

Toward Automatic Verification of Quantum Programs

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Outline

Motivation

A Quantum Programming Language

Floyd-Hoare Logic for Quantum Programs

Invariant Generation

Summary

Verification of Quantum Programs

Motivation

- ▶ quantum programs: *less intuitive* and *error-prone*.

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- ▶ QPL practice: Quipper, QWIRE, Scaffold, Q#, qiskit, Forrest, ProjectQ, ...

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Issues with Verifications

- ▶ The object of verification?

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Possible Long-term Target

- ▶ **Scalable and Principled Verification of Quantum Programs!**
- ▶ a library of verified quantum programs; automated tools to assist programmer; ...

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Quantum While-Language

Syntax

A *core* language for imperative quantum programming

$$\begin{aligned} S ::= & \mathbf{skip} \mid q := |0\rangle \\ & \mid S_1; S_2 \\ & \mid \bar{q} := U[\bar{q}] \\ & \mid \mathbf{if} (\square m \cdot M[\bar{q}] = m \rightarrow S_m) \mathbf{fi} \\ & \mid \mathbf{while} M[\bar{q}] = 1 \mathbf{do} S \mathbf{od} \end{aligned}$$

Operational Semantics

A *configuration*: $\langle S, \rho \rangle$

- ▶ S is a quantum program or E (the empty program)
- ▶ ρ is a partial density operator in

$$\mathcal{H}_{\text{all}} = \bigotimes_{\text{all } q} \mathcal{H}_q$$

Operational Semantics

$$(Sk) \quad \frac{}{\langle \mathbf{skip}, \rho \rangle \rightarrow \langle E, \rho \rangle}$$

$$(Ini) \quad \frac{}{\langle q := |0\rangle, \rho \rangle \rightarrow \langle E, \rho_0^q \rangle}$$

- ▶ $type(q) = \mathbf{Boolean}$:

$$\rho_0^q = |0\rangle_q \langle 0| \rho |0\rangle_q \langle 0| + |0\rangle_q \langle 1| \rho |1\rangle_q \langle 0|$$

- ▶ $type(q) = \mathbf{integer}$:

$$\rho_0^q = \sum_{n=-\infty}^{\infty} |0\rangle_q \langle n| \rho |n\rangle_q \langle 0|$$

Operational Semantics

$$(Uni) \quad \frac{}{\langle \bar{q} := U[\bar{q}], \rho \rangle \rightarrow \langle E, U\rho U^+ \rangle}$$

$$(Seq) \quad \frac{\langle S_1, \rho \rangle \rightarrow \langle S'_1, \rho' \rangle}{\langle S_1; S_2, \rho \rangle \rightarrow \langle S'_1; S_2, \rho' \rangle}$$

Convention : $E; S_2 = S_2$.

$$(IF) \quad \frac{}{\langle \mathbf{if} (\Box m \cdot M[\bar{q}] = m \rightarrow S_m) \mathbf{fi}, \rho \rangle \rightarrow \langle S_m, M_m \rho M_m^+ \rangle}$$

for each outcome m

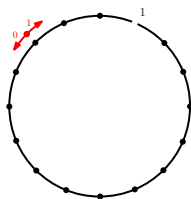
Operational Semantics

$$(L0) \quad \frac{}{\langle \mathbf{while} \ M[\bar{q}] = 1 \ \mathbf{do} \ S \ \mathbf{od}, \rho \rangle \rightarrow \langle E, M_0 \rho M_0^+ \rangle}$$

$$(L1) \quad \frac{}{\langle \mathbf{while} \ M[\bar{q}] = 1 \ \mathbf{do} \ S, \rho \rangle \rightarrow \langle S; \mathbf{while} \ M[\bar{q}] = 1 \ \mathbf{do} \ S, M_1 \rho M_1^+ \rangle}$$

Quantum 1-D Loop Walk

```
QW  $\equiv$   $c := |L\rangle$ ;  
     $p := |0\rangle$ ;  
    while  $M[p] = no$  do  
         $c := H[c]$ ;  
         $c, p := S[c, p]$   
    od
```



Operator Definition

$$S = \sum_{i=0}^{n-1} |L\rangle\langle L| \otimes |i \ominus 1\rangle\langle i| + \sum_{i=0}^{n-1} |R\rangle\langle R| \otimes |i \oplus 1\rangle\langle i|.$$

Denotational Semantics

Semantic function of quantum program S :

$$\llbracket S \rrbracket : \mathcal{D}(\mathcal{H}_{\text{all}}) \rightarrow \mathcal{D}(\mathcal{H}_{\text{all}})$$

$$\llbracket S \rrbracket(\rho) = \sum \{ |\rho'\rangle : \langle S, \rho \rangle \rightarrow^* \langle E, \rho' \rangle | \} \text{ for all } \rho \in \mathcal{D}(\mathcal{H}_{\text{all}})$$

Observation:

$$\text{tr}(\llbracket S \rrbracket(\rho)) \leq \text{tr}(\rho)$$

for any quantum program S and all $\rho \in \mathcal{D}(\mathcal{H}_{\text{all}})$.

- ▶ $\text{tr}(\rho) - \text{tr}(\llbracket S \rrbracket(\rho))$ is the probability that program S diverges from input state ρ .

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Definitions

- ▶ A *quantum predicate* is a Hermitian operator (observable) P such that $0 \sqsubseteq P \sqsubseteq I$.

[1] E. D'Hondt and P. Panangaden, Quantum weakest preconditions, *Mathematical Structures in Computer Science* 2006.

- ▶ A *correctness formula* is a statement of the form:

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

where:

- ▶ S is a quantum program
- ▶ P and Q are quantum predicates.
- ▶ Operator P is called the *precondition* and Q the *postcondition*.

Definitions

1. $\{P\}S\{Q\}$ is true in the sense of *total correctness*:

$$\models_{\text{tot}} \{P\}S\{Q\}$$

if

$$\text{tr}(P\rho) \leq \text{tr}(Q\llbracket S \rrbracket(\rho)) \text{ for all } \rho.$$

2. $\{P\}S\{Q\}$ is true in the sense of *partial correctness*:

$$\models_{\text{par}} \{P\}S\{Q\},$$

if

$$\text{tr}(P\rho) \leq \text{tr}(Q\llbracket S \rrbracket(\rho)) + [\text{tr}(\rho) - \text{tr}(\llbracket S \rrbracket(\rho))]$$

for all ρ .

Proof System for Partial Correctness

$$(Axiom\ Sk) \quad \{P\} \mathbf{Skip} \{P\}$$

$$(Axiom\ Ini)$$

$$type(q) = \mathbf{Boolean} :$$

$$\{|0\rangle_q \langle 0|P|0\rangle_q \langle 0| + |1\rangle_q \langle 0|P|0\rangle_q \langle 1|\}q := |0\rangle \{P\}$$

$$type(q) = \mathbf{integer} :$$

$$\left\{ \sum_{n=-\infty}^{\infty} |n\rangle_q \langle 0|P|0\rangle_q \langle n| \right\}q := |0\rangle \{P\}$$

$$(Axiom\ Uni) \quad \{U^\dagger P U\} \bar{q} := U[\bar{q}] \{P\}$$

Proof System for Partial Correctness

$$(Rule\ Seq) \quad \frac{\{P\}S_1\{Q\} \quad \{Q\}S_2\{R\}}{\{P\}S_1;S_2\{R\}}$$

$$(Rule\ IF) \quad \frac{\{P_m\}S_m\{Q\} \text{ for all } m}{\{\sum_m M_m^+ P_m M_m\} \mathbf{if} (\square m \cdot M[\bar{q}] = m \rightarrow S_m) \mathbf{fi}\{Q\}}$$

$$(Rule\ LP) \quad \frac{\{Q\}S\{M_0^+ P M_0 + M_1^+ Q M_1\}}{\{M_0^+ P M_0 + M_1^+ Q M_1\} \mathbf{while} M[\bar{q}] = 1 \mathbf{do} S\{P\}}$$

$$(Rule\ Ord) \quad \frac{P \sqsubseteq P' \quad \{P'\}S\{Q'\} \quad Q' \sqsubseteq Q}{\{P\}S\{Q\}}$$

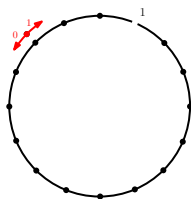
Theorem (Soundness and Completeness)

For any quantum program S and quantum predicates P, Q ,

$$\models_{\text{par}} \{P\}S\{Q\} \text{ if and only if } \vdash_{PD} \{P\}S\{Q\}.$$

Quantum 1-D Loop Walk

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QW  $\equiv$   $c := |L\rangle$ ;  
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Operator Definition

$$S = \sum_{i=0}^{n-1} |L\rangle\langle L| \otimes |i \ominus 1\rangle\langle i| + \sum_{i=0}^{n-1} |R\rangle\langle R| \otimes |i \oplus 1\rangle\langle i|.$$

Proof System for Total Correctness

Let P be a quantum predicate and $\epsilon > 0$. A function

$$t : \mathcal{D}(\mathcal{H}_{\text{all}}) \text{ (density operators)} \rightarrow \mathbb{N}$$

is called a (P, ϵ) -*ranking function* of quantum loop:

while $M[\bar{q}] = 1$ **do** S **od**

if for all ρ :

1. $t(\llbracket S \rrbracket(M_1 \rho M_1^\dagger)) \leq t(\rho)$;
2. $\text{tr}(P\rho) \geq \epsilon$ implies $t(\llbracket S \rrbracket(M_1 \rho M_1^\dagger)) < t(\rho)$

Proof System for Total Correctness

(1) $\{Q\}S\{M_0^\dagger PM_0 + M_1^\dagger QM_1\}$

(2) for any $\epsilon > 0$, t_ϵ is a $(M_1^\dagger QM_1, \epsilon)$ -ranking
function of loop

(Rule LT)
$$\frac{\{M_0^\dagger PM_0 + M_1^\dagger QM_1\} \mathbf{while} M[\bar{q}] = 1 \mathbf{do} S \mathbf{od} \{P\}}{\{M_0^\dagger PM_0 + M_1^\dagger QM_1\} \mathbf{while} M[\bar{q}] = 1 \mathbf{do} S \mathbf{od} \{P\}}$$

Theorem (Soundness and Completeness)

For any quantum program S and quantum predicates $P Q$,

$$\models_{\text{tot}} \{P\}S\{Q\} \text{ if and only if } \vdash_{TD} \{P\}S\{Q\}.$$

[2] M. S. Ying, Floyd-Hoare logic for quantum programs, *ACM Transactions on Programming Languages and Systems* 2011

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Super-Operator Labelled Graphs

A super-operator labelled graph is a 4-tuple $\mathcal{G} = \langle \mathcal{H}, L, l_0, \rightarrow \rangle$:

1. \mathcal{H} is a Hilbert space;
2. L is a finite set of locations;
3. $l_0 \in L$ is the initial location
4. transition relation

$$l \xrightarrow{\mathcal{E}} l'$$

with $l, l' \in L$, \mathcal{E} a super-operator: for every $l \in L$,

$$\sum \{ |\mathcal{E} : l \xrightarrow{\mathcal{E}} l' \text{ for some } l' | \} \approx \mathcal{I}.$$

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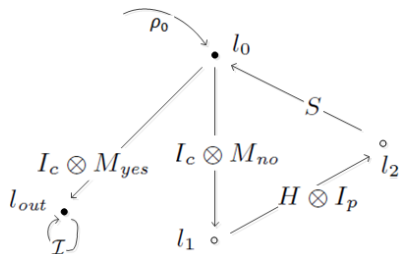
$$\sum \{ |\mathcal{E} : l \xrightarrow{\mathcal{E}} l' \text{ for some } l' | \} \approx \mathcal{I}.$$

Control-Flow Graph of Quantum Programs

A quantum program P can be represented by a graph \mathcal{G}_P .

Quantum 1-D Loop Walk

$QW \equiv c := |L\rangle;$
 $p := |0\rangle;$
while $M[p] = no$ **do**
 $c := H[c];$
 $c, p := S[c, p]$
od



Operator Definition

$$S = \sum_{i=0}^{n-1} |L\rangle\langle L| \otimes |i \ominus 1\rangle\langle i| + \sum_{i=0}^{n-1} |R\rangle\langle R| \otimes |i \oplus 1\rangle\langle i|.$$

Invariants

- ▶ A set Π of paths is *prime* if for each

$$\pi = l_1 \xrightarrow{\mathcal{E}_1} \dots \xrightarrow{\mathcal{E}_{n-1}} l_n \in \Pi$$

its proper initial segments $l_1 \xrightarrow{\mathcal{E}_1} \dots \xrightarrow{\mathcal{E}_{k-1}} l_k \notin \Pi$ for all $k < n$.

- ▶ Let $\mathcal{G} = \langle \mathcal{H}, L, l_0, \rightarrow \rangle$, Θ a quantum predicate (initial condition), $l \in L$. An *invariant* at l is a quantum predicate O such that for any density operator ρ , any prime set Π of paths from l_0 to l :

$$\text{tr}(\Theta\rho) \leq 1 - \text{tr}(\mathcal{E}_\Pi(\rho)) + \text{tr}(O\mathcal{E}_\Pi(\rho))$$

where $\mathcal{E}_\Pi = \sum \{|\mathcal{E}_\pi : \pi \in \Pi|\}$.

Theorem (Partial Correctness)

Let P be a quantum program. If O is an invariant at l_{out}^P in \mathcal{S}_P , then

$$\models_{par} \{\Theta\}P\{O\}$$

Inductive Assertion Maps

- ▶ Given $\mathcal{G} = \langle \mathcal{H}, L, l_0, \rightarrow \rangle$ with a cutset C and initial condition Θ .
- ▶ An *assertion map* is a mapping η from each cutpoint $l \in C$ to a quantum predicate $\eta(l)$.
- ▶ Π_l : the set of all basic paths from l to some cutpoint.
- ▶ l_π : the last location in a path π .
- ▶ An assertion map η is *inductive* if:
 - ▶ **Initiation:** for any density operator ρ :

$$\text{tr}(\Theta\rho) \leq 1 - \text{tr}(\mathcal{E}_{\Pi_{l_0}}(\rho)) + \sum_{\pi \in \Pi_{l_0}} \text{tr}(\eta(l_\pi)\mathcal{E}_\pi(\rho));$$

- ▶ **Consecution:** for any density operator ρ , each cutpoint $l \in C$:

$$\text{tr}(\eta(l)\rho) \leq 1 - \text{tr}(\mathcal{E}_{\Pi_l}(\rho)) + \sum_{\pi \in \Pi_l} \text{tr}(\eta(l_\pi)\mathcal{E}_\pi(\rho)).$$

Theorem (Invariance)

If η is an inductive assertion map, then for every cutpoint $l \in C$, $\eta(l)$ is an invariant at l .

Invariant Generation Problem

Given $\mathcal{G} = \langle \mathcal{H}, L, l_0, \Theta, \rightarrow \rangle$ with a cutset $C \subseteq L$. For each cutpoint $l \in C$, find a quantum predicate $\eta(l)$ such that $\eta : l \mapsto \eta(l)$ is an inductive map.

Reduce to a SDP (Semi-Definite Programming) Problem

- ▶ Assume $C = \{l_0, l_1, \dots, l_m\}$.
- ▶ Write $O_i = \eta(l_i)$ for $i = 0, 1, \dots, m$.
- ▶ $\mathcal{E}_{ij}^* = \sum\{|\mathcal{E}_\pi^* : \text{basic path } l_i \xrightarrow{\pi} l_j \mid\}$ for $i, j = 0, 1, \dots, m$.

Theorem

Invariant Generation Problem is equivalent to find complex matrices O_0, O_1, \dots, O_m satisfying the constraints:

$$0 \sqsubseteq \sum_j \mathcal{E}_{0j}^*(O_j) + A,$$

$$0 \sqsubseteq \sum_{j \neq i} \mathcal{E}_{ij}^*(O_j) + (\mathcal{E}_{ii}^* - \mathcal{I})(O_i) + A_i \quad (i = 0, 1, \dots, m),$$

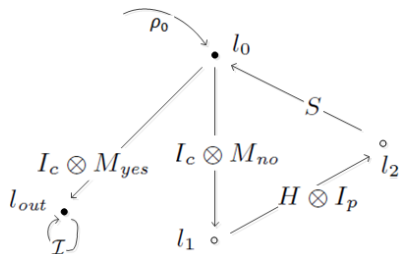
$$0 \sqsubseteq O_i \sqsubseteq I \quad (i = 0, 1, \dots, m),$$

where:

$$\begin{cases} A = I - \sum_j \mathcal{E}_{0j}^*(I) - \Theta, \\ A_i = I - \sum_j \mathcal{E}_{ij}^*(I) \quad (i = 0, 1, \dots, m). \end{cases}$$

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Invariant SDPs for Quantum 1-D Loop Walk

Choose cut-set $C = \{l_0, l_3\}$ with $l_3 = l_{out}$. $\Theta = I$. Invariants O_0 and O_3 satisfy the following constraints:

$$0 \sqsubseteq \mathcal{E}_{00}^*(O_0) + \mathcal{E}_{03}^*(O_3) - \Theta, \quad (1)$$

$$0 \sqsubseteq (\mathcal{E}_{00}^* - \mathcal{I})(O_0) + \mathcal{E}_{03}^*(O_3), \quad (2)$$

$$0 \sqsubseteq (\mathcal{E}_{33}^* - \mathcal{I})(O_3) - (I - \mathcal{E}_{33}^*(I)), \quad (3)$$

$$0 \sqsubseteq O_0, O_3 \sqsubseteq I \quad (4)$$

$$\mathbb{E}_{00} = E_{00} \circ E_{00}^\dagger, \mathbb{E}_{03} = E_{03} \circ E_{03}^\dagger, \mathbb{E}_{33} = \mathcal{I},$$

$$E_{00} = S(H \otimes I_p)(I_c \otimes M_{no}), E_{03} = I_c \otimes M_{yes}, \text{ and } I_c, I_p \text{ identities.}$$

Invariant SDPs for Quantum 1-D Loop Walk

Choose cut-set $C = \{l_0, l_3\}$ with $l_3 = l_{out}$. $\Theta = I$. Invariants O_0 and O_3 satisfy the following constraints:

$$0 \sqsubseteq \mathcal{E}_{00}^*(O_0) + \mathcal{E}_{03}^*(O_3) - \Theta, \quad (1)$$

$$0 \sqsubseteq (\mathcal{E}_{00}^* - \mathcal{I})(O_0) + \mathcal{E}_{03}^*(O_3), \quad (2)$$

$$0 \sqsubseteq (\mathcal{E}_{33}^* - \mathcal{I})(O_3) - (I - \mathcal{E}_{33}^*(I)), \quad (3)$$

$$0 \sqsubseteq O_0, O_3 \sqsubseteq I \quad (4)$$

$\mathbb{E}_{00} = E_{00} \circ E_{00}^\dagger$, $\mathbb{E}_{03} = E_{03} \circ E_{03}^\dagger$, $\mathbb{E}_{33} = \mathcal{I}$,
 $E_{00} = S(H \otimes I_p)(I_c \otimes M_{no})$, $E_{03} = I_c \otimes M_{yes}$, and I_c, I_p identities.

Solution

- ▶ $O_3 = I_c \otimes |1\rangle\langle 1| \rightarrow \text{tr}(O_3 \rho_{out}) \geq \text{tr}(\Theta \rho_{in}) = 1$, i.e., always terminates at the position $|1\rangle$ regardless of the input state ρ_0 . (O_0 omitted.)

Solving Constraints: *Use SDP solvers!*

Applications

- ▶ Quantum walk on an n -circle. [3]
- ▶ Quantum Metropolis sampling on n -qubits. (1-qubit in [3])
- ▶ Repeat-Until-Success.
- ▶ Quantum Search.
- ▶ Quantum Bernoulli Factory.
- ▶ Recursively written Quantum Fourier Transformation.

[3] M. S. Ying, S. G. Ying and X. Wu, Invariants of quantum programs: characterisations and generation, *POPL* 2017.

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Toward Automatic Verification of Quantum Programs

- ▶ scalable and principled verification!

Existing Techniques

- ▶ Quantum While-language (c. control, q. data).
- ▶ Quantum Hoare logic.
- ▶ Invariant Generation by SDPs.

Progress & Targets

- ▶ expressibility: quantum functionality, codespace,
- ▶ scalability: succinct or template representations, quantum verification,

Thank you!

Q & A

Quantum states

- ▶ The *state space* of a quantum system is a *Hilbert space* \mathcal{H} , i.e. a complex vector space with an inner product that is complete in the sense that every Cauchy sequence has a limit.
- ▶ For finite n , an n -dimensional Hilbert space is essentially the space \mathbb{C}^n of complex vectors.
- ▶ A *pure quantum state* is represented by a *unit vector*, i.e. a vector with length 1.
- ▶ We use Dirac's notation $|\varphi\rangle, |\psi\rangle, \dots$ to denote pure states.

Qubits

- ▶ A *Quantum bit* (qubit) is the quantum counterpart of *bit*.
- ▶ The state space of a qubit is the 2-dimensional Hilbert space.
- ▶ A pure state of qubit is:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad \text{with } |\alpha|^2 + |\beta|^2 = 1.$$

- ▶ A qubit can be in the basis states:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- ▶ A qubit can also be in a superposition of $|0\rangle, |1\rangle$, e.g.

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Mixed states

- ▶ A *mixed state* is represented by an *ensemble*

$$\{(p_1, |\psi_1\rangle), \dots, (p_k, |\psi_k\rangle)\}$$

meaning that the system is in state $|\psi_i\rangle$ with probability p_i .

- ▶ It is a quantum generalisation of a probability distribution over states.

Density matrices

- ▶ In the n -dimensional Hilbert space \mathbb{C}^n , an operator is represented by an $n \times n$ complex matrix A .
- ▶ The trace of an operator A is $tr(A) = \sum_i A_{ii}$ (the sum of the entries on the main diagonal).
- ▶ A positive semidefinite matrix ρ is called a *partial density matrix* if $tr(\rho) \leq 1$; in particular, a *density matrix* ρ is a partial density matrix with $tr(\rho) = 1$.

Mixed states = density matrices

- ▶ Matrix $|\psi\rangle\langle\psi|$ is the multiplication of column vector $|\psi\rangle$ and the row vector $\langle\psi|$ (the conjugate and transpose of $|\psi\rangle$).
- ▶ For any mixed state $\{(p_1, |\psi_1\rangle), \dots, (p_k, |\psi_k\rangle)\}$,

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

is a density operator

- ▶ For any density operator ρ , there is a mixed state $\{(p_1, |\psi_1\rangle), \dots, (p_k, |\psi_k\rangle)\}$ such that

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|.$$

- ▶ In particular, a pure state $|\psi\rangle$ is identified with the density operator $\rho = |\psi\rangle\langle\psi|$.

Mixed states = density matrices

- ▶ Mixed state of a qubit:

$$\left\{ \left(\frac{2}{3}, |0\rangle \right), \left(\frac{1}{3}, |-\rangle \right) \right\} \text{ with } |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

- ▶ Density matrix:

$$\rho = \frac{2}{3}|0\rangle\langle 0| + \frac{1}{3}|-\rangle\langle -| = \frac{1}{6} \begin{pmatrix} 5 & -1 \\ -1 & 1 \end{pmatrix}$$

Unitary matrices

- ▶ *Dynamics* of a closed quantum system is described by a *unitary matrix*:

$$|\psi\rangle \mapsto U|\psi\rangle$$

- ▶ A matrix U is unitary if $U^\dagger U = I$, where U^\dagger is the conjugate and transpose of U
- ▶ Hadamard matrix

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

is an unitary operator in the 2-dimensional Hilbert space

- ▶ $H|0\rangle = |+\rangle$, $H|1\rangle = |-\rangle$

Quantum gates – one-qubit gates

- ▶ Pauli gates:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- ▶ Hadarmard gate:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

- ▶ Rotation about x -axis of the Bloch sphere:

$$R_x(\theta) = \begin{pmatrix} \cos \frac{\theta}{2} & -i \sin \frac{\theta}{2} \\ -i \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix}$$

Quantum gates – two-qubit gate

- ▶ The controlled-NOT (CNOT) gate:

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

- ▶ *CNOT generates entanglement*: separable state $|+0\rangle$ is transformed to EPR (Einstein-Podolsky-Rosen) pair:

$$CNOT(|+0\rangle) = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Super-operators

- ▶ *Dynamics* of an open quantum system is described by a *super-operator*:

$$\rho \mapsto \mathcal{E}(\rho)$$

- ▶ A super-operator is a mapping \mathcal{E} from partial density operators to themselves:
 - ▶ completely positive;
 - ▶ $\text{tr}(\mathcal{E}(\rho)) \leq \text{tr}(\rho)$ for all ρ .
- ▶ A super-operator can be seen as a quantum counterpart of a transformation of probability distributions.

Kraus representation

- ▶ Löwner order: $A \sqsubseteq B$ if and only if $B - A$ is positive semidefinite.
- ▶ Each super-operator \mathcal{E} has a Kraus representation:

$$\mathcal{E}(\rho) = \sum_i E_i \rho E_i^\dagger$$

for all density matrices ρ , where the set $\{E_i\}$ of matrices satisfies the sub-normalisation condition: $\sum_i E_i^\dagger E_i \sqsubseteq I$

- ▶ We often write $\mathcal{E} = \sum_i E_i \circ E_i^\dagger$.

Quantum measurements

- ▶ The way to extract information about a quantum system is quantum measurement.
- ▶ In quantum computation, measurement is used to read out a computational result.
- ▶ A *measurement* is modelled as a set of operators $M = \{M_m\}$ with $\sum_m M_m^\dagger M_m = I$.
- ▶ If a quantum system was in pure state $|\psi\rangle$ before the measurement, then:
 - ▶ the probability that measurement outcome is λ :

$$p(m) = \|M_m|\psi\rangle\|^2$$

where $\|\cdot\|$ is the length of vector.

- ▶ the state of the system after the measurement:

$$\frac{M_m|\psi\rangle}{\sqrt{p(m)}}$$

Quantum measurements

- ▶ If we perform a measurement M on a system in state ρ , then:
 - ▶ an outcome m is observed with probability
$$p(m) = \text{tr}(M_m \rho M_m^\dagger);$$
 - ▶ after that, the system will be in state $M_m \rho M_m^\dagger / p(m)$.

- ▶ A major difference between classical and quantum systems:
 - ▶ *Measuring a classical system does not change its state.*
 - ▶ *The state of a quantum systems is changed after measuring it.*

Quantum measurements – example

- ▶ The measurement on a qubit in the computational basis $\{|0\rangle, |1\rangle\}$ is $M = \{M_0, M_1\}$:

$$M_0 = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad M_1 = |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

- ▶ If we perform M on a qubit in state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$:
 - ▶ the probability that we get outcome 0 is $|\alpha|^2$;
 - ▶ the probability that we get outcome 1 is $|\beta|^2$.
- ▶ If we perform M on a qubit in (mixed) state

$$\rho = \frac{2}{3}|0\rangle\langle 0| + \frac{1}{3}|+\rangle\langle +| = \frac{1}{6} \begin{pmatrix} 5 & 1 \\ 1 & 1 \end{pmatrix}$$

- ▶ the probability that we get outcome 0 is $p(0) = \text{tr}(M_0\rho M_0) = \frac{5}{6}$ and then the qubit is in state $|0\rangle$.
- ▶ Outcome 1 is obtained with probability $p(1) = \frac{1}{6}$ and after that the qubit is in $|1\rangle$.