}^{\infty} \mathcal{E}_0 \circ ([\![S]\!] \circ \mathcal{E}_1)^k(\rho),$
where $\mathcal{E}_i(\rho) = M_i \rho M_i^\dagger$ for $i = 0, 1$.

# Quantum Hoare logic: semantic correctness

The correctness formula $\{P\}S\{Q\}$ is true in the sense of partial correctness, written

$$\models_p \{P\}S\{Q\}$$

if we have

$$\mathrm{tr}(P\rho) \leq \mathrm{tr}(Q[\![S]\!](\rho)) + [\mathrm{tr}(\rho) - \mathrm{tr}([\![S]\!](\rho))]$$

for all density operator $\rho$ in the state space of $S$.

# Quantum Hoare logic: reasoning rules

**(Skip)** $\{P\}\ \mathbf{skip}\ \{P\}$

**(UT)** $\{U^\dagger P U\}\ \overline{q} := U\overline{q}\ \{P\}$

**(Seq)** $$\frac{\{P\}\ S_1\ \{Q\} \qquad \{Q\}\ S_2\ \{R\}}{\{P\}\ S_1; S_2\ \{R\}}$$

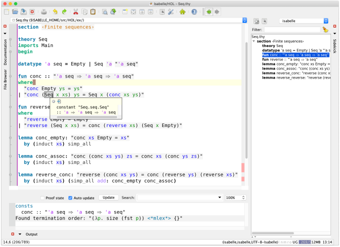
**(Mea)** $$\frac{\{P_m\}\ S_m\ \{Q\}\ \text{for all}\ m}{\{\sum_m {M_m}^\dagger P_m M_m\}\ \mathbf{measure}\ M[\overline{q}] : \overline{S}\ \{Q\}}$$

**(Loop)** $$\frac{\{Q\}\ S\ \{M_0^\dagger P M_0 + M_1^\dagger Q M_1\}}{\{M_0^\dagger P M_0 + M_1^\dagger Q M_1\}\ \mathbf{while}\ M[\overline{q}] = 1\ \mathbf{do}\ S\ \{P\}}$$

**(Order)** $$\frac{P \leq_L P' \quad \{P'\}\ S\ \{Q'\} \quad Q' \leq_L Q}{\{P\}\ S\ \{Q\}}$$

# Isabelle/HOL

- Proof assistant based on higher-order logic.
- Extensive library for analysis and linear algebra, including some material on complex matrices.



# Formalization of Quantum Hoare logic

Our work:

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Our work:

- Continued development of Isabelle/HOL's library in linear algebra, adding properties of positivity, hermitian and unitary matrices.
- Results about limits of matrices.
- Formally verified soundness and completeness of the deduction system (for partial correctness).
- Library for working with tensor products of vectors and matrices (for reasoning about operations on a subset of variables).

# Syntax

```
datatype com =
  SKIP
| Utrans "complex mat"
| Seq com com  ("_;;/ _" [60, 61] 60)
| Measure nat "nat ⇒ complex mat" "com list"
| While "nat ⇒ complex mat" com
```

# Semantics

```
fun denote :: "com ⇒ state ⇒ state" where
   "denote SKIP ϱ = ϱ"
 | "denote (Utrans U) ϱ = U * ϱ * adjoint U"
 | "denote (Seq S1 S2) ϱ = denote S2 (denote S1 ϱ)"
 | "denote (Measure n M S) ϱ =
      denote_measure n M (map denote S) ϱ"
 | "denote (While M S) ϱ =
       denote_while (M 0) (M 1) (denote S) ϱ"
```

# Reasoning rules

```
inductive hoare_partial :: "complex mat ⇒ com ⇒ complex mat ⇒ bool"
  ("⊢p ({(1_)}/ (_)/ {(1_)})" 50) where
  "is_quantum_predicate P ⟹ ⊢p {P} SKIP {P}"
| "is_quantum_predicate P ⟹ ⊢p {adjoint U * P * U} Utrans U {P}"
| "is_quantum_predicate P ⟹ is_quantum_predicate Q ⟹ is_quantum_predicate R ⟹
   ⊢p {P} S1 {Q} ⟹ ⊢p {Q} S2 {R} ⟹
   ⊢p {P} Seq S1 S2 {R}"
| "(⋀k. k < n ⟹ is_quantum_predicate (P k)) ⟹ is_quantum_predicate Q ⟹
   (⋀k. k < n ⟹ ⊢p {P k} S ! k {Q}) ⟹
   ⊢p {matrix_sum d (λk. adjoint (M k) * P k  * M k) n} Measure n M S {Q}"
| "is_quantum_predicate P ⟹ is_quantum_predicate Q ⟹
   ⊢p {Q} S {adjoint (M 0) * P * M 0 + adjoint (M 1) * Q * M 1} ⟹
   ⊢p {adjoint (M 0) * P * M 0 + adjoint (M 1) * Q * M 1} While M S {P}"
| "is_quantum_predicate P ⟹ is_quantum_predicate Q ⟹ is_quantum_predicate P' ⟹
   is_quantum_predicate Q' ⟹ P ≤L P' ⟹ ⊢p {P'} S {Q'} ⟹ Q' ≤L Q ⟹ ⊢p {P} S {Q}"
```

# Soundness and completeness

```
theorem hoare_partial_sound:
  "⊢p {P} S {Q} ⟹ well_com S ⟹
   ⊨p {P} S {Q}"

theorem hoare_partial_complete:
  "⊨p {P} S {Q} ⟹ well_com S ⟹
   is_quantum_predicate P ⟹
   is_quantum_predicate Q ⟹
   ⊢p {P} S {Q}"
```

# Application: Grover's algorithm

- Given a set of $N$ elements, $M$ of which satisfy $f(x) = 1$ for some boolean function $f$ (think $M \ll N$). Find one such element.

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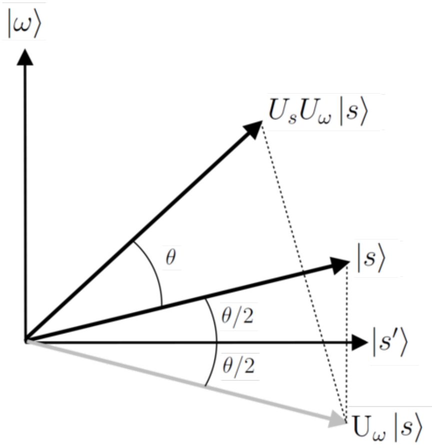
- Grover's algorithm finds a solution in $O(\sqrt{N/M})$ calls to the oracle.

# Grover's algorithm: intuition




- $|s'\rangle$ contains *bad* elements, $|\omega\rangle$ contains *good* elements.

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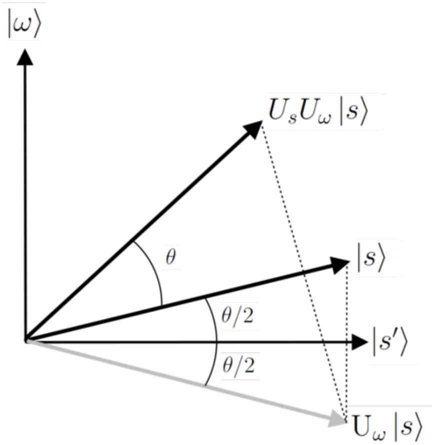


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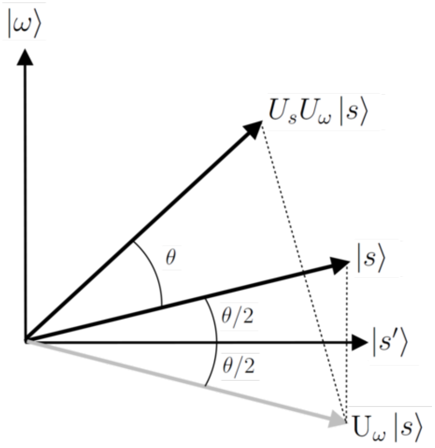


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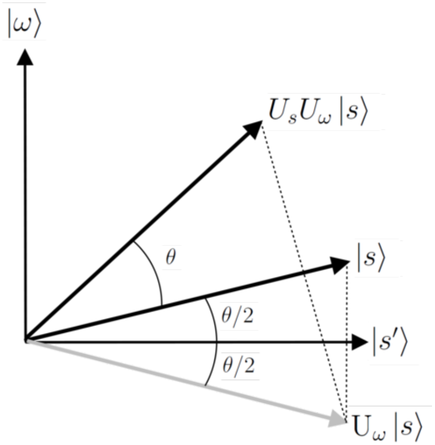


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- Start from $|s\rangle$, a linear combination of $|s'\rangle$ and $|\omega\rangle$, closer to $|s'\rangle$.
- Each iteration rotates the state towards $|\omega\rangle$.
- The number of rotations is $O(\sqrt{N/M})$.

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# Grover's algorithm: the verification

$$
\begin{array}{l}
q_0 q_1 \ldots q_{n-1} := H^{\otimes n}[q_0 q_1 \ldots q_{n-1}]; \\
\textbf{while } M[q_n] = 1 \textbf{ do} \\
\quad q_0 q_1 \ldots q_{n-1} := U_f[q_0 q_1 \ldots q_{n-1}]; \\
\quad q_0 q_1 \ldots q_{n-1} := H^{\otimes n}[q_0 q_1 \ldots q_{n-1}]; \\
\quad q_0 q_1 \ldots q_{n-1} := Ph[q_0 q_1 \ldots q_{n-1}]; \\
\quad q_0 q_1 \ldots q_{n-1} := H^{\otimes n}[q_0 q_1 \ldots q_{n-1}]; \\
\quad q_n := Inc[q_n]; \\
\textbf{measure } N[q_0 q_1 \ldots q_{n-1}] : \overline{\textbf{skip}}
\end{array}
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**while** $M[q_n] = 1$ **do** *Compare counter*

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\quad q_0 q_1 \ldots q_{n-1} := U_f[q_0 q_1 \ldots q_{n-1}]; & \textit{Oracle call} \\
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$\{\ |0\rangle_{\overline{q}}\langle 0| \otimes |0\rangle_{q_n}\langle 0|\ \}$

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$\quad \{\ \sum_{k=0}^{R} |\psi_k\rangle_{\overline{q}}\langle \psi_k| \otimes |k\rangle_{q_n}\langle k|\ \}$

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# Grover's algorithm: end of proof

```
theorem grover_partial_correct:
  "⊨p
   {tensor_P pre (proj_k 0)}
    Grover
   {tensor_P post (1m K)}"
  using grover_partial_deduct well_com_Grover qp_pre qp_post
        hoare_partial_sound by auto
```

# Statistics

| Description | Files | Lines of proof |
|---|---|---|
| Preliminaries | *Complex_Matrix, ...* | 4193 |
| Semantics | *Quantum_Program* | 1110 |
| Hoare logic | *Quantum_Hoare* | 1417 |
| Tensor product | *Partial_State* | 1664 |
| Grover's algorithm | *Grover* | 3184 |
| Total | | 11568 |

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- Automation for working with linear algebra is very helpful.
- Currently, can automatically prove:

$$
\begin{aligned}
\mathrm{tr}(MM^\dagger(PP^\dagger)) &= \mathrm{tr}((P^\dagger M)(P^\dagger M)^\dagger) \\
\mathrm{tr}(M_0AM_0^\dagger) + \mathrm{tr}(M_1AM_1^\dagger) &= \mathrm{tr}((M_0^\dagger M_0 + M_1^\dagger M_1)A) \\
H^\dagger(Ph^\dagger(H^\dagger Q_2 H)Ph)H &= (HPhH)^\dagger Q_2(HPhH)
\end{aligned}
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