

Quantum Hoare Logic

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Abstract

We formalize quantum Hoare logic as given in [1]. In particular, we specify the syntax and denotational semantics of a simple model of quantum programs. Then, we write down the rules of quantum Hoare logic for partial correctness, and show the soundness and completeness of the resulting proof system. As an application, we verify the correctness of Grover’s algorithm.

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1 Complex matrices

```
theory Complex-Matrix
imports
  Jordan-Normal-Form.Matrix
  Jordan-Normal-Form.Conjugate
  Jordan-Normal-Form.Jordan-Normal-Form-Existence
begin
```

1.1 Trace of a matrix

```
definition trace :: 'a::ring mat ⇒ 'a where
  trace A = (Σ i ∈ {0 .. < dim-row A}. A $$ (i,i))
```

```
lemma trace-zero [simp]:
```

```
  trace (0m n n) = 0
  ⟨proof⟩
```

```
lemma trace-id [simp]:
```

```
  trace (1m n) = n
  ⟨proof⟩
```

```

lemma trace-comm:
  fixes A B :: 'a::comm-ring mat
  assumes A: A ∈ carrier-mat n n and B: B ∈ carrier-mat n n
  shows trace (A * B) = trace (B * A)
  ⟨proof⟩

lemma trace-add-linear:
  fixes A B :: 'a::comm-ring mat
  assumes A: A ∈ carrier-mat n n and B: B ∈ carrier-mat n n
  shows trace (A + B) = trace A + trace B (is ?lhs = ?rhs)
  ⟨proof⟩

lemma trace-minus-linear:
  fixes A B :: 'a::comm-ring mat
  assumes A: A ∈ carrier-mat n n and B: B ∈ carrier-mat n n
  shows trace (A - B) = trace A - trace B (is ?lhs = ?rhs)
  ⟨proof⟩

lemma trace-smult:
  assumes A ∈ carrier-mat n n
  shows trace (c ·m A) = c * trace A
  ⟨proof⟩

```

1.2 Conjugate of a vector

```

lemma conjugate-scalar-prod:
  fixes v w :: 'a::conjugatable-ring vec
  assumes dim-vec v = dim-vec w
  shows conjugate (v · w) = conjugate v · conjugate w
  ⟨proof⟩

```

1.3 Inner product

```

abbreviation inner-prod :: 'a vec ⇒ 'a vec ⇒ 'a :: conjugatable-ring
  where inner-prod v w ≡ w · c v

```

```

lemma conjugate-scalar-prod-Im [simp]:
  Im (v · c v) = 0
  ⟨proof⟩

```

```

lemma conjugate-scalar-prod-Re [simp]:
  Re (v · c v) ≥ 0
  ⟨proof⟩

```

```

lemma self-cscalar-prod-geq-0:
  fixes v :: 'a::conjugatable-ordered-field vec
  shows v · c v ≥ 0
  ⟨proof⟩

```

```

lemma inner-prod-distrib-left:
  fixes u v w :: ('a::conjugatable-field) vec
  assumes dimu: u ∈ carrier-vec n and dimv:v ∈ carrier-vec n and dimw: w ∈
carrier-vec n
  shows inner-prod (v + w) u = inner-prod v u + inner-prod w u (is ?lhs = ?rhs)
⟨proof⟩

lemma inner-prod-distrib-right:
  fixes u v w :: ('a::conjugatable-field) vec
  assumes dimu: u ∈ carrier-vec n and dimv:v ∈ carrier-vec n and dimw: w ∈
carrier-vec n
  shows inner-prod u (v + w) = inner-prod u v + inner-prod u w (is ?lhs = ?rhs)
⟨proof⟩

lemma inner-prod-minus-distrib-right:
  fixes u v w :: ('a::conjugatable-field) vec
  assumes dimu: u ∈ carrier-vec n and dimv:v ∈ carrier-vec n and dimw: w ∈
carrier-vec n
  shows inner-prod u (v - w) = inner-prod u v - inner-prod u w (is ?lhs = ?rhs)
⟨proof⟩

lemma inner-prod-smult-right:
  fixes u v :: complex vec
  assumes dimu: u ∈ carrier-vec n and dimv:v ∈ carrier-vec n
  shows inner-prod (a ·v u) v = conjugate a * inner-prod u v (is ?lhs = ?rhs)
⟨proof⟩

lemma inner-prod-smult-left:
  fixes u v :: complex vec
  assumes dimu: u ∈ carrier-vec n and dimv: v ∈ carrier-vec n
  shows inner-prod u (a ·v v) = a * inner-prod u v (is ?lhs = ?rhs)
⟨proof⟩

lemma inner-prod-smult-left-right:
  fixes u v :: complex vec
  assumes dimu: u ∈ carrier-vec n and dimv: v ∈ carrier-vec n
  shows inner-prod (a ·v u) (b ·v v) = conjugate a * b * inner-prod u v (is ?lhs
= ?rhs)
⟨proof⟩

lemma inner-prod-swap:
  fixes x y :: complex vec
  assumes y ∈ carrier-vec n and x ∈ carrier-vec n
  shows inner-prod y x = conjugate (inner-prod x y)
⟨proof⟩

```

Cauchy-Schwarz theorem for complex vectors. This is analogous to aux_Cauchy and Cauchy_Schwarz_ineq in Generalizations2.thy in QR_Decomposition. Consider merging and moving to Isabelle library.

```

lemma aux-Cauchy:
  fixes  $x \ y :: \text{complex vec}$ 
  assumes  $x \in \text{carrier-vec } n$  and  $y \in \text{carrier-vec } n$ 
  shows  $0 \leq \text{inner-prod } x \ x + a * (\text{inner-prod } x \ y) + (\text{cnj } a) * ((\text{cnj } (\text{inner-prod } x \ y)) + a * (\text{inner-prod } y \ y))$ 
   $\langle \text{proof} \rangle$ 

```

```

lemma Cauchy-Schwarz-complex-vec:
  fixes  $x \ y :: \text{complex vec}$ 
  assumes  $x \in \text{carrier-vec } n$  and  $y \in \text{carrier-vec } n$ 
  shows  $\text{inner-prod } x \ y * \text{inner-prod } y \ x \leq \text{inner-prod } x \ x * \text{inner-prod } y \ y$ 
   $\langle \text{proof} \rangle$ 

```

1.4 Hermitian adjoint of a matrix

abbreviation adjoint **where** $\text{adjoint} \equiv \text{mat-adjoint}$

```

lemma adjoint-dim-row [simp]:
   $\text{dim-row } (\text{adjoint } A) = \text{dim-col } A$ 
   $\langle \text{proof} \rangle$ 

```

```

lemma adjoint-dim-col [simp]:
   $\text{dim-col } (\text{adjoint } A) = \text{dim-row } A$ 
   $\langle \text{proof} \rangle$ 

```

```

lemma adjoint-dim:
   $A \in \text{carrier-mat } n \ n \implies \text{adjoint } A \in \text{carrier-mat } n \ n$ 
   $\langle \text{proof} \rangle$ 

```

```

lemma adjoint-def:
   $\text{adjoint } A = \text{mat } (\text{dim-col } A) (\text{dim-row } A) (\lambda(i,j). \text{conjugate } (A \$\$ (j,i)))$ 
   $\langle \text{proof} \rangle$ 

```

```

lemma adjoint-eval:
  assumes  $i < \text{dim-col } A$   $j < \text{dim-row } A$ 
  shows  $(\text{adjoint } A) \$\$ (i,j) = \text{conjugate } (A \$\$ (j,i))$ 
   $\langle \text{proof} \rangle$ 

```

```

lemma adjoint-row:
  assumes  $i < \text{dim-col } A$ 
  shows  $\text{row } (\text{adjoint } A) i = \text{conjugate } (\text{col } A i)$ 
   $\langle \text{proof} \rangle$ 

```

```

lemma adjoint-col:
  assumes  $i < \text{dim-row } A$ 
  shows  $\text{col } (\text{adjoint } A) i = \text{conjugate } (\text{row } A i)$ 
   $\langle \text{proof} \rangle$ 

```

The identity $\langle v, A w \rangle = \langle A^* v, w \rangle$

```

lemma adjoint-def-alter:
  fixes  $v \ w :: 'a::\text{conjugatable-field} \text{ vec}$ 
  and  $A :: 'a::\text{conjugatable-field} \text{ mat}$ 

```

```

assumes dims:  $v \in \text{carrier-vec } n$   $w \in \text{carrier-vec } m$   $A \in \text{carrier-mat } n m$ 
shows inner-prod  $v (A *_v w) = \text{inner-prod} (\text{adjoint } A *_v v) w$  (is ?lhs = ?rhs)
⟨proof⟩

lemma adjoint-one:
fixes  $A :: 'a::\text{conjugatable-field mat}$ 
shows adjoint  $(1_m n) = (1_m n::\text{complex mat})$ 
⟨proof⟩

lemma adjoint-scale:
fixes  $A :: 'a::\text{conjugatable-field mat}$ 
shows adjoint  $(a \cdot_m A) = (\text{conjugate } a) \cdot_m \text{adjoint } A$ 
⟨proof⟩

lemma adjoint-add:
fixes  $A B :: 'a::\text{conjugatable-field mat}$ 
assumes  $A \in \text{carrier-mat } n m$   $B \in \text{carrier-mat } n m$ 
shows adjoint  $(A + B) = \text{adjoint } A + \text{adjoint } B$ 
⟨proof⟩

lemma adjoint-minus:
fixes  $A B :: 'a::\text{conjugatable-field mat}$ 
assumes  $A \in \text{carrier-mat } n m$   $B \in \text{carrier-mat } n m$ 
shows adjoint  $(A - B) = \text{adjoint } A - \text{adjoint } B$ 
⟨proof⟩

lemma adjoint-mult:
fixes  $A B :: 'a::\text{conjugatable-field mat}$ 
assumes  $A \in \text{carrier-mat } n m$   $B \in \text{carrier-mat } m l$ 
shows adjoint  $(A * B) = \text{adjoint } B * \text{adjoint } A$ 
⟨proof⟩

lemma adjoint-adjoint:
fixes  $A :: 'a::\text{conjugatable-field mat}$ 
shows adjoint  $(\text{adjoint } A) = A$ 
⟨proof⟩

lemma trace-adjoint-positive:
fixes  $A :: \text{complex mat}$ 
shows trace  $(A * \text{adjoint } A) \geq 0$ 
⟨proof⟩

```

1.5 Algebraic manipulations on matrices

```

lemma right-add-zero-mat[simp]:
 $(A :: 'a :: \text{monoid-add mat}) \in \text{carrier-mat } nr nc \implies A + 0_m nr nc = A$ 
⟨proof⟩

lemma add-carrier-mat':
 $A \in \text{carrier-mat } nr nc \implies B \in \text{carrier-mat } nr nc \implies A + B \in \text{carrier-mat } nr$ 

```

nc
⟨proof⟩

lemma *minus-carrier-mat'*:

A ∈ carrier-mat nr *nc* ⇒ *B* ∈ carrier-mat nr *nc* ⇒ *A* − *B* ∈ carrier-mat nr
nc
⟨proof⟩

lemma *swap-plus-mat*:

fixes *A B C* :: 'a::semiring-1 mat
assumes *A* ∈ carrier-mat *n n* *B* ∈ carrier-mat *n n* *C* ∈ carrier-mat *n n*
shows *A* + *B* + *C* = *A* + *C* + *B*
⟨proof⟩

lemma *uminus-mat*:

fixes *A* :: complex mat
assumes *A* ∈ carrier-mat *n n*
shows −*A* = (−1) ·_{*m*} *A*
⟨proof⟩

⟨ML⟩

lemma *mat-assoc-test*:

fixes *A B C D* :: complex mat
assumes *A* ∈ carrier-mat *n n* *B* ∈ carrier-mat *n n* *C* ∈ carrier-mat *n n* *D* ∈ carrier-mat *n n*
shows

$$(A * B) * (C * D) = A * B * C * D$$

$$\text{adjoint } (A * \text{adjoint } B) * C = B * (\text{adjoint } A * C)$$

$$A * 1_m n * 1_m n * B * 1_m n = A * B$$

$$(A - B) + (B - C) = A + (-B) + B + (-C)$$

$$A + (B - C) = A + B - C$$

$$A - (B + C + D) = A - B - C - D$$

$$(A + B) * (B + C) = A * B + B * B + A * C + B * C$$

$$A - B = A + (-1) \cdot_m B$$

$$A * (B - C) * D = A * B * D - A * C * D$$

$$\text{trace } (A * B * C) = \text{trace } (B * C * A)$$

$$\text{trace } (A * B * C * D) = \text{trace } (C * D * A * B)$$

$$\text{trace } (A + B * C) = \text{trace } A + \text{trace } (C * B)$$

$$A + B = B + A$$

$$A + B + C = C + B + A$$

$$A + B + (C + D) = A + C + (B + D)$$
⟨proof⟩

1.6 Hermitian matrices

A Hermitian matrix is a matrix that is equal to its Hermitian adjoint.

definition *hermitian* :: 'a::conjugatable-field mat ⇒ bool where
hermitian A ↔ (adjoint *A* = *A*)

```

lemma hermitian-one:
  shows hermitian (( $1_m n$ )::('a::conjugatable-field mat))
  ⟨proof⟩

```

1.7 Inverse matrices

```

lemma inverts-mat-symm:
  fixes A B :: 'a::field mat
  assumes dim: A ∈ carrier-mat n n B ∈ carrier-mat n n
    and AB: inverts-mat A B
  shows inverts-mat B A
  ⟨proof⟩

lemma inverts-mat-unique:
  fixes A B C :: 'a::field mat
  assumes dim: A ∈ carrier-mat n n B ∈ carrier-mat n n C ∈ carrier-mat n n
    and AB: inverts-mat A B and AC: inverts-mat A C
  shows B = C
  ⟨proof⟩

```

1.8 Unitary matrices

A unitary matrix is a matrix whose Hermitian adjoint is also its inverse.

```

definition unitary :: 'a::conjugatable-field mat ⇒ bool where
  unitary A ↔ A ∈ carrier-mat (dim-row A) (dim-row A) ∧ inverts-mat A (adjoint A)

lemma unitaryD2:
  assumes A ∈ carrier-mat n n
  shows unitary A ⇒ inverts-mat (adjoint A) A
  ⟨proof⟩

lemma unitary-simps [simp]:
  A ∈ carrier-mat n n ⇒ unitary A ⇒ adjoint A * A =  $1_m n$ 
  A ∈ carrier-mat n n ⇒ unitary A ⇒ A * adjoint A =  $1_m n$ 
  ⟨proof⟩

lemma unitary-adjoint [simp]:
  assumes A ∈ carrier-mat n n unitary A
  shows unitary (adjoint A)
  ⟨proof⟩

lemma unitary-one:
  shows unitary (( $1_m n$ )::('a::conjugatable-field mat))
  ⟨proof⟩

lemma unitary-zero:
  fixes A :: 'a::conjugatable-field mat

```

```

assumes  $A \in \text{carrier-mat } 0\ 0$ 
shows unitary  $A$ 
⟨proof⟩

lemma unitary-elim:
assumes dims:  $A \in \text{carrier-mat } n\ n$   $B \in \text{carrier-mat } n\ n$   $P \in \text{carrier-mat } n\ n$ 
    and  $uP$ : unitary  $P$  and eq:  $P * A * \text{adjoint } P = P * B * \text{adjoint } P$ 
shows  $A = B$ 
⟨proof⟩

lemma unitary-is-corthogonal:
fixes  $U :: 'a::\text{conjugatable-field mat}$ 
assumes dim:  $U \in \text{carrier-mat } n\ n$ 
    and  $U$ : unitary  $U$ 
shows corthogonal-mat  $U$ 
⟨proof⟩

lemma unitary-times-unitary:
fixes  $P\ Q :: 'a::\text{conjugatable-field mat}$ 
assumes dim:  $P \in \text{carrier-mat } n\ n$   $Q \in \text{carrier-mat } n\ n$ 
    and  $uP$ : unitary  $P$  and  $uQ$ : unitary  $Q$ 
shows unitary  $(P * Q)$ 
⟨proof⟩

lemma unitary-operator-keep-trace:
fixes  $U\ A :: \text{complex mat}$ 
assumes  $dU$ :  $U \in \text{carrier-mat } n\ n$  and  $dA$ :  $A \in \text{carrier-mat } n\ n$  and  $u$ : unitary  $U$ 
shows  $\text{trace } A = \text{trace } (\text{adjoint } U * A * U)$ 
⟨proof⟩

```

1.9 Normalization of vectors

```

definition vec-norm :: complex vec  $\Rightarrow$  complex where
  vec-norm  $v \equiv \text{csqrt} (v \cdot c v)$ 

```

```

lemma vec-norm-geq-0:
fixes  $v :: \text{complex vec}$ 
shows vec-norm  $v \geq 0$ 
⟨proof⟩

```

```

lemma vec-norm-zero:
fixes  $v :: \text{complex vec}$ 
assumes dim:  $v \in \text{carrier-vec } n$ 
shows vec-norm  $v = 0 \longleftrightarrow v = 0_v$   $n$ 
⟨proof⟩

```

```

lemma vec-norm-ge-0:
fixes  $v :: \text{complex vec}$ 

```

```

assumes dim- $v$ :  $v \in \text{carrier-vec } n$  and neq0:  $v \neq 0_v \ n$ 
shows vec-norm  $v > 0$ 
⟨proof⟩

definition vec-normalize :: complex vec  $\Rightarrow$  complex vec where
  vec-normalize  $v = (\text{if } (v = 0_v \ (\text{dim-vec } v)) \text{ then } v \text{ else } 1 / (\text{vec-norm } v) \cdot_v v)$ 

lemma normalized-vec-dim[simp]:
  assumes ( $v::\text{complex vec}$ )  $\in \text{carrier-vec } n$ 
  shows vec-normalize  $v \in \text{carrier-vec } n$ 
  ⟨proof⟩

lemma vec-eq-norm-smult-normalized:
  shows  $v = \text{vec-norm } v \cdot_v \text{vec-normalize } v$ 
  ⟨proof⟩

lemma normalized-cscalar-prod:
  fixes  $v \ w :: \text{complex vec}$ 
  assumes dim- $v$ :  $v \in \text{carrier-vec } n$  and dim- $w$ :  $w \in \text{carrier-vec } n$ 
  shows  $v \cdot c \ w = (\text{vec-norm } v * \text{vec-norm } w) * (\text{vec-normalize } v \cdot c \ \text{vec-normalize } w)$ 
  ⟨proof⟩

lemma normalized-vec-norm :
  fixes  $v :: \text{complex vec}$ 
  assumes dim- $v$ :  $v \in \text{carrier-vec } n$ 
    and neq0:  $v \neq 0_v \ n$ 
  shows vec-normalize  $v \cdot c \ \text{vec-normalize } v = 1$ 
  ⟨proof⟩

lemma normalize-zero:
  assumes  $v \in \text{carrier-vec } n$ 
  shows vec-normalize  $v = 0_v \ n \longleftrightarrow v = 0_v \ n$ 
  ⟨proof⟩

lemma normalize-normalize[simp]:
  vec-normalize (vec-normalize  $v$ ) = vec-normalize  $v$ 
  ⟨proof⟩

```

1.10 Spectral decomposition of normal complex matrices

```

lemma normalize-keep-corthogonal:
  fixes  $vs :: \text{complex vec list}$ 
  assumes cor:  $\text{corthogonal } vs$  and dims:  $\text{set } vs \subseteq \text{carrier-vec } n$ 
  shows corthogonal (map vec-normalize  $vs$ )
  ⟨proof⟩

lemma normalized-corthogonal-mat-is-unitary:
  assumes  $W: \text{set } ws \subseteq \text{carrier-vec } n$ 

```

```

and orth: corthogonal ws
and len: length ws = n
shows unitary (mat-of-cols n (map vec-normalize ws)) (is unitary ?W)
<proof>

```

```

lemma normalize-keep-eigenvector:
assumes ev: eigenvector A v e
and dim: A ∈ carrier-mat n n v ∈ carrier-vec n
shows eigenvector A (vec-normalize v) e
<proof>

```

```

lemma four-block-mat-adjoint:
fixes A B C D :: 'a::conjugatable-field mat
assumes dim: A ∈ carrier-mat nr1 nc1 B ∈ carrier-mat nr1 nc2
C ∈ carrier-mat nr2 nc1 D ∈ carrier-mat nr2 nc2
shows adjoint (four-block-mat A B C D)
 $= \text{four-block-mat}(\text{adjoint } A)(\text{adjoint } C)(\text{adjoint } B)(\text{adjoint } D)$ 
<proof>

```

```

fun unitary-schur-decomposition :: complex mat ⇒ complex list ⇒ complex mat ×
complex mat × complex mat where
unitary-schur-decomposition A [] = (A, 1_m (dim-row A), 1_m (dim-row A))
| unitary-schur-decomposition A (e # es) = (let
n = dim-row A;
n1 = n - 1;
v' = find-eigenvector A e;
v = vec-normalize v';
ws0 = gram-schmidt n (basis-completion v);
ws = map vec-normalize ws0;
W = mat-of-cols n ws;
W' = corthogonal-inv W;
A' = W' * A * W;
(A1, A2, A0, A3) = split-block A' 1 1;
(B, P, Q) = unitary-schur-decomposition A3 es;
z-row = (0_m 1 n1);
z-col = (0_m n1 1);
one-1 = 1_m 1
in (four-block-mat A1 (A2 * P) A0 B,
W * four-block-mat one-1 z-row z-col P,
four-block-mat one-1 z-row z-col Q * W'))

```

```

theorem unitary-schur-decomposition:
assumes A: (A::complex mat) ∈ carrier-mat n n
and c: char-poly A = (Π (e :: complex) ← es. [:- e, 1:])
and B: unitary-schur-decomposition A es = (B, P, Q)
shows similar-mat-wit A B P Q ∧ upper-triangular B ∧ diag-mat B = es ∧
unitary P ∧ (Q = adjoint P)
<proof>

```

```

lemma complex-mat-char-poly-factorizable:
  fixes A :: complex mat
  assumes A ∈ carrier-mat n n
  shows ∃ as. char-poly A = (Π a ← as. [:- a, 1:]) ∧ length as = n
  ⟨proof⟩

lemma complex-mat-has-unitary-schur-decomposition:
  fixes A :: complex mat
  assumes A ∈ carrier-mat n n
  shows ∃ B P es. similar-mat-wit A B P (adjoint P) ∧ unitary P
    ∧ char-poly A = (Π (e :: complex) ← es. [:- e, 1:]) ∧ diag-mat B = es
  ⟨proof⟩

lemma normal-upper-triangular-matrix-is-diagonal:
  fixes A :: 'a::conjugatable-ordered-field mat
  assumes A ∈ carrier-mat n n
  and tri: upper-triangular A
  and norm: A * adjoint A = adjoint A * A
  shows diagonal-mat A
  ⟨proof⟩

lemma normal-complex-mat-has-spectral-decomposition:
  assumes A: (A::complex mat) ∈ carrier-mat n n
  and normal: A * adjoint A = adjoint A * A
  and c: char-poly A = (Π (e :: complex) ← es. [:- e, 1:])
  and B: unitary-schur-decomposition A es = (B,P,Q)
  shows similar-mat-wit A B P (adjoint P) ∧ diagonal-mat B ∧ diag-mat B = es
  ∧ unitary P
  ⟨proof⟩

lemma complex-mat-has-jordan-nf:
  fixes A :: complex mat
  assumes A ∈ carrier-mat n n
  shows ∃ n-as. jordan-nf A n-as
  ⟨proof⟩

lemma hermitian-is-normal:
  assumes hermitian A
  shows A * adjoint A = adjoint A * A
  ⟨proof⟩

lemma hermitian-eigenvalue-real:
  assumes dim: (A::complex mat) ∈ carrier-mat n n
  and hA: hermitian A
  and c: char-poly A = (Π (e :: complex) ← es. [:- e, 1:])
  and B: unitary-schur-decomposition A es = (B,P,Q)
  shows similar-mat-wit A B P (adjoint P) ∧ diagonal-mat B ∧ diag-mat B = es
  ∧ unitary P ∧ (∀ i < n. B$$i, i) ∈ Reals)
  ⟨proof⟩

```

```

lemma hermitian-inner-prod-real:
  assumes dimA: (A::complex mat) ∈ carrier-mat n n
    and dimv: v ∈ carrier-vec n
    and hA: hermitian A
  shows inner-prod v (A *v v) ∈ Reals
  ⟨proof⟩

lemma unit-vec-bracket:
  fixes A :: complex mat
  assumes dimA: A ∈ carrier-mat n n and i: i < n
  shows inner-prod (unit-vec n i) (A *v (unit-vec n i)) = A$$⟨i, i⟩
  ⟨proof⟩

lemma spectral-decomposition-extract-diag:
  fixes P B :: complex mat
  assumes dimP: P ∈ carrier-mat n n and dimB: B ∈ carrier-mat n n
    and uP: unitary P and dB: diagonal-mat B and i: i < n
  shows inner-prod (col P i) (P * B * (adjoint P) *v (col P i)) = B$$⟨i, i⟩
  ⟨proof⟩

lemma hermitian-inner-prod-zero:
  fixes A :: complex mat
  assumes dimA: A ∈ carrier-mat n n and hA: hermitian A
    and zero: ∀ v ∈ carrier-vec n. inner-prod v (A *v v) = 0
  shows A = 0m n n
  ⟨proof⟩

lemma complex-mat-decomposition-to-hermitian:
  fixes A :: complex mat
  assumes dim: A ∈ carrier-mat n n
  shows ∃ B C. hermitian B ∧ hermitian C ∧ A = B + i ·m C ∧ B ∈ carrier-mat n n ∧ C ∈ carrier-mat n n
  ⟨proof⟩

```

1.11 Outer product

```

definition outer-prod :: 'a::conjugatable-field vec ⇒ 'a vec ⇒ 'a mat where
  outer-prod v w = mat (dim-vec v) 1 (λ(i, j). v $ i) * mat 1 (dim-vec w) (λ(i, j).
    (conjugate w) $ j)

```

```

lemma outer-prod-dim[simp]:
  fixes v w :: 'a::conjugatable-field vec
  assumes v: v ∈ carrier-vec n and w: w ∈ carrier-vec m
  shows outer-prod v w ∈ carrier-mat n m
  ⟨proof⟩

```

```

lemma mat-of-vec-mult-eq-scalar-prod:
  fixes v w :: 'a::conjugatable-field vec

```

```

assumes  $v \in \text{carrier-vec } n$  and  $w \in \text{carrier-vec } n$ 
shows  $\text{mat } 1 (\text{dim-vec } v) (\lambda(i, j). (\text{conjugate } v) \$ j) * \text{mat } (\text{dim-vec } w) 1 (\lambda(i, j). w \$ i)$ 
 $= \text{mat } 1 1 (\lambda k. \text{inner-prod } v w)$ 
{proof}

lemma one-dim-mat-mult-is-scale:
fixes  $A B :: 'a::\text{conjugatable-field mat}$ 
assumes  $B \in \text{carrier-mat } 1 n$ 
shows  $(\text{mat } 1 1 (\lambda k. a)) * B = a \cdot_m B$ 
{proof}

lemma outer-prod-mult-outer-prod:
fixes  $a b c d :: 'a::\text{conjugatable-field vec}$ 
assumes  $a: a \in \text{carrier-vec } d1$  and  $b: b \in \text{carrier-vec } d2$ 
and  $c: c \in \text{carrier-vec } d2$  and  $d: d \in \text{carrier-vec } d3$ 
shows  $\text{outer-prod } a b * \text{outer-prod } c d = \text{inner-prod } b c \cdot_m \text{outer-prod } a d$ 
{proof}

lemma index-outer-prod:
fixes  $v w :: 'a::\text{conjugatable-field vec}$ 
assumes  $v: v \in \text{carrier-vec } n$  and  $w: w \in \text{carrier-vec } m$ 
and  $ij: i < n \ j < m$ 
shows  $(\text{outer-prod } v w) \$\$ (i, j) = v \$ i * \text{conjugate } (w \$ j)$ 
{proof}

lemma mat-of-vec-mult-vec:
fixes  $a b c :: 'a::\text{conjugatable-field vec}$ 
assumes  $a: a \in \text{carrier-vec } d$  and  $b: b \in \text{carrier-vec } d$ 
shows  $\text{mat } 1 d (\lambda(i, j). (\text{conjugate } a) \$ j) *_v b = \text{vec } 1 (\lambda k. \text{inner-prod } a b)$ 
{proof}

lemma mat-of-vec-mult-one-dim-vec:
fixes  $a b :: 'a::\text{conjugatable-field vec}$ 
assumes  $a: a \in \text{carrier-vec } d$ 
shows  $\text{mat } d 1 (\lambda(i, j). a \$ i) *_v \text{vec } 1 (\lambda k. c) = c \cdot_v a$ 
{proof}

lemma outer-prod-mult-vec:
fixes  $a b c :: 'a::\text{conjugatable-field vec}$ 
assumes  $a: a \in \text{carrier-vec } d1$  and  $b: b \in \text{carrier-vec } d2$ 
and  $c: c \in \text{carrier-vec } d2$ 
shows  $\text{outer-prod } a b *_v c = \text{inner-prod } b c \cdot_v a$ 
{proof}

lemma trace-outer-prod-right:
fixes  $A :: 'a::\text{conjugatable-field mat}$  and  $v w :: 'a \text{ vec}$ 
assumes  $A: A \in \text{carrier-mat } n n$ 
and  $v: v \in \text{carrier-vec } n$  and  $w: w \in \text{carrier-vec } n$ 

```

```

shows trace (A * outer-prod v w) = inner-prod w (A *_v v) (is ?lhs = ?rhs)
⟨proof⟩

```

```
lemma trace-outer-prod:
```

```

fixes v w :: ('a::conjugatable-field vec)
assumes v: v ∈ carrier-vec n and w: w ∈ carrier-vec n
shows trace (outer-prod v w) = inner-prod w v (is ?lhs = ?rhs)
⟨proof⟩

```

```
lemma inner-prod-outer-prod:
```

```

fixes a b c d :: 'a::conjugatable-field vec
assumes a: a ∈ carrier-vec n and b: b ∈ carrier-vec n
and c: c ∈ carrier-vec m and d: d ∈ carrier-vec m
shows inner-prod a (outer-prod b c *_v d) = inner-prod a b * inner-prod c d (is
?lhs = ?rhs)
⟨proof⟩

```

1.12 Semi-definite matrices

```
definition positive :: complex mat ⇒ bool where
```

```

positive A ↔
A ∈ carrier-mat (dim-col A) (dim-col A) ∧
(∀ v. dim-vec v = dim-col A → inner-prod v (A *_v v) ≥ 0)

```

```
lemma positive-iff-normalized-vec:
```

```

positive A ↔
A ∈ carrier-mat (dim-col A) (dim-col A) ∧
(∀ v. (dim-vec v = dim-col A ∧ vec-norm v = 1) → inner-prod v (A *_v v) ≥
0)
⟨proof⟩

```

```
lemma positive-is-hermitian:
```

```

fixes A :: complex mat
assumes pA: positive A
shows hermitian A
⟨proof⟩

```

```
lemma positive-eigenvalue-positive:
```

```

assumes dimA: (A::complex mat) ∈ carrier-mat n n
and pA: positive A
and c: char-poly A = (Π (e :: complex) ← es. [:- e, 1:])
and B: unitary-schur-decomposition A es = (B,P,Q)
shows ∀i. i < n ⇒ B$$(i, i) ≥ 0
⟨proof⟩

```

```
lemma diag-mat-mult-diag-mat:
```

```

fixes B D :: 'a::semiring-0 mat
assumes dimB: B ∈ carrier-mat n n and dimD: D ∈ carrier-mat n n
and dB: diagonal-mat B and dD: diagonal-mat D

```

shows $B * D = \text{mat } n \ n (\lambda(i,j). (\text{if } i = j \text{ then } (B\$$(i, i)) * (D\$$(i, i)) \text{ else } 0))$
 $\langle \text{proof} \rangle$

lemma *positive-only-if-decomp*:

assumes $\text{dimA}: A \in \text{carrier-mat } n \ n$ **and** $pA: \text{positive } A$
shows $\exists M \in \text{carrier-mat } n \ n. M * \text{adjoint } M = A$
 $\langle \text{proof} \rangle$

lemma *positive-if-decomp*:

assumes $\text{dimA}: A \in \text{carrier-mat } n \ n$ **and** $\exists M. M * \text{adjoint } M = A$
shows *positive A*
 $\langle \text{proof} \rangle$

lemma *positive-iff-decomp*:

assumes $\text{dimA}: A \in \text{carrier-mat } n \ n$
shows *positive A* $\longleftrightarrow (\exists M \in \text{carrier-mat } n \ n. M * \text{adjoint } M = A)$
 $\langle \text{proof} \rangle$

lemma *positive-dim-eq*:

assumes *positive A*
shows *dim-row A = dim-col A*
 $\langle \text{proof} \rangle$

lemma *positive-zero*:

positive (0_m n n)
 $\langle \text{proof} \rangle$

lemma *positive-one*:

positive (1_m n)
 $\langle \text{proof} \rangle$

lemma *positive-antisym*:

assumes $pA: \text{positive } A$ **and** $pnA: \text{positive } (-A)$
shows $A = 0_m (\text{dim-col } A) (\text{dim-col } A)$
 $\langle \text{proof} \rangle$

lemma *positive-add*:

assumes $pA: \text{positive } A$ **and** $pB: \text{positive } B$
and $\text{dimA}: A \in \text{carrier-mat } n \ n$ **and** $\text{dimB}: B \in \text{carrier-mat } n \ n$
shows *positive (A + B)*
 $\langle \text{proof} \rangle$

lemma *positive-trace*:

assumes $A \in \text{carrier-mat } n \ n$ **and** *positive A*
shows *trace A ≥ 0*
 $\langle \text{proof} \rangle$

lemma *positive-close-under-left-right-mult-adjoint*:

fixes $M A :: \text{complex mat}$

```

assumes  $dM: M \in \text{carrier-mat } n \ n$  and  $dA: A \in \text{carrier-mat } n \ n$ 
and  $pA: \text{positive } A$ 
shows  $\text{positive} (M * A * \text{adjoint } M)$ 
⟨proof⟩

lemma  $\text{positive-same-outer-prod}:$ 
fixes  $v \ w :: \text{complex vec}$ 
assumes  $v: v \in \text{carrier-vec } n$ 
shows  $\text{positive} (\text{outer-prod } v \ v)$ 
⟨proof⟩

lemma  $\text{smult-smult-mat}:$ 
fixes  $k :: \text{complex}$  and  $l :: \text{complex}$ 
assumes  $A \in \text{carrier-mat } nr \ n$ 
shows  $k \cdot_m (l \cdot_m A) = (k * l) \cdot_m A$  ⟨proof⟩

lemma  $\text{positive-smult}:$ 
assumes  $A \in \text{carrier-mat } n \ n$ 
and  $\text{positive } A$ 
and  $c \geq 0$ 
shows  $\text{positive} (c \cdot_m A)$ 
⟨proof⟩

```

Version of previous theorem for real numbers

```

lemma  $\text{positive-scale}:$ 
fixes  $c :: \text{real}$ 
assumes  $A \in \text{carrier-mat } n \ n$ 
and  $\text{positive } A$ 
and  $c \geq 0$ 
shows  $\text{positive} (c \cdot_m A)$ 
⟨proof⟩

```

1.13 Löwner partial order

```

definition  $\text{lowner-le} :: \text{complex mat} \Rightarrow \text{complex mat} \Rightarrow \text{bool}$  (infix  $\leq_L$  50)
where
 $A \leq_L B \longleftrightarrow \text{dim-row } A = \text{dim-row } B \wedge \text{dim-col } A = \text{dim-col } B \wedge \text{positive} (B - A)$ 

```

```

lemma  $\text{lowner-le-refl}:$ 
assumes  $A \in \text{carrier-mat } n \ n$ 
shows  $A \leq_L A$ 
⟨proof⟩

```

```

lemma  $\text{lowner-le-antisym}:$ 
assumes  $A: A \in \text{carrier-mat } n \ n$  and  $B: B \in \text{carrier-mat } n \ n$ 
and  $L1: A \leq_L B$  and  $L2: B \leq_L A$ 
shows  $A = B$ 
⟨proof⟩

```

```

lemma lowner-le-inner-prod-le:
  fixes A B :: complex mat and v :: complex vec
  assumes A: A ∈ carrier-mat n n and B: B ∈ carrier-mat n n
    and v: v ∈ carrier-vec n
    and A ≤L B
  shows inner-prod v (A *v v) ≤ inner-prod v (B *v v)
  ⟨proof⟩

lemma lowner-le-trans:
  fixes A B C :: complex mat
  assumes A: A ∈ carrier-mat n n and B: B ∈ carrier-mat n n and C: C ∈
    carrier-mat n n
    and L1: A ≤L B and L2: B ≤L C
  shows A ≤L C
  ⟨proof⟩

lemma lowner-le-imp-trace-le:
  assumes A ∈ carrier-mat n n and B ∈ carrier-mat n n
    and A ≤L B
  shows trace A ≤ trace B
  ⟨proof⟩

lemma lowner-le-add:
  assumes A ∈ carrier-mat n n B ∈ carrier-mat n n C ∈ carrier-mat n n D ∈
    carrier-mat n n
    and A ≤L B C ≤L D
  shows A + C ≤L B + D
  ⟨proof⟩

lemma lowner-le-swap:
  assumes A ∈ carrier-mat n n B ∈ carrier-mat n n
    and A ≤L B
  shows -B ≤L -A
  ⟨proof⟩

lemma lowner-le-minus:
  assumes A ∈ carrier-mat n n B ∈ carrier-mat n n C ∈ carrier-mat n n D ∈
    carrier-mat n n
    and A ≤L B C ≤L D
  shows A - D ≤L B - C
  ⟨proof⟩

lemma outer-prod-le-one:
  assumes v ∈ carrier-vec n
    and inner-prod v v ≤ 1
  shows outer-prod v v ≤L 1m n
  ⟨proof⟩

lemma zero-lowner-le-positiveD:

```

```

fixes A :: complex mat
assumes dA: A ∈ carrier-mat n n and le: 0m n n ≤L A
shows positive A
⟨proof⟩

lemma zero-lowner-le-positiveI:
fixes A :: complex mat
assumes dA: A ∈ carrier-mat n n and le: positive A
shows 0m n n ≤L A
⟨proof⟩

lemma lowner-le-trans-positiveI:
fixes A B :: complex mat
assumes dA: A ∈ carrier-mat n n and pA: positive A and le: A ≤L B
shows positive B
⟨proof⟩

lemma lowner-le-keep-under-measurement:
fixes M A B :: complex mat
assumes dM: M ∈ carrier-mat n n and dA: A ∈ carrier-mat n n and dB: B ∈
carrier-mat n n
and le: A ≤L B
shows adjoint M * A * M ≤L adjoint M * B * M
⟨proof⟩

lemma smult-distrib-left-minus-mat:
fixes A B :: 'a::comm-ring-1 mat
assumes A ∈ carrier-mat n n B ∈ carrier-mat n n
shows c ·m (B - A) = c ·m B - c ·m A
⟨proof⟩

lemma lowner-le-smultc:
fixes c :: complex
assumes c ≥ 0 A ≤L B A ∈ carrier-mat n n B ∈ carrier-mat n n
shows c ·m A ≤L c ·m B
⟨proof⟩

lemma lowner-le-smult:
fixes c :: real
assumes c ≥ 0 A ≤L B A ∈ carrier-mat n n B ∈ carrier-mat n n
shows c ·m A ≤L c ·m B
⟨proof⟩

lemma minus-smult-vec-distrib:
fixes w :: 'a::comm-ring-1 vec
shows (a - b) ·v w = a ·v w - b ·v w
⟨proof⟩

lemma smult-mat-mult-mat-vec-assoc:

```

```

fixes A :: 'a::comm-ring-1 mat
assumes A: A ∈ carrier-mat n m and w: w ∈ carrier-vec m
shows a ·m A *v w = a ·v (A *v w)
⟨proof⟩

lemma mult-mat-vec-smult-vec-assoc:
fixes A :: 'a::comm-ring-1 mat
assumes A: A ∈ carrier-mat n m and w: w ∈ carrier-vec m
shows A *v (a ·v w) = a ·v (A *v w)
⟨proof⟩

lemma outer-prod-left-right-mat:
fixes A B :: complex mat
assumes du: u ∈ carrier-vec d2 and dv: v ∈ carrier-vec d3
and dA: A ∈ carrier-mat d1 d2 and dB: B ∈ carrier-mat d3 d4
shows A * (outer-prod u v) * B = (outer-prod (A *v u) (adjoint B *v v))
⟨proof⟩

```

1.14 Density operators

```

definition density-operator :: complex mat ⇒ bool where
density-operator A ↔ positive A ∧ trace A = 1

definition partial-density-operator :: complex mat ⇒ bool where
partial-density-operator A ↔ positive A ∧ trace A ≤ 1

lemma pure-state-self-outer-prod-is-partial-density-operator:
fixes v :: complex vec
assumes dimv: v ∈ carrier-vec n and nv: vec-norm v = 1
shows partial-density-operator (outer-prod v v)
⟨proof⟩

```

```

lemma lowner-le-trace:
assumes A: A ∈ carrier-mat n n
and B: B ∈ carrier-mat n n
shows A ≤L B ↔ (∀ ρ ∈ carrier-mat n n. partial-density-operator ρ → trace (A * ρ) ≤ trace (B * ρ))
⟨proof⟩

lemma lowner-le-traceI:
assumes A ∈ carrier-mat n n
and B ∈ carrier-mat n n
and ⋀ ρ. ρ ∈ carrier-mat n n ⇒ partial-density-operator ρ ⇒ trace (A * ρ) ≤ trace (B * ρ)
shows A ≤L B
⟨proof⟩

lemma trace-pdo-eq-imp-eq:

```

```

assumes A:  $A \in carrier\text{-mat } n \ n$ 
and B:  $B \in carrier\text{-mat } n \ n$ 
and teq:  $\bigwedge \varrho. \varrho \in carrier\text{-mat } n \ n \implies partial\text{-density-operator } \varrho \implies trace (A * \varrho) = trace (B * \varrho)$ 
shows A = B
⟨proof⟩

lemma lowner-le-traceD:
assumes A:  $A \in carrier\text{-mat } n \ n$  B:  $B \in carrier\text{-mat } n \ n$   $\varrho \in carrier\text{-mat } n \ n$ 
and  $A \leq_L B$ 
and partial-density-operator  $\varrho$ 
shows  $trace (A * \varrho) \leq trace (B * \varrho)$ 
⟨proof⟩

lemma sum-only-one-neq-0:
assumes finite A and  $j \in A$  and  $\bigwedge i. i \in A \implies i \neq j \implies g i = 0$ 
shows sum g A = g j
⟨proof⟩

end

```

2 Matrix limits

```

theory Matrix-Limit
imports Complex-Matrix
begin

```

2.1 Definition of limit of matrices

```

definition limit-mat ::  $(nat \Rightarrow complex\ mat) \Rightarrow complex\ mat \Rightarrow nat \Rightarrow bool$  where
  limit-mat X A m  $\longleftrightarrow$   $(\forall n. X n \in carrier\text{-mat } m \ m \wedge A \in carrier\text{-mat } m \ m \wedge$ 
 $(\forall i < m. \forall j < m. (\lambda n. (X n) \$\$ (i, j)) \longrightarrow (A \$\$ (i, j))))$ 

lemma limit-mat-unique:
assumes limA: limit-mat X A m and limB: limit-mat X B m
shows A = B
⟨proof⟩

lemma limit-mat-const:
fixes A :: complex mat
assumes A:  $A \in carrier\text{-mat } m \ m$ 
shows limit-mat ( $\lambda k. A$ ) A m
⟨proof⟩

lemma limit-mat-scale:
fixes X ::  $nat \Rightarrow complex\ mat$  and A ::  $complex\ mat$ 
assumes limX: limit-mat X A m
shows limit-mat ( $\lambda n. c \cdot_m X n$ ) ( $c \cdot_m A$ ) m
⟨proof⟩

```

```

lemma limit-mat-add:
  fixes X :: nat  $\Rightarrow$  complex mat and Y :: nat  $\Rightarrow$  complex mat and A :: complex
  mat
    and m :: nat and B :: complex mat
  assumes limX: limit-mat X A m and limY: limit-mat Y B m
  shows limit-mat ( $\lambda k. X k + Y k$ ) (A + B) m
  (proof)

lemma limit-mat-minus:
  fixes X :: nat  $\Rightarrow$  complex mat and Y :: nat  $\Rightarrow$  complex mat and A :: complex
  mat
    and m :: nat and B :: complex mat
  assumes limX: limit-mat X A m and limY: limit-mat Y B m
  shows limit-mat ( $\lambda k. X k - Y k$ ) (A - B) m
  (proof)

lemma limit-mat-mult:
  fixes X :: nat  $\Rightarrow$  complex mat and Y :: nat  $\Rightarrow$  complex mat and A :: complex
  mat
    and m :: nat and B :: complex mat
  assumes limX: limit-mat X A m and limY: limit-mat Y B m
  shows limit-mat ( $\lambda k. X k * Y k$ ) (A * B) m
  (proof)

```

Adding matrix A to the sequence X

```

definition mat-add-seq :: complex mat  $\Rightarrow$  (nat  $\Rightarrow$  complex mat)  $\Rightarrow$  nat  $\Rightarrow$  complex
mat where
  mat-add-seq A X = ( $\lambda n. A + X n$ )

```

```

lemma mat-add-limit:
  fixes X :: nat  $\Rightarrow$  complex mat and A :: complex mat and m :: nat and B :: complex
  mat
  assumes dimB: B  $\in$  carrier-mat m m and limX: limit-mat X A m
  shows limit-mat (mat-add-seq B X) (B + A) m
  (proof)

```

```

lemma mat-minus-limit:
  fixes X :: nat  $\Rightarrow$  complex mat and A :: complex mat and m :: nat and B :: complex
  mat
  assumes dimB: B  $\in$  carrier-mat m m and limX: limit-mat X A m
  shows limit-mat ( $\lambda n. B - X n$ ) (B - A) m
  (proof)

```

Multiply matrix A by the sequence X

```

definition mat-mult-seq :: complex mat  $\Rightarrow$  (nat  $\Rightarrow$  complex mat)  $\Rightarrow$  nat  $\Rightarrow$  com-
plex mat where
  mat-mult-seq A X = ( $\lambda n. A * X n$ )

```

```

lemma mat-mult-limit:
  fixes X :: nat  $\Rightarrow$  complex mat and A B :: complex mat and m :: nat
  assumes dimB: B  $\in$  carrier-mat m m and limX: limit-mat X A m
  shows limit-mat (mat-mult-seq B X) (B * A) m
  ⟨proof⟩

lemma mult-mat-limit:
  fixes X :: nat  $\Rightarrow$  complex mat and A B :: complex mat and m :: nat
  assumes dimB: B  $\in$  carrier-mat m m and limX: limit-mat X A m
  shows limit-mat ( $\lambda k. X k * B$ ) (A * B) m
  ⟨proof⟩

lemma quadratic-form-mat:
  fixes A :: complex mat and v :: complex vec and m :: nat
  assumes dimv: dim-vec v = m and dimA: A  $\in$  carrier-mat m m
  shows inner-prod v (A *v v) = ( $\sum i=0..<m.$  ( $\sum j=0..<m.$  conjugate (v\$i) * A$(i, j) * v\$j))
  ⟨proof⟩

lemma sum-subtractff:
  fixes h g :: nat  $\Rightarrow$  nat  $\Rightarrow$  'a::ab-group-add
  shows ( $\sum x \in A. \sum y \in B. h x y - g x y$ ) = ( $\sum x \in A. \sum y \in B. h x y$ ) - ( $\sum x \in A. \sum y \in B. g x y$ )
  ⟨proof⟩

lemma sum-abs-complex:
  fixes h :: nat  $\Rightarrow$  nat  $\Rightarrow$  complex
  shows cmod ( $\sum x \in A. \sum y \in B. h x y$ )  $\leq$  ( $\sum x \in A. \sum y \in B. cmod(h x y)$ )
  ⟨proof⟩

lemma hermitian-mat-lim-is-hermitian:
  fixes X :: nat  $\Rightarrow$  complex mat and A :: complex mat and m :: nat
  assumes limX: limit-mat X A m and herX:  $\forall n. \text{hermitian } (X n)$ 
  shows hermitian A
  ⟨proof⟩

lemma quantifier-change-order-once:
  fixes P :: nat  $\Rightarrow$  nat  $\Rightarrow$  bool and m :: nat
  shows  $\forall j < m. \exists no. \forall n \geq no. P n j \implies \exists no. \forall j < m. \forall n \geq no. P n j$ 
  ⟨proof⟩

lemma quantifier-change-order-twice:
  fixes P :: nat  $\Rightarrow$  nat  $\Rightarrow$  nat  $\Rightarrow$  bool and m n :: nat
  shows  $\forall i < m. \forall j < n. \exists no. \forall n \geq no. P n i j \implies \exists no. \forall i < m. \forall j < n. \forall n \geq no. P n i j$ 
  ⟨proof⟩

lemma pos-mat-lim-is-pos:
  fixes X :: nat  $\Rightarrow$  complex mat and A :: complex mat and m :: nat

```

```

assumes limX: limit-mat X A m and posX:  $\forall n.$  positive (X n)
shows positive A
⟨proof⟩

```

```

lemma limit-mat-ignore-initial-segment:
  limit-mat g A d  $\implies$  limit-mat ( $\lambda n.$  g (n + k)) A d
⟨proof⟩

```

```

lemma mat-trace-limit:
  limit-mat g A d  $\implies$  ( $\lambda n.$  trace (g n))  $\longrightarrow$  trace A
⟨proof⟩

```

2.2 Existence of least upper bound for the Löwner order

```

definition lowner-is-lub :: (nat  $\Rightarrow$  complex mat)  $\Rightarrow$  complex mat  $\Rightarrow$  bool where
  lowner-is-lub f M  $\longleftrightarrow$  ( $\forall n.$  f n  $\leq_L$  M)  $\wedge$  ( $\forall M'.$  ( $\forall n.$  f n  $\leq_L$  M')  $\longrightarrow$  M  $\leq_L$  M')

```

```

locale matrix-seq =
  fixes dim :: nat
  and f :: nat  $\Rightarrow$  complex mat
assumes
  dim:  $\bigwedge n.$  f n  $\in$  carrier-mat dim dim and
  pdo:  $\bigwedge n.$  partial-density-operator (f n) and
  inc:  $\bigwedge n.$  lowner-le (f n) (f (Suc n))
begin

definition lowner-is-lub :: complex mat  $\Rightarrow$  bool where
  lowner-is-lub M  $\longleftrightarrow$  ( $\forall n.$  f n  $\leq_L$  M)  $\wedge$  ( $\forall M'.$  ( $\forall n.$  f n  $\leq_L$  M')  $\longrightarrow$  M  $\leq_L$  M')

```

```

lemma lowner-is-lub-dim:
  assumes lowner-is-lub M
  shows M  $\in$  carrier-mat dim dim
⟨proof⟩

```

```

lemma trace-adjoint-eq-u:
  fixes A :: complex mat
  shows trace (A * adjoint A) = ( $\sum i \in \{0 .. < \text{dim-row } A\}.$   $\sum j \in \{0 .. < \text{dim-col } A\}.$  (norm(A $$ (i,j)))^2)
⟨proof⟩

```

```

lemma trace-adjoint-element-ineq:
  fixes A :: complex mat
  assumes rindex:  $i \in \{0 .. < \text{dim-row } A\}$ 
  and cindex:  $j \in \{0 .. < \text{dim-col } A\}$ 
  shows (norm(A $$ (i,j)))^2  $\leq$  trace (A * adjoint A)
⟨proof⟩

```

```

lemma positive-is-normal:

```

```

fixes A :: complex mat
assumes pos: positive A
shows A * adjoint A = adjoint A * A
⟨proof⟩

lemma diag-mat-mul-diag-diag:
fixes A B :: complex mat
assumes dimA: A ∈ carrier-mat n n and dimB: B ∈ carrier-mat n n
and dA: diagonal-mat A and dB: diagonal-mat B
shows diagonal-mat (A * B)
⟨proof⟩

lemma diag-mat-mul-diag-ele:
fixes A B :: complex mat
assumes dimA: A ∈ carrier-mat n n and dimB: B ∈ carrier-mat n n
and dA: diagonal-mat A and dB: diagonal-mat B
shows ∀ i < n. (A * B) $(i, i) = A$(i, i) * B$(i, i)
⟨proof⟩

lemma trace-square-less-square-trace:
fixes B :: complex mat
assumes dimB: B ∈ carrier-mat n n
and dB: diagonal-mat B and pB: ∀ i. i < n ⇒ B$(i, i) ≥ 0
shows trace (B * B) ≤ (trace B)2
⟨proof⟩

lemma trace-positive-eq:
fixes A :: complex mat
assumes pos: positive A
shows trace (A * adjoint A) ≤ (trace A)2
⟨proof⟩

```

```

lemma lowner-le-transitive:
fixes m n :: nat
assumes re: n ≥ m
shows positive (f n - f m)
⟨proof⟩

```

The sequence of matrices converges pointwise.

```

lemma inc-partial-density-operator-converge:
assumes i: i ∈ {0 .. < dim} and j: j ∈ {0 .. < dim}
shows convergent (λn. f n $(i, j))
⟨proof⟩

```

```

definition mat-seq-minus :: (nat ⇒ complex mat) ⇒ complex mat ⇒ nat ⇒
complex mat where
mat-seq-minus X A = (λn. X n - A)

```

```

definition minus-mat-seq :: complex mat  $\Rightarrow$  (nat  $\Rightarrow$  complex mat)  $\Rightarrow$  nat  $\Rightarrow$  complex mat where
  minus-mat-seq A X = ( $\lambda n.$  A  $-$  X n)

lemma pos-mat-lim-is-pos-aux:
  fixes X :: nat  $\Rightarrow$  complex mat and A :: complex mat and m :: nat
  assumes limX: limit-mat X A m and posX:  $\exists k.$   $\forall n \geq k.$  positive (X n)
  shows positive A
  ⟨proof⟩

lemma minus-mat-limit:
  fixes X :: nat  $\Rightarrow$  complex mat and A :: complex mat and m :: nat and B :: complex mat
  assumes dimB: B  $\in$  carrier-mat m m and limX: limit-mat X A m
  shows limit-mat (mat-seq-minus X B) (A  $-$  B) m
  ⟨proof⟩

lemma mat-minus-limit:
  fixes X :: nat  $\Rightarrow$  complex mat and A :: complex mat and m :: nat and B :: complex mat
  assumes dimA: A  $\in$  carrier-mat m m and limX: limit-mat X A m
  shows limit-mat (minus-mat-seq B X) (B  $-$  A) m
  ⟨proof⟩

lemma lowner-lub-form:
  lowner-is-lub (mat dim dim ( $\lambda (i, j).$  (lim ( $\lambda n.$  (f n)  $\$$ (i, j)))))$ 
```

Lowner partial order is a complete partial order.

```

lemma lowner-lub-exists:  $\exists M.$  lowner-is-lub M
  ⟨proof⟩
```

```

lemma lowner-lub-unique:  $\exists !M.$  lowner-is-lub M
  ⟨proof⟩
```

```

definition lowner-lub :: complex mat where
  lowner-lub = (THE M. lowner-is-lub M)
```

```

lemma lowner-lub-prop: lowner-is-lub lowner-lub
  ⟨proof⟩
```

```

lemma lowner-lub-is-limit:
  limit-mat f lowner-lub dim
  ⟨proof⟩
```

```

lemma lowner-lub-trace:
  assumes  $\forall n.$  trace (f n)  $\leq x$ 
  shows trace lowner-lub  $\leq x$ 
  ⟨proof⟩
```

```
lemma lowner-lub-is-positive:
```

```
  shows positive lowner-lub
```

```
  ⟨proof⟩
```

```
end
```

2.3 Finite sum of matrices

```
Add f in the interval [0, n)
```

```
fun matrix-sum :: nat ⇒ (nat ⇒ 'b::semiring-1 mat) ⇒ nat ⇒ 'b mat where
  matrix-sum d f 0 = 0m d d
  | matrix-sum d f (Suc n) = f n + matrix-sum d f n
```

```
definition matrix-inf-sum :: nat ⇒ (nat ⇒ complex mat) ⇒ complex mat where
  matrix-inf-sum d f = matrix-seq.lowner-lub (λn. matrix-sum d f n)
```

```
lemma matrix-sum-dim:
```

```
  fixes f :: nat ⇒ 'b::semiring-1 mat
```

```
  shows (¬k. k < n ⇒ f k ∈ carrier-mat d d) ⇒ matrix-sum d f n ∈ carrier-mat
    d d
```

```
  ⟨proof⟩
```

```
lemma matrix-sum-cong:
```

```
  fixes f :: nat ⇒ 'b::semiring-1 mat
```

```
  shows (¬k. k < n ⇒ f k = f' k) ⇒ matrix-sum d f n = matrix-sum d f' n
```

```
  ⟨proof⟩
```

```
lemma matrix-sum-add:
```

```
  fixes f :: nat ⇒ 'b::semiring-1 mat and g :: nat ⇒ 'b::semiring-1 mat and h
    :: nat ⇒ 'b::semiring-1 mat
```

```
  shows (¬k. k < n ⇒ f k ∈ carrier-mat d d) ⇒ (¬k. k < n ⇒ g k ∈
    carrier-mat d d) ⇒ (¬k. k < n ⇒ h k ∈ carrier-mat d d) ⇒
```

```
  (¬k. k < n ⇒ f k = g k + h k) ⇒ matrix-sum d f n = matrix-sum d g n
    + matrix-sum d h n
```

```
  ⟨proof⟩
```

```
lemma matrix-sum-smult:
```

```
  fixes f :: nat ⇒ 'b::semiring-1 mat
```

```
  shows (¬k. k < n ⇒ f k ∈ carrier-mat d d) ⇒
```

```
  matrix-sum d (λ k. c ·m f k) n = c ·m matrix-sum d f n
```

```
  ⟨proof⟩
```

```
lemma matrix-sum-remove:
```

```
  fixes f :: nat ⇒ 'b::semiring-1 mat
```

```
  assumes j: j < n
```

```
  and df: (¬k. k < n ⇒ f k ∈ carrier-mat d d)
```

```
  and f': (¬k. f' k = (if k = j then 0m d d else f k))
```

```
  shows matrix-sum d f n = f j + matrix-sum d f' n
```

$\langle proof \rangle$

lemma *matrix-sum-Suc-remove-head*:
fixes $f :: nat \Rightarrow complex\ mat$
shows $(\bigwedge k. k < n + 1 \Rightarrow f k \in carrier\text{-}mat d d) \Rightarrow$
 $matrix\text{-}sum\ d\ f\ (n + 1) = f\ 0 + matrix\text{-}sum\ d\ (\lambda k. f\ (k + 1))\ n$
 $\langle proof \rangle$

lemma *matrix-sum-positive*:
fixes $f :: nat \Rightarrow complex\ mat$
shows $(\bigwedge k. k < n \Rightarrow f k \in carrier\text{-}mat d d) \Rightarrow (\bigwedge k. k < n \Rightarrow positive\ (f k))$
 $\Rightarrow positive\ (matrix\text{-}sum\ d\ f\ n)$
 $\langle proof \rangle$

lemma *matrix-sum-mult-right*:
shows $(\bigwedge k. k < n \Rightarrow f k \in carrier\text{-}mat d d) \Rightarrow A \in carrier\text{-}mat d d$
 $\Rightarrow matrix\text{-}sum\ d\ (\lambda k. (f k) * A)\ n = matrix\text{-}sum\ d\ (\lambda k. f k)\ n * A$
 $\langle proof \rangle$

lemma *matrix-sum-add-distrib*:
shows $(\bigwedge k. k < n \Rightarrow f k \in carrier\text{-}mat d d) \Rightarrow (\bigwedge k. k < n \Rightarrow g k \in carrier\text{-}mat d d)$
 $\Rightarrow matrix\text{-}sum\ d\ (\lambda k. (f k) + (g k))\ n = matrix\text{-}sum\ d\ f\ n + matrix\text{-}sum\ d\ g\ n$
 $\langle proof \rangle$

lemma *matrix-sum-minus-distrib*:
fixes $f g :: nat \Rightarrow complex\ mat$
shows $(\bigwedge k. k < n \Rightarrow f k \in carrier\text{-}mat d d) \Rightarrow (\bigwedge k. k < n \Rightarrow g k \in carrier\text{-}mat d d)$
 $\Rightarrow matrix\text{-}sum\ d\ (\lambda k. (f k) - (g k))\ n = matrix\text{-}sum\ d\ f\ n - matrix\text{-}sum\ d\ g\ n$
 $\langle proof \rangle$

lemma *matrix-sum-shift-Suc*:
shows $(\bigwedge k. k < (Suc\ n) \Rightarrow f k \in carrier\text{-}mat d d)$
 $\Rightarrow matrix\text{-}sum\ d\ f\ (Suc\ n) = f\ 0 + matrix\text{-}sum\ d\ (\lambda k. f\ (Suc\ k))\ n$
 $\langle proof \rangle$

lemma *lowner-le-matrix-sum*:
fixes $f g :: nat \Rightarrow complex\ mat$
shows $(\bigwedge k. k < n \Rightarrow f k \in carrier\text{-}mat d d) \Rightarrow (\bigwedge k. k < n \Rightarrow g k \in carrier\text{-}mat d d)$
 $\Rightarrow (\bigwedge k. k < n \Rightarrow f k \leq_L g k)$
 $\Rightarrow matrix\text{-}sum\ d\ f\ n \leq_L matrix\text{-}sum\ d\ g\ n$
 $\langle proof \rangle$

lemma *lowner-lub-add*:
assumes $matrix\text{-}seq\ d\ f\ matrix\text{-}seq\ d\ g\ \forall\ n. trace\ (f\ n + g\ n) \leq 1$
shows $matrix\text{-}seq.lowner-lub\ (\lambda n. f\ n + g\ n) = matrix\text{-}seq.lowner-lub\ f + matrix\text{-}seq.lowner-lub\ g$

$\langle proof \rangle$

```
lemma lowner-lub-scale:
  fixes c :: real
  assumes matrix-seq d f  $\forall n. trace(c \cdot_m f n) \leq 1 \quad c \geq 0$ 
  shows matrix-seq.lowner-lub ( $\lambda n. c \cdot_m f n$ ) =  $c \cdot_m$  matrix-seq.lowner-lub f
⟨proof⟩
```

```
lemma trace-matrix-sum-linear:
  fixes f :: nat  $\Rightarrow$  complex mat
  shows  $(\bigwedge k. k < n \Rightarrow f k \in carrier\text{-}mat d d) \Rightarrow trace(matrix\text{-}sum d f n) =$ 
    sum  $(\lambda k. trace(f k)) \{0..<n\}$ 
⟨proof⟩
```

```
lemma matrix-sum-distrib-left:
  fixes f :: nat  $\Rightarrow$  complex mat
  shows  $P \in carrier\text{-}mat d d \Rightarrow (\bigwedge k. k < n \Rightarrow f k \in carrier\text{-}mat d d) \Rightarrow$ 
    matrix-sum d  $(\lambda k. P * (f k)) n = P * (matrix\text{-}sum d f n)$ 
⟨proof⟩
```

2.4 Measurement

```
definition measurement :: nat  $\Rightarrow$  nat  $\Rightarrow$  (nat  $\Rightarrow$  complex mat)  $\Rightarrow$  bool where
  measurement d n M  $\longleftrightarrow$   $(\forall j < n. M j \in carrier\text{-}mat d d)$ 
     $\wedge$  matrix-sum d  $(\lambda j. (adjoint(M j)) * M j) n = 1_m d$ 
```

```
lemma measurement-dim:
  assumes measurement d n M
  shows  $\bigwedge k. k < n \Rightarrow (M k) \in carrier\text{-}mat d d$ 
⟨proof⟩
```

```
lemma measurement-id2:
  assumes measurement d 2 M
  shows adjoint(M 0) * M 0 + adjoint(M 1) * M 1 = 1_m d
⟨proof⟩
```

Result of measurement on ρ by matrix M

```
definition measurement-res :: complex mat  $\Rightarrow$  complex mat  $\Rightarrow$  complex mat where
  measurement-res M  $\varrho = M * \varrho * adjoint M$ 
```

```
lemma add-positive-le-reduce1:
  assumes dA: A  $\in$  carrier-mat n n and dB: B  $\in$  carrier-mat n n and dC: C  $\in$ 
    carrier-mat n n
    and pB: positive B and le: A + B  $\leq_L C$ 
  shows A  $\leq_L C$ 
⟨proof⟩
```

```
lemma add-positive-le-reduce2:
  assumes dA: A  $\in$  carrier-mat n n and dB: B  $\in$  carrier-mat n n and dC: C  $\in$ 
    carrier-mat n n
```

and pB : positive B **and** $le: B + A \leq_L C$
shows $A \leq_L C$
 $\langle proof \rangle$

lemma *measurement-le-one-mat*:
assumes measurement $d n f$
shows $\bigwedge j. j < n \implies \text{adjoint}(f j) * f j \leq_L 1_m d$
 $\langle proof \rangle$

lemma *pdo-close-under-measurement*:
fixes $M \varrho :: \text{complex mat}$
assumes $dM: M \in \text{carrier-mat } n n$ **and** $dr: \varrho \in \text{carrier-mat } n n$
and $pdor: \text{partial-density-operator } \varrho$
and $le: \text{adjoint } M * M \leq_L 1_m n$
shows partial-density-operator $(M * \varrho * \text{adjoint } M)$
 $\langle proof \rangle$

lemma *trace-measurement*:
assumes $m: \text{measurement } d n M$ **and** $dA: A \in \text{carrier-mat } d d$
shows $\text{trace}(\text{matrix-sum } d (\lambda k. (M k) * A * \text{adjoint}(M k)) n) = \text{trace } A$
 $\langle proof \rangle$

lemma *mat-inc-seq-positive-transform*:
assumes $dfn: \bigwedge n. f n \in \text{carrier-mat } d d$
and $inc: \bigwedge n. f n \leq_L f(Suc n)$
shows $\bigwedge n. f n - f 0 \in \text{carrier-mat } d d$ **and** $\bigwedge n. (f n - f 0) \leq_L (f(Suc n) - f 0)$
 $\langle proof \rangle$

lemma *mat-inc-seq-lub*:
assumes $dfn: \bigwedge n. f n \in \text{carrier-mat } d d$
and $inc: \bigwedge n. f n \leq_L f(Suc n)$
and $ub: \bigwedge n. f n \leq_L A$
shows $\exists B. \text{lowner-is-lub } f B \wedge \text{limit-mat } f B d$
 $\langle proof \rangle$

end

3 Quantum programs

theory *Quantum-Program*
imports *Matrix-Limit*
begin

3.1 Syntax

Datatype for quantum programs

datatype *com* =

```

 $\text{SKIP}$ 
|  $\text{Utrans complex mat}$ 
|  $\text{Seq com com } (\langle-;;/\rightarrow [60, 61] 60)$ 
|  $\text{Measure nat nat} \Rightarrow \text{complex mat com list}$ 
|  $\text{While nat} \Rightarrow \text{complex mat com}$ 

```

A state corresponds to the density operator

```
type-synonym state = complex mat
```

List of dimensions of quantum states

```

locale state-sig =
  fixes dims :: nat list
begin

```

```

definition d :: nat where
  d = prod-list dims

```

Wellformedness of commands

```

fun well-com :: com  $\Rightarrow$  bool where
  well-com SKIP = True
  | well-com ( $\text{Utrans } U$ ) = ( $U \in \text{carrier-mat } d$   $\wedge$  unitary  $U$ )
  | well-com (Seq S1 S2) = (well-com S1  $\wedge$  well-com S2)
  | well-com (Measure n M S) =
    (measurement d n M  $\wedge$  length S = n  $\wedge$  list-all well-com S)
  | well-com (While M S) =
    (measurement d 2 M  $\wedge$  well-com S)

```

3.2 Denotational semantics

Denotation of going through the while loop n times

```

fun denote-while-n-iter :: complex mat  $\Rightarrow$  complex mat  $\Rightarrow$  (state  $\Rightarrow$  state)  $\Rightarrow$  nat
 $\Rightarrow$  state  $\Rightarrow$  state where
  denote-while-n-iter M0 M1 DS 0  $\varrho$  =  $\varrho$ 
  | denote-while-n-iter M0 M1 DS (Suc n)  $\varrho$  = denote-while-n-iter M0 M1 DS n (DS
  (M1 *  $\varrho$  * adjoint M1))

```

```

fun denote-while-n :: complex mat  $\Rightarrow$  complex mat  $\Rightarrow$  (state  $\Rightarrow$  state)  $\Rightarrow$  nat  $\Rightarrow$ 
state  $\Rightarrow$  state where
  denote-while-n M0 M1 DS n  $\varrho$  = M0 * denote-while-n-iter M0 M1 DS n  $\varrho$  *
adjoint M0

```

```

fun denote-while-n-comp :: complex mat  $\Rightarrow$  complex mat  $\Rightarrow$  (state  $\Rightarrow$  state)  $\Rightarrow$  nat
 $\Rightarrow$  state  $\Rightarrow$  state where
  denote-while-n-comp M0 M1 DS n  $\varrho$  = M1 * denote-while-n-iter M0 M1 DS n  $\varrho$  *
* adjoint M1

```

lemma denote-while-n-iter-assoc:

```

denote-while-n-iter M0 M1 DS (Suc n)  $\varrho$  = DS (M1 * (denote-while-n-iter M0
M1 DS n  $\varrho$ ) * adjoint M1)

```

$\langle proof \rangle$

lemma *denote-while-n-iter-dim*:

$$\begin{aligned} & \varrho \in \text{carrier-mat } m \ m \implies \text{partial-density-operator } \varrho \implies M1 \in \text{carrier-mat } m \ m \\ & \implies \text{adjoint } M1 * M1 \leq_L 1_m \ m \\ & \implies (\bigwedge \varrho. \varrho \in \text{carrier-mat } m \ m \implies \text{partial-density-operator } \varrho \implies DS \varrho \in \text{carrier-mat } m \ m \wedge \text{partial-density-operator } (DS \varrho)) \\ & \implies \text{denote-while-n-iter } M0 \ M1 \ DS \ n \ \varrho \in \text{carrier-mat } m \ m \wedge \text{partial-density-operator } (\text{denote-while-n-iter } M0 \ M1 \ DS \ n \ \varrho) \end{aligned}$$

$\langle proof \rangle$

lemma *pdo-denote-while-n-iter*:

$$\begin{aligned} & \varrho \in \text{carrier-mat } m \ m \implies \text{partial-density-operator } \varrho \implies M1 \in \text{carrier-mat } m \ m \\ & \implies \text{adjoint } M1 * M1 \leq_L 1_m \ m \\ & \implies (\bigwedge \varrho. \varrho \in \text{carrier-mat } m \ m \wedge \text{partial-density-operator } \varrho \implies \text{partial-density-operator } (DS \varrho)) \\ & \implies (\bigwedge \varrho. \varrho \in \text{carrier-mat } m \ m \wedge \text{partial-density-operator } \varrho \implies DS \varrho \in \text{carrier-mat } m \ m) \\ & \implies \text{partial-density-operator } (\text{denote-while-n-iter } M0 \ M1 \ DS \ n \ \varrho) \end{aligned}$$

$\langle proof \rangle$

Denotation of while is simply the infinite sum of denote_while_n

definition *denote-while* :: *complex mat* \Rightarrow *complex mat* \Rightarrow (*state* \Rightarrow *state*) \Rightarrow *state* \Rightarrow *state* **where**

$$\text{denote-while } M0 \ M1 \ DS \ \varrho = \text{matrix-inf-sum } d \ (\lambda n. \text{denote-while-n } M0 \ M1 \ DS \ n \ \varrho)$$

lemma *denote-while-n-dim*:

assumes $\varrho \in \text{carrier-mat } d \ d$
 $M0 \in \text{carrier-mat } d \ d$
 $M1 \in \text{carrier-mat } d \ d$
 $\text{partial-density-operator } \varrho$
 $\bigwedge \varrho'. \varrho' \in \text{carrier-mat } d \ d \implies \text{partial-density-operator } \varrho' \implies \text{positive } (DS \varrho')$
 $\wedge \text{trace } (DS \varrho') \leq \text{trace } \varrho' \wedge DS \varrho' \in \text{carrier-mat } d \ d$
shows $\text{denote-while-n } M0 \ M1 \ DS \ n \ \varrho \in \text{carrier-mat } d \ d$
 $\langle proof \rangle$

lemma *denote-while-n-sum-dim*:

assumes $\varrho \in \text{carrier-mat } d \ d$
 $M0 \in \text{carrier-mat } d \ d$
 $M1 \in \text{carrier-mat } d \ d$
 $\text{partial-density-operator } \varrho$
 $\bigwedge \varrho'. \varrho' \in \text{carrier-mat } d \ d \implies \text{partial-density-operator } \varrho' \implies \text{positive } (DS \varrho')$
 $\wedge \text{trace } (DS \varrho') \leq \text{trace } \varrho' \wedge DS \varrho' \in \text{carrier-mat } d \ d$
shows $\text{matrix-sum } d \ (\lambda n. \text{denote-while-n } M0 \ M1 \ DS \ n \ \varrho) \ n \in \text{carrier-mat } d \ d$
 $\langle proof \rangle$

lemma *trace-decrease-mul-adj*:

assumes *pdo*: *partial-density-operator* ϱ **and** *dimr*: $\varrho \in \text{carrier-mat } d \ d$

and $\text{dim}x: x \in \text{carrier-mat } d \ d$ **and** $\text{un}: \text{adjoint } x * x \leq_L 1_m \ d$
shows $\text{trace}(x * \varrho * \text{adjoint } x) \leq \text{trace } \varrho$
 $\langle \text{proof} \rangle$

lemma *denote-while-n-positive*:

assumes $\text{dim}0: M0 \in \text{carrier-mat } d \ d$ **and** $\text{dim}1: M1 \in \text{carrier-mat } d \ d$ **and**
 $\text{un}: \text{adjoint } M1 * M1 \leq_L 1_m \ d$
and $\text{DS}: \bigwedge \varrho. \varrho \in \text{carrier-mat } d \ d \implies \text{partial-density-operator } \varrho \implies \text{positive}$
 $(\text{DS } \varrho) \wedge \text{trace } (\text{DS } \varrho) \leq \text{trace } \varrho \wedge \text{DS } \varrho \in \text{carrier-mat } d \ d$
shows $\text{partial-density-operator } \varrho \wedge \varrho \in \text{carrier-mat } d \ d \implies \text{positive } (\text{denote-while-n } M0 \ M1 \ \text{DS } n \ \varrho)$
 $\langle \text{proof} \rangle$

lemma *denote-while-n-sum-positive*:

assumes $\text{dim}0: M0 \in \text{carrier-mat } d \ d$ **and** $\text{dim}1: M1 \in \text{carrier-mat } d \ d$ **and**
 $\text{un}: \text{adjoint } M1 * M1 \leq_L 1_m \ d$
and $\text{DS}: \bigwedge \varrho. \varrho \in \text{carrier-mat } d \ d \implies \text{partial-density-operator } \varrho \implies \text{positive}$
 $(\text{DS } \varrho) \wedge \text{trace } (\text{DS } \varrho) \leq \text{trace } \varrho \wedge \text{DS } \varrho \in \text{carrier-mat } d \ d$
and $\text{pdo}: \text{partial-density-operator } \varrho \text{ and } r: \varrho \in \text{carrier-mat } d \ d$
shows $\text{positive } (\text{matrix-sum } d (\lambda n. \text{denote-while-n } M0 \ M1 \ \text{DS } n \ \varrho) \ n)$
 $\langle \text{proof} \rangle$

lemma *trace-measure2-id*:

assumes $dM0: M0 \in \text{carrier-mat } n \ n$ **and** $dM1: M1 \in \text{carrier-mat } n \ n$
and $\text{id}: \text{adjoint } M0 * M0 + \text{adjoint } M1 * M1 = 1_m \ n$
and $dA: A \in \text{carrier-mat } n \ n$
shows $\text{trace } (M0 * A * \text{adjoint } M0) + \text{trace } (M1 * A * \text{adjoint } M1) = \text{trace } A$
 $\langle \text{proof} \rangle$

lemma *measurement-lowner-le-one1*:

assumes $\text{dim}0: M0 \in \text{carrier-mat } d \ d$ **and** $\text{dim}1: M1 \in \text{carrier-mat } d \ d$ **and** $\text{id}:$
 $\text{adjoint } M0 * M0 + \text{adjoint } M1 * M1 = 1_m \ d$
shows $\text{adjoint } M1 * M1 \leq_L 1_m \ d$
 $\langle \text{proof} \rangle$

lemma *denote-while-n-sum-trace*:

assumes $\text{dim}0: M0 \in \text{carrier-mat } d \ d$ **and** $\text{dim}1: M1 \in \text{carrier-mat } d \ d$ **and** $\text{id}:$
 $\text{adjoint } M0 * M0 + \text{adjoint } M1 * M1 = 1_m \ d$
and $\text{DS}: \bigwedge \varrho. \varrho \in \text{carrier-mat } d \ d \implies \text{partial-density-operator } \varrho \implies \text{positive}$
 $(\text{DS } \varrho) \wedge \text{trace } (\text{DS } \varrho) \leq \text{trace } \varrho \wedge \text{DS } \varrho \in \text{carrier-mat } d \ d$
and $r: \varrho \in \text{carrier-mat } d \ d$
and $\text{pdor}: \text{partial-density-operator } \varrho$
shows $\text{trace } (\text{matrix-sum } d (\lambda n. \text{denote-while-n } M0 \ M1 \ \text{DS } n \ \varrho) \ n) \leq \text{trace } \varrho$
 $\langle \text{proof} \rangle$

lemma *denote-while-n-sum-partial-density*:

assumes $\text{dim}0: M0 \in \text{carrier-mat } d \ d$ **and** $\text{dim}1: M1 \in \text{carrier-mat } d \ d$ **and** $\text{id}:$
 $\text{adjoint } M0 * M0 + \text{adjoint } M1 * M1 = 1_m \ d$
and $\text{DS}: \bigwedge \varrho. \varrho \in \text{carrier-mat } d \ d \implies \text{partial-density-operator } \varrho \implies \text{positive}$

$(DS \varrho) \wedge \text{trace}(DS \varrho) \leq \text{trace} \varrho \wedge DS \varrho \in \text{carrier-mat } d d$
and pdo: partial-density-operator ϱ **and** r: $\varrho \in \text{carrier-mat } d d$
shows (partial-density-operator (matrix-sum d ($\lambda n.$ denote-while-n M0 M1 DS n ϱ) n))
 $\langle proof \rangle$

lemma denote-while-n-sum-lowner-le:
assumes dim0: $M0 \in \text{carrier-mat } d d$ **and** dim1: $M1 \in \text{carrier-mat } d d$ **and** id:
 $\text{adjoint } M0 * M0 + \text{adjoint } M1 * M1 = 1_m d$
and DS: $\bigwedge \varrho. \varrho \in \text{carrier-mat } d d \implies \text{partial-density-operator } \varrho \implies \text{positive}$
 $(DS \varrho) \wedge \text{trace}(DS \varrho) \leq \text{trace} \varrho \wedge DS \varrho \in \text{carrier-mat } d d$
and pdo: partial-density-operator ϱ **and** dimr: $\varrho \in \text{carrier-mat } d d$
shows (matrix-sum d ($\lambda n.$ denote-while-n M0 M1 DS n ϱ) n \leq_L matrix-sum d
 $(\lambda n.$ denote-while-n M0 M1 DS n ϱ) (Suc n))
 $\langle proof \rangle$

lemma lowner-is-lub-matrix-sum:
assumes dim0: $M0 \in \text{carrier-mat } d d$ **and** dim1: $M1 \in \text{carrier-mat } d d$ **and** id:
 $\text{adjoint } M0 * M0 + \text{adjoint } M1 * M1 = 1_m d$
and DS: $\bigwedge \varrho. \varrho \in \text{carrier-mat } d d \implies \text{partial-density-operator } \varrho \implies \text{positive}$
 $(DS \varrho) \wedge \text{trace}(DS \varrho) \leq \text{trace} \varrho \wedge DS \varrho \in \text{carrier-mat } d d$
and pdo: partial-density-operator ϱ **and** dimr: $\varrho \in \text{carrier-mat } d d$
shows matrix-seq.lowner-is-lub (matrix-sum d ($\lambda n.$ denote-while-n M0 M1 DS n ϱ)) (matrix-seq.lowner-lub (matrix-sum d ($\lambda n.$ denote-while-n M0 M1 DS n ϱ)))
 $\langle proof \rangle$

lemma denote-while-dim-positive:
assumes dim0: $M0 \in \text{carrier-mat } d d$ **and** dim1: $M1 \in \text{carrier-mat } d d$ **and** id:
 $\text{adjoint } M0 * M0 + \text{adjoint } M1 * M1 = 1_m d$
and DS: $\bigwedge \varrho. \varrho \in \text{carrier-mat } d d \implies \text{partial-density-operator } \varrho \implies \text{positive}$
 $(DS \varrho) \wedge \text{trace}(DS \varrho) \leq \text{trace} \varrho \wedge DS \varrho \in \text{carrier-mat } d d$
and pdo: partial-density-operator ϱ **and** dimr: $\varrho \in \text{carrier-mat } d d$
shows
 $\text{denote-while } M0 M1 DS \varrho \in \text{carrier-mat } d d \wedge \text{positive}(\text{denote-while } M0 M1 DS \varrho) \wedge \text{trace}(\text{denote-while } M0 M1 DS \varrho) \leq \text{trace} \varrho$
 $\langle proof \rangle$

definition denote-measure :: nat \Rightarrow (nat \Rightarrow complex mat) \Rightarrow ((state \Rightarrow state) list)
 \Rightarrow state \Rightarrow state **where**
 $\text{denote-measure } n M DS \varrho = \text{matrix-sum } d (\lambda k. (DS!k) ((M k) * \varrho * \text{adjoint } (M k))) n$

lemma denote-measure-dim:
assumes $\varrho \in \text{carrier-mat } d d$
measurement d n M
 $\bigwedge \varrho' k. \varrho' \in \text{carrier-mat } d d \implies k < n \implies (DS!k) \varrho' \in \text{carrier-mat } d d$
shows
 $\text{denote-measure } n M DS \varrho \in \text{carrier-mat } d d$
 $\langle proof \rangle$

```

lemma measure-well-com:
  assumes well-com (Measure n M S)
  shows  $\bigwedge k. k < n \implies$  well-com (S ! k)
  (proof)

  Semantics of commands

fun denote :: com  $\Rightarrow$  state  $\Rightarrow$  state where
  denote SKIP  $\varrho = \varrho$ 
  | denote (Utrans U)  $\varrho = U * \varrho * \text{adjoint } U$ 
  | denote (Seq S1 S2)  $\varrho = \text{denote } S2 (\text{denote } S1 \varrho)$ 
  | denote (Measure n M S)  $\varrho = \text{denote-measure } n M (\text{map denote } S) \varrho$ 
  | denote (While M S)  $\varrho = \text{denote-while } (M 0) (M 1) (\text{denote } S) \varrho$ 

```

```

lemma denote-measure-expand:
  assumes m:  $m \leq n$  and wc: well-com (Measure n M S)
  shows denote (Measure m M S)  $\varrho = \text{matrix-sum } d (\lambda k. \text{denote } (S!k) ((M k) * \varrho$ 
   $* \text{adjoint } (M k))) m$ 
  (proof)

```

```

lemma matrix-sum-trace-le:
  fixes f :: nat  $\Rightarrow$  complex mat and g :: nat  $\Rightarrow$  complex mat
  assumes ( $\bigwedge k. k < n \implies f k \in \text{carrier-mat } d d$ )
    ( $\bigwedge k. k < n \implies g k \in \text{carrier-mat } d d$ )
    ( $\bigwedge k. k < n \implies \text{trace } (f k) \leq \text{trace } (g k)$ )
  shows trace (matrix-sum d f n)  $\leq$  trace (matrix-sum d g n)
  (proof)

```

```

lemma map-denote-positive-trace-dim:
  assumes well-com (Measure x1 x2a x3a)
  x4  $\in$  carrier-mat d d
  partial-density-operator x4
   $\bigwedge x3aa \varrho. x3aa \in \text{set } x3a \implies$  well-com x3aa  $\implies \varrho \in \text{carrier-mat } d d \implies$ 
  partial-density-operator  $\varrho$ 
   $\implies \text{positive } (\text{denote } x3aa \varrho) \wedge \text{trace } (\text{denote } x3aa \varrho) \leq \text{trace } \varrho \wedge \text{denote } x3aa$ 
   $\varrho \in \text{carrier-mat } d d$ 
  shows  $\forall k < x1. \text{positive } ((\text{map denote } x3a ! k) (x2a k * x4 * \text{adjoint } (x2a k)))$ 
     $\wedge ((\text{map denote } x3a ! k) (x2a k * x4 * \text{adjoint } (x2a k))) \in \text{carrier-mat}$ 
    d d
     $\wedge \text{trace } ((\text{map denote } x3a ! k) (x2a k * x4 * \text{adjoint } (x2a k))) \leq \text{trace }$ 
    (x2a k * x4 * adjoint (x2a k))
  (proof)

```

```

lemma denote-measure-positive-trace-dim:
  assumes well-com (Measure x1 x2a x3a)
  x4  $\in$  carrier-mat d d
  partial-density-operator x4
   $\bigwedge x3aa \varrho. x3aa \in \text{set } x3a \implies$  well-com x3aa  $\implies \varrho \in \text{carrier-mat } d d \implies$ 

```

partial-density-operator ϱ
 $\implies \text{positive}(\text{denote } x3aa \varrho) \wedge \text{trace}(\text{denote } x3aa \varrho) \leq \text{trace } \varrho \wedge \text{denote } x3aa$
 $\varrho \in \text{carrier-mat } d$
shows $\text{positive}(\text{denote}(\text{Measure } x1 x2a x3a) x4) \wedge \text{trace}(\text{denote}(\text{Measure } x1 x2a x3a) x4) \leq \text{trace } x4$
 $\wedge (\text{denote}(\text{Measure } x1 x2a x3a) x4) \in \text{carrier-mat } d$
 $\langle \text{proof} \rangle$

lemma *denote-positive-trace-dim*:

$\text{well-com } S \implies \varrho \in \text{carrier-mat } d$ $d \implies \text{partial-density-operator } \varrho$
 $\implies (\text{positive}(\text{denote } S \varrho) \wedge \text{trace}(\text{denote } S \varrho) \leq \text{trace } \varrho \wedge \text{denote } S \varrho \in$
 $\text{carrier-mat } d)$
 $\langle \text{proof} \rangle$

lemma *denote-dim-pdo*:

$\text{well-com } S \implies \varrho \in \text{carrier-mat } d$ $d \implies \text{partial-density-operator } \varrho$
 $\implies (\text{denote } S \varrho \in \text{carrier-mat } d)$ $d \wedge (\text{partial-density-operator}(\text{denote } S \varrho))$
 $\langle \text{proof} \rangle$

lemma *denote-dim*:

$\text{well-com } S \implies \varrho \in \text{carrier-mat } d$ $d \implies \text{partial-density-operator } \varrho$
 $\implies (\text{denote } S \varrho \in \text{carrier-mat } d)$
 $\langle \text{proof} \rangle$

lemma *denote-trace*:

$\text{well-com } S \implies \varrho \in \text{carrier-mat } d$ $d \implies \text{partial-density-operator } \varrho$
 $\implies \text{trace}(\text{denote } S \varrho) \leq \text{trace } \varrho$
 $\langle \text{proof} \rangle$

lemma *denote-partial-density-operator*:

assumes $\text{well-com } S$ $\text{partial-density-operator } \varrho$ $\varrho \in \text{carrier-mat } d$ d
shows $\text{partial-density-operator}(\text{denote } S \varrho)$
 $\langle \text{proof} \rangle$

lemma *denote-while-n-sum-mat-seq*:

assumes $\varrho \in \text{carrier-mat } d$ d **and**
 $x1 0 \in \text{carrier-mat } d$ d **and**
 $x1 1 \in \text{carrier-mat } d$ d **and**
 $\text{partial-density-operator } \varrho$ **and**
 $\text{wc: well-com } x2$ **and** $\text{mea: measurement } d 2 x1$
shows $\text{matrix-seq } d (\text{matrix-sum } d (\lambda n. \text{denote-while-n} (x1 0) (x1 1) (\text{denote } x2)$
 $n \varrho))$
 $\langle \text{proof} \rangle$

lemma *denote-while-n-add*:

assumes $M0: x1 0 \in \text{carrier-mat } d$ d **and**
 $M1: x1 1 \in \text{carrier-mat } d$ d **and**
 $\text{wc: well-com } x2$ **and** $\text{mea: measurement } d 2 x1$ **and**

$DS: (\bigwedge \varrho_1 \varrho_2. \varrho_1 \in carrier\text{-}mat d d \implies \varrho_2 \in carrier\text{-}mat d d \implies partial\text{-}density\text{-}operator$
 $\varrho_1 \implies$
 $partial\text{-}density\text{-}operator \varrho_2 \implies trace(\varrho_1 + \varrho_2) \leq 1 \implies denote x2(\varrho_1 + \varrho_2)$
 $= denote x2 \varrho_1 + denote x2 \varrho_2$
shows $\varrho_1 \in carrier\text{-}mat d d \implies \varrho_2 \in carrier\text{-}mat d d \implies partial\text{-}density\text{-}operator$
 $\varrho_1 \implies partial\text{-}density\text{-}operator \varrho_2 \implies trace(\varrho_1 + \varrho_2) \leq 1 \implies$
 $denote\text{-}while\text{-}n(x1 0)(x1 1)(denote x2)k(\varrho_1 + \varrho_2) = denote\text{-}while\text{-}n(x1 0)$
 $(x1 1)(denote x2)k\varrho_1 + denote\text{-}while\text{-}n(x1 0)(x1 1)(denote x2)k\varrho_2$
 $\langle proof \rangle$

lemma *denote-while-add*:

assumes $r1: \varrho_1 \in carrier\text{-}mat d d$ **and**
 $r2: \varrho_2 \in carrier\text{-}mat d d$ **and**
 $M0: x1 0 \in carrier\text{-}mat d d$ **and**
 $M1: x1 1 \in carrier\text{-}mat d d$ **and**
 $pdo1: partial\text{-}density\text{-}operator \varrho_1$ **and**
 $pdo2: partial\text{-}density\text{-}operator \varrho_2$ **and** $tr12: trace(\varrho_1 + \varrho_2) \leq 1$ **and**
 $wc: well\text{-}com x2$ **and** $mea: measurement d 2 x1$ **and**
 $DS: (\bigwedge \varrho_1 \varrho_2. \varrho_1 \in carrier\text{-}mat d d \implies \varrho_2 \in carrier\text{-}mat d d \implies partial\text{-}density\text{-}operator$
 $\varrho_1 \implies$
 $partial\text{-}density\text{-}operator \varrho_2 \implies trace(\varrho_1 + \varrho_2) \leq 1 \implies denote x2(\varrho_1 + \varrho_2)$
 $= denote x2 \varrho_1 + denote x2 \varrho_2$
shows
 $denote\text{-}while(x1 0)(x1 1)(denote x2)(\varrho_1 + \varrho_2) = denote\text{-}while(x1 0)(x1 1)$
 $(denote x2)\varrho_1 + denote\text{-}while(x1 0)(x1 1)(denote x2)\varrho_2$
 $\langle proof \rangle$

lemma *denote-add*:

$well\text{-}com S \implies \varrho_1 \in carrier\text{-}mat d d \implies \varrho_2 \in carrier\text{-}mat d d \implies$
 $partial\text{-}density\text{-}operator \varrho_1 \implies partial\text{-}density\text{-}operator \varrho_2 \implies trace(\varrho_1 + \varrho_2)$
 $\leq 1 \implies$
 $denote S(\varrho_1 + \varrho_2) = denote S \varrho_1 + denote S \varrho_2$
 $\langle proof \rangle$

lemma *mulfact*:

fixes $c: real$ **and** $a: complex$ **and** $b: complex$
assumes $c \geq 0$ $a \leq b$
shows $c * a \leq c * b$
 $\langle proof \rangle$

lemma *denote-while-n-scale*:

fixes $c: real$
assumes $c \geq 0$
 $measurement d 2 x1 well\text{-}com x2$
 $(\bigwedge \varrho. \varrho \in carrier\text{-}mat d d \implies partial\text{-}density\text{-}operator \varrho \implies trace(c \cdot_m \varrho) \leq 1$
 \implies
 $denote x2(c \cdot_m \varrho) = c \cdot_m denote x2 \varrho)$
shows $\varrho \in carrier\text{-}mat d d \implies partial\text{-}density\text{-}operator \varrho \implies trace(c \cdot_m \varrho) \leq$

```

1 ==>
  denote-while-n (x1 0) (x1 1) (denote x2) n (complex-of-real c ·m ρ) = c ·m
  (denote-while-n (x1 0) (x1 1) (denote x2) n ρ)
  ⟨proof⟩

```

```

lemma denote-while-scale:
  fixes c:: real
  assumes ρ ∈ carrier-mat d d
    partial-density-operator ρ
    trace (c ·m ρ) ≤ 1 c ≥ 0
    measurement d 2 x1 well-com x2
    (Λρ. ρ ∈ carrier-mat d d ==> partial-density-operator ρ ==> trace (c ·m ρ) ≤ 1
  ==>
    denote x2 (c ·m ρ) = c ·m denote x2 ρ)
  shows denote-while (x1 0) (x1 1) (denote x2) (c ·m ρ) = c ·m denote-while (x1
  0) (x1 1) (denote x2) ρ
  ⟨proof⟩

```

```

lemma denote-scale:
  fixes c :: real
  assumes c ≥ 0
  shows well-com S ==> ρ ∈ carrier-mat d d ==> partial-density-operator ρ ==>
    trace (c ·m ρ) ≤ 1 ==> denote S (c ·m ρ) = c ·m denote S ρ
  ⟨proof⟩

```

```

lemma limit-mat-denote-while-n:
  assumes wc: well-com (While M S) and dr: ρ ∈ carrier-mat d d and pdor:
    partial-density-operator ρ
  shows limit-mat (matrix-sum d (λk. denote-while-n (M 0) (M 1) (denote S) k
  ρ)) (denote (While M S) ρ) d
  ⟨proof⟩
end
end

```

4 Partial state

```

theory Partial-State
  imports Quantum-Program Deep-Learning.Tensor-Matricization
begin

```

```

lemma nths-intersection-eq:
  assumes {0..} ⊆ A
  shows nths xs B = nths xs (A ∩ B)
  ⟨proof⟩

```

```

lemma nths-minus-eq:
  assumes {0..} ⊆ A

```

shows $nths\ xs\ (-B) = nths\ xs\ (A - B)$
 $\langle proof \rangle$

lemma *nths-split-complement-eq*:

assumes $A \cap B = \{\}$
and $\{0..<\text{length}\ xs\} \subseteq A \cup B$
shows $nths\ xs\ A = nths\ xs\ (-B)$
 $\langle proof \rangle$

lemma *lt-set-card-lt*:

fixes $A :: \text{nat set}$
assumes *finite A* **and** $x \in A$
shows $\text{card}\ \{y. y \in A \wedge y < x\} < \text{card}\ A$
 $\langle proof \rangle$

definition *ind-in-set* **where**

ind-in-set A x = $\text{card}\ \{i. i \in A \wedge i < x\}$

lemma *bij-ind-in-set-bound*:

fixes $M :: \text{nat}$ **and** $v0 :: \text{nat set}$
assumes $\bigwedge x. f\ x = \text{card}\ \{y. y \in v0 \wedge y < x\}$
shows *bij-betw f ({0..<M} ∩ v0) {0..<card ({0..<M} ∩ v0)}*
 $\langle proof \rangle$

lemma *ind-in-set-bound*:

fixes $A :: \text{nat set}$ **and** $M\ N :: \text{nat}$
assumes $N \geq M$
shows *ind-in-set A N* \notin *(ind-in-set A ‘ ({0..<M} ∩ A))*
 $\langle proof \rangle$

lemma *bij-minus-subset*:

bij-betw f A B \implies $C \subseteq A \implies (f ` A) - (f ` C) = f ` (A - C)$
 $\langle proof \rangle$

lemma *ind-in-set-minus-subset-bound*:

fixes $A\ B :: \text{nat set}$ **and** $M :: \text{nat}$
assumes $B \subseteq A$
shows *(ind-in-set A ‘ ({0..<M} ∩ A)) - (ind-in-set A ‘ B) = (ind-in-set A ‘ ({0..<M} ∩ A)) ∩ (ind-in-set A ‘ (A - B))*
 $\langle proof \rangle$

lemma *ind-in-set-iff*:

fixes $A\ B :: \text{nat set}$
assumes $x \in A$ **and** $B \subseteq A$
shows *ind-in-set A x* \in *(ind-in-set A ‘ B) = (x ∈ B)*
 $\langle proof \rangle$

lemma *nths-reencode-eq*:

```

assumes  $B \subseteq A$ 
shows  $\text{nths}(\text{nths } xs \ A) (\text{ind-in-set } A \setminus B) = \text{nths } xs \ B$ 
⟨proof⟩

lemma nths-reencode-eq-comp:
assumes  $B \subseteq A$ 
shows  $\text{nths}(\text{nths } xs \ A) (- \text{ ind-in-set } A \setminus B) = \text{nths } xs \ (A - B)$ 
⟨proof⟩

lemma nths-prod-list-split:
fixes  $A :: \text{nat set}$  and  $xs :: \text{nat list}$ 
assumes  $B \subseteq A$ 
shows  $\text{prod-list}(\text{nths } xs \ A) = (\text{prod-list}(\text{nths } xs \ B)) * (\text{prod-list}(\text{nths } xs \ (A - B)))$ 
⟨proof⟩

```

4.1 Encodings

```

lemma digit-encode-take:
 $\text{take } n \ (\text{digit-encode } ds \ a) = \text{digit-encode}(\text{take } n \ ds) \ a$ 
⟨proof⟩

lemma nths-minus-upt-eq-drop:
 $\text{nths } l \ (-\{\dots < n\}) = \text{drop } n \ l$ 
⟨proof⟩

lemma digit-encode-drop:
 $\text{drop } n \ (\text{digit-encode } ds \ a) = \text{digit-encode}(\text{drop } n \ ds) \ (a \text{ div } (\text{prod-list}(\text{take } n \ ds)))$ 
⟨proof⟩

```

List of active variables in the partial state

```

locale partial-state = state-sig +
fixes  $vars :: \text{nat set}$ 

context partial-state
begin

    Dimensions of active variables

abbreviation  $avars :: \text{nat set}$  where
 $avars \equiv \{0..\text{length } dims\}$ 

definition  $dims1 :: \text{nat list}$  where
 $dims1 = \text{nths } dims \ vars$ 

definition  $dims2 :: \text{nat list}$  where
 $dims2 = \text{nths } dims \ (-vars)$ 

lemma dims1-alter:
assumes  $avars \subseteq A$ 

```

```

shows dims1 = nths dims (A ∩ vars)
⟨proof⟩

lemma dims2-alter:
assumes avars ⊆ A
shows dims2 = nths dims (A − vars)
⟨proof⟩

    Total dimension for the active variables

definition d1 :: nat where
d1 = prod-list dims1

    Total dimension for the non-active variables

definition d2 :: nat where
d2 = prod-list dims2

    Translating dimension in d to dimension in d1

definition encode1 :: nat ⇒ nat where
encode1 i = digit-decode dims1 (nths (digit-encode dims i) vars)

lemma encode1-alter:
assumes avars ⊆ A
shows encode1 i = digit-decode dims1 (nths (digit-encode dims i) (A ∩ vars))
⟨proof⟩

    Translating dimension in d to dimension in d2

definition encode2 :: nat ⇒ nat where
encode2 i = digit-decode dims2 (nths (digit-encode dims i) (−vars))

lemma encode2-alter:
assumes avars ⊆ A
shows encode2 i = digit-decode dims2 (nths (digit-encode dims i) (A − vars))
⟨proof⟩

lemma encode1-lt [simp]:
assumes i < d
shows encode1 i < d1
⟨proof⟩

lemma encode2-lt [simp]:
assumes i < d
shows encode2 i < d2
⟨proof⟩

    Given dimensions in d1 and d2, form dimension in d

fun encode12 :: nat × nat ⇒ nat where
encode12 (i, j) = digit-decode dims (weave vars (digit-encode dims1 i) (digit-encode
dims2 j))
declare encode12.simps [simp del]

```

```

lemma encode12-inv:
  assumes k < d
  shows encode12 (encode1 k, encode2 k) = k
  {proof}

lemma encode12-inv1:
  assumes i < d1 j < d2
  shows encode1 (encode12 (i, j)) = i
  {proof}

lemma encode12-inv2:
  assumes i < d1 j < d2
  shows encode2 (encode12 (i, j)) = j
  {proof}

lemma encode12-lt:
  assumes i < d1 j < d2
  shows encode12 (i, j) < d
  {proof}

lemma sum-encode: ( $\sum i = 0..< d1. \sum j = 0..< d2. f i j$ ) = sum ( $\lambda k. f (encode1 k) (encode2 k)$ ) {0..< d}
  {proof}

```

4.2 Tensor product of vectors and matrices

Given vector v1 of dimension d1, and vector v2 of dimension d2, form the tensor vector of dimension d1 * d2 = d

```

definition tensor-vec :: 'a::times vec  $\Rightarrow$  'a vec  $\Rightarrow$  'a vec where
  tensor-vec v1 v2 = Matrix.vec d ( $\lambda i. v1 \$ encode1 i * v2 \$ encode2 i$ )

lemma tensor-vec-dim [simp]:
  dim-vec (tensor-vec v1 v2) = d
  {proof}

lemma tensor-vec-carrier:
  tensor-vec v1 v2  $\in$  carrier-vec d
  {proof}

lemma tensor-vec-eval:
  assumes i < d
  shows tensor-vec v1 v2 $ i = v1 $ encode1 i * v2 $ encode2 i
  {proof}

lemma tensor-vec-add1:
  fixes v1 v2 v3 :: 'a::comm-ring vec
  assumes v1  $\in$  carrier-vec d1
  and v2  $\in$  carrier-vec d1

```

and $v3 \in carrier\text{-}vec d2$
shows $tensor\text{-}vec(v1 + v2) v3 = tensor\text{-}vec v1 v3 + tensor\text{-}vec v2 v3$
 $\langle proof \rangle$

lemma *tensor-vec-add2*:
fixes $v1 v2 v3 :: 'a::comm-ring vec$
assumes $v1 \in carrier\text{-}vec d1$
and $v2 \in carrier\text{-}vec d2$
and $v3 \in carrier\text{-}vec d2$
shows $tensor\text{-}vec v1 (v2 + v3) = tensor\text{-}vec v1 v2 + tensor\text{-}vec v1 v3$
 $\langle proof \rangle$

Given d1-by-d1 matrix m1, and d2-by-d2 matrix m2, form d-by-d matrix

definition *tensor-mat* :: ' $a::comm-ring$ -1 mat \Rightarrow 'a mat \Rightarrow 'a mat **where**
 $tensor\text{-}mat m1 m2 = Matrix.mat d d (\lambda(i,j).$
 $m1 \$\$ (encode1 i, encode1 j) * m2 \$\$ (encode2 i, encode2 j))$

lemma *tensor-mat-dim-row* [*simp*]:
 $dim\text{-}row(tensor\text{-}mat m1 m2) = d$
 $\langle proof \rangle$

lemma *tensor-mat-dim-col* [*simp*]:
 $dim\text{-}col(tensor\text{-}mat m1 m2) = d$
 $\langle proof \rangle$

lemma *tensor-mat-carrier*:
 $tensor\text{-}mat m1 m2 \in carrier\text{-}mat d d$
 $\langle proof \rangle$

lemma *tensor-mat-eval*:
assumes $i < d j < d$
shows $tensor\text{-}mat m1 m2 \$\$ (i, j) = m1 \$\$ (encode1 i, encode1 j) * m2 \$\$ (encode2 i, encode2 j)$
 $\langle proof \rangle$

lemma *tensor-mat-zero1*:
shows $tensor\text{-}mat (0_m d1 d1) m1 = 0_m d d$
 $\langle proof \rangle$

lemma *tensor-mat-zero2*:
shows $tensor\text{-}mat m1 (0_m d2 d2) = 0_m d d$
 $\langle proof \rangle$

lemma *tensor-mat-add1*:
assumes $m1 \in carrier\text{-}mat d1 d1$
and $m2 \in carrier\text{-}mat d1 d1$
and $m3 \in carrier\text{-}mat d2 d2$
shows $tensor\text{-}mat (m1 + m2) m3 = tensor\text{-}mat m1 m3 + tensor\text{-}mat m2 m3$
 $\langle proof \rangle$

```

lemma tensor-mat-add2:
  assumes m1 ∈ carrier-mat d1 d1
  and m2 ∈ carrier-mat d2 d2
  and m3 ∈ carrier-mat d2 d2
  shows tensor-mat m1 (m2 + m3) = tensor-mat m1 m2 + tensor-mat m1 m3
  ⟨proof⟩

lemma tensor-mat-minus1:
  assumes m1 ∈ carrier-mat d1 d1
  and m2 ∈ carrier-mat d1 d1
  and m3 ∈ carrier-mat d2 d2
  shows tensor-mat (m1 - m2) m3 = tensor-mat m1 m3 - tensor-mat m2 m3
  ⟨proof⟩

lemma tensor-mat-matrix-sum2:
  assumes m1 ∈ carrier-mat d1 d1
  shows ( $\bigwedge k. k < n \implies f k \in \text{carrier-mat } d2 d2$ )
     $\implies \text{matrix-sum } d (\lambda k. \text{tensor-mat } m1 (f k)) n = \text{tensor-mat } m1 (\text{matrix-sum } d2 f n)$ 
  ⟨proof⟩

lemma tensor-mat-scale1:
  assumes m1 ∈ carrier-mat d1 d1
  and m2 ∈ carrier-mat d2 d2
  shows tensor-mat (a ·m m1) m2 = a ·m tensor-mat m1 m2
  ⟨proof⟩

lemma tensor-mat-scale2:
  assumes m1 ∈ carrier-mat d1 d1
  and m2 ∈ carrier-mat d2 d2
  shows tensor-mat m1 (a ·m m2) = a ·m tensor-mat m1 m2
  ⟨proof⟩

lemma tensor-mat-trace:
  assumes m1 ∈ carrier-mat d1 d1
  and m2 ∈ carrier-mat d2 d2
  shows trace (tensor-mat m1 m2) = trace m1 * trace m2
  ⟨proof⟩

lemma tensor-mat-id:
  tensor-mat (1m d1) (1m d2) = 1m d
  ⟨proof⟩

lemma tensor-mat-mult-vec:
  assumes m1 ∈ carrier-mat d1 d1
  and m2 ∈ carrier-mat d2 d2
  and v1 ∈ carrier-vec d1
  and v2 ∈ carrier-vec d2

```

```

shows tensor-vec ( $m1 *_v v1$ ) ( $m2 *_v v2$ ) = tensor-mat  $m1 m2 *_v$  tensor-vec  $v1$ 
 $v2$ 
⟨proof⟩

lemma tensor-mat-mult:
assumes  $m1 \in$  carrier-mat  $d1 d1$ 
and  $m2 \in$  carrier-mat  $d1 d1$ 
and  $m3 \in$  carrier-mat  $d2 d2$ 
and  $m4 \in$  carrier-mat  $d2 d2$ 
shows tensor-mat ( $m1 * m2$ ) ( $m3 * m4$ ) = tensor-mat  $m1 m3 *$  tensor-mat  $m2$ 
 $m4$ 
⟨proof⟩

lemma tensor-mat-adjoint:
assumes  $m1 \in$  carrier-mat  $d1 d1$ 
and  $m2 \in$  carrier-mat  $d2 d2$ 
shows adjoint (tensor-mat  $m1 m2$ ) = tensor-mat (adjoint  $m1$ ) (adjoint  $m2$ )
⟨proof⟩

lemma tensor-mat-hermitian:
assumes  $m1 \in$  carrier-mat  $d1 d1$ 
and  $m2 \in$  carrier-mat  $d2 d2$ 
and hermitian  $m1$ 
and hermitian  $m2$ 
shows hermitian (tensor-mat  $m1 m2$ )
⟨proof⟩

lemma tensor-mat-unitary:
assumes  $m1 \in$  carrier-mat  $d1 d1$ 
and  $m2 \in$  carrier-mat  $d2 d2$ 
and unitary  $m1$ 
and unitary  $m2$ 
shows unitary (tensor-mat  $m1 m2$ )
⟨proof⟩

lemma tensor-mat-positive:
assumes  $m1 \in$  carrier-mat  $d1 d1$ 
and  $m2 \in$  carrier-mat  $d2 d2$ 
and positive  $m1$ 
and positive  $m2$ 
shows positive (tensor-mat  $m1 m2$ )
⟨proof⟩

lemma tensor-mat-positive-le:
assumes  $m1 \in$  carrier-mat  $d1 d1$ 
and  $m2 \in$  carrier-mat  $d2 d2$ 
and positive  $m1$ 
and positive  $m2$ 
and  $m1 \leq_L A$ 

```

```

and  $m2 \leq_L B$ 
shows tensor-mat  $m1\ m2 \leq_L \text{tensor-mat } A\ B$ 
⟨proof⟩

```

```

lemma tensor-mat-le-one:
assumes  $m1 \in \text{carrier-mat } d1\ d1$ 
and  $m2 \in \text{carrier-mat } d2\ d2$ 
and positive  $m1$ 
and positive  $m2$ 
and  $m1 \leq_L 1_m\ d1$ 
and  $m2 \leq_L 1_m\ d2$ 
shows tensor-mat  $m1\ m2 \leq_L 1_m\ d$ 
⟨proof⟩

```

4.3 Extension of matrices

```

definition mat-extension :: 'a::comm-ring-1 mat ⇒ 'a mat where
mat-extension  $m = \text{tensor-mat } m (1_m\ d2)$ 

```

```

lemma mat-extension-carrier:
mat-extension  $m \in \text{carrier-mat } d\ d$ 
⟨proof⟩

```

```

lemma mat-extension-add:
assumes  $m1 \in \text{carrier-mat } d1\ d1$ 
and  $m2 \in \text{carrier-mat } d1\ d1$ 
shows mat-extension  $(m1 + m2) = \text{mat-extension } m1 + \text{mat-extension } m2$ 
⟨proof⟩

```

```

lemma mat-extension-trace:
assumes  $m \in \text{carrier-mat } d1\ d1$ 
shows trace  $(\text{mat-extension } m) = d2 * \text{trace } m$ 
⟨proof⟩

```

```

lemma mat-extension-id:
mat-extension  $(1_m\ d1) = 1_m\ d$ 
⟨proof⟩

```

```

lemma mat-extension-mult:
assumes  $m1 \in \text{carrier-mat } d1\ d1$ 
and  $m2 \in \text{carrier-mat } d1\ d1$ 
shows mat-extension  $(m1 * m2) = \text{mat-extension } m1 * \text{mat-extension } m2$ 
⟨proof⟩

```

```

lemma mat-extension-hermitian:
assumes  $m \in \text{carrier-mat } d1\ d1$ 
and hermitian  $m$ 
shows hermitian  $(\text{mat-extension } m)$ 
⟨proof⟩

```

```

lemma mat-extension-unitary:
  assumes m ∈ carrier-mat d1 d1
    and unitary m
  shows unitary (mat-extension m)
  ⟨proof⟩

end

abbreviation tensor-mat ≡ partial-state.tensor-mat
abbreviation mat-extension ≡ partial-state.mat-extension

context state-sig
begin

  Swapping the order of matrices, as well as switching vars, should have
  no effect

lemma tensor-mat-comm:
  assumes vars1 ∩ vars2 = {}
    and {0..<length dims} ⊆ vars1 ∪ vars2
    and m1 ∈ carrier-mat (prod-list (nths dims vars1)) (prod-list (nths dims vars1))
      and m2 ∈ carrier-mat (prod-list (nths dims vars2)) (prod-list (nths dims vars2))
    shows tensor-mat dims vars1 m1 m2 = tensor-mat dims vars2 m2 m1
  ⟨proof⟩
end

```

4.4 Partial tensor product

In this context, we assume two disjoint sets of variables, and define the tensor product of two matrices on these variables

```

locale partial-state2 = state-sig +
  fixes vars1 :: nat set
    and vars2 :: nat set
  assumes disjoint: vars1 ∩ vars2 = {}

begin

definition vars0 :: nat set where
  vars0 = vars1 ∪ vars2

definition dims0 :: nat list where
  dims0 = nths dims vars0

definition dims1 :: nat list where
  dims1 = nths dims vars1

definition dims2 :: nat list where
  dims2 = nths dims vars2

```

```
definition d0 :: nat where
d0 = prod-list dims0
```

```
definition d1 :: nat where
d1 = prod-list dims1
```

```
definition d2 :: nat where
d2 = prod-list dims2
```

lemma dims-product:
 $d0 = d1 * d2$
 $\langle proof \rangle$

Locations of variables in vars1 relative to vars0. For example: if vars0 = 0,1,2,4,5,6,9 and vars1 = 1,4,6,9, then vars1' should be 1,3,5,6.

```
definition vars1' :: nat set where
vars1' = (ind-in-set vars0) ` vars1
```

```
definition vars2' :: nat set where
vars2' = (ind-in-set vars0) ` vars2
```

lemma vars1'I:
 $x \in vars1 \implies card \{y \in vars0. y < x\} \in vars1'$
 $\langle proof \rangle$

lemma vars1'D:
 $i \in vars1' \implies \exists x \in vars1. card \{y \in vars0. y < x\} = i$
 $\langle proof \rangle$

Main property of vars1'

lemma ind-in-set-bij:
 $bij\text{-}betw (ind-in-set vars0) (\{0..<\text{length } dims\} \cap vars0) \{0..<\text{card } (\{0..<\text{length } dims\} \cap vars0)\}$
 $\langle proof \rangle$

lemma length-dims0:
 $\text{length } dims0 = \text{card } (\{0..<\text{length } dims\} \cap vars0)$
 $\langle proof \rangle$

lemma length-dims0-minus-vars2'-is-vars1':
 $\{0..<\text{length } dims0\} - vars2' = \{0..<\text{length } dims0\} \cap vars1'$
 $\langle proof \rangle$

lemma length-dims0-minus-vars1'-is-vars2':
 $\{0..<\text{length } dims0\} - vars1' = \{0..<\text{length } dims0\} \cap vars2'$
 $\langle proof \rangle$

lemma nths-vars1':
 $nths \ dims0 \ vars1' = dims1$

$\langle proof \rangle$

lemma *nths-vars1'-comp*:
nths dims0 (-vars2') = dims1
 $\langle proof \rangle$

lemma *nths-vars2'*:
nths dims0 (-vars1') = dims2
 $\langle proof \rangle$

lemma *nths-vars2'-comp*:
nths dims0 (vars2') = dims2
 $\langle proof \rangle$

lemma *ptensor-encode1-encode2*:
partial-state.encode1 dims0 vars1' = partial-state.encode2 dims0 vars2'
 $\langle proof \rangle$

lemma *ptensor-encode2-encode1*:
partial-state.encode1 dims0 vars2' = partial-state.encode2 dims0 vars1'
 $\langle proof \rangle$

Given vector v1 of dimension d1, and vector v2 of dimension d2, form the tensor vector of dimension $d1 * d2 = d0$

definition *ptensor-vec* :: '*a::times vec* \Rightarrow '*a vec* \Rightarrow '*a vec* **where**
ptensor-vec v1 v2 = partial-state.tensor-vec dims0 vars1' v1 v2

lemma *ptensor-vec-dim [simp]*:
dim-vec (ptensor-vec v1 v2) = d0
 $\langle proof \rangle$

lemma *ptensor-vec-carrier*:
ptensor-vec v1 v2 ∈ carrier-vec d0
 $\langle proof \rangle$

lemma *ptensor-vec-add*:
fixes *v1 v2 v3 :: 'a::comm-ring vec*
assumes *v1 ∈ carrier-vec d1*
and *v2 ∈ carrier-vec d1*
and *v3 ∈ carrier-vec d2*
shows *ptensor-vec (v1 + v2) v3 = ptensor-vec v1 v3 + ptensor-vec v2 v3*
 $\langle proof \rangle$

definition *ptensor-mat* :: '*a::comm-ring-1 mat* \Rightarrow '*a mat* \Rightarrow '*a mat* **where**
ptensor-mat m1 m2 = partial-state.tensor-mat dims0 vars1' m1 m2

lemma *ptensor-mat-dim-row [simp]*:
dim-row (ptensor-mat m1 m2) = d0
 $\langle proof \rangle$

```

lemma ptensor-mat-dim-col [simp]:
  dim-col (ptensor-mat m1 m2) = d0
  ⟨proof⟩

lemma ptensor-mat-carrier:
  ptensor-mat m1 m2 ∈ carrier-mat d0 d0
  ⟨proof⟩

lemma ptensor-mat-add:
  assumes m1 ∈ carrier-mat d1 d1
  and m2 ∈ carrier-mat d1 d1
  and m3 ∈ carrier-mat d2 d2
  shows ptensor-mat (m1 + m2) m3 = ptensor-mat m1 m3 + ptensor-mat m2
  m3
  ⟨proof⟩

lemma ptensor-mat-trace:
  assumes m1 ∈ carrier-mat d1 d1
  and m2 ∈ carrier-mat d2 d2
  shows trace (ptensor-mat m1 m2) = trace m1 * trace m2
  ⟨proof⟩

lemma ptensor-mat-id:
  ptensor-mat (1m d1) (1m d2) = 1m d0
  ⟨proof⟩

lemma ptensor-mat-mult:
  assumes m1 ∈ carrier-mat d1 d1
  and m2 ∈ carrier-mat d1 d1
  and m3 ∈ carrier-mat d2 d2
  and m4 ∈ carrier-mat d2 d2
  shows ptensor-mat (m1 * m2) (m3 * m4) = ptensor-mat m1 m3 * ptensor-mat
  m2 m4
  ⟨proof⟩

lemma ptensor-mat-mult-vec:
  assumes m1 ∈ carrier-mat d1 d1
  and v1 ∈ carrier-vec d1
  and m2 ∈ carrier-mat d2 d2
  and v2 ∈ carrier-vec d2
  shows ptensor-vec (m1 *_v v1) (m2 *_v v2) = ptensor-mat m1 m2 *_v ptensor-vec
  v1 v2
  ⟨proof⟩

```

4.5 Partial extensions

```

definition pmat-extension :: 'a::comm-ring-1 mat ⇒ 'a mat where
  pmat-extension m = ptensor-mat m (1m d2)

```

```

lemma pmat-extension-carrier:
  pmat-extension m ∈ carrier-mat d0 d0
  ⟨proof⟩

lemma pmat-extension-add:
  assumes m1 ∈ carrier-mat d1 d1
  and m2 ∈ carrier-mat d1 d1
  shows pmat-extension (m1 + m2) = pmat-extension m1 + pmat-extension m2
  ⟨proof⟩

lemma pmat-extension-trace:
  assumes m ∈ carrier-mat d1 d1
  shows trace (pmat-extension m) = d2 * trace m
  ⟨proof⟩

lemma pmat-extension-id:
  pmat-extension (1_m d1) = 1_m d0
  ⟨proof⟩

lemma pmat-extension-mult:
  assumes m1 ∈ carrier-mat d1 d1
  and m2 ∈ carrier-mat d1 d1
  shows pmat-extension (m1 * m2) = pmat-extension m1 * pmat-extension m2
  ⟨proof⟩

end

context state-sig
begin

```

```

abbreviation ptensor-vec ≡ partial-state2.ptensor-vec
abbreviation ptensor-mat ≡ partial-state2.ptensor-mat
abbreviation pmat-extension ≡ partial-state2.pmat-extension

```

Key property: commutativity of tensor product

```

lemma ptensor-mat-comm:
  fixes m1 m2 :: complex mat
  assumes vars1 ∩ vars2 = {}
  shows ptensor-mat dims vars1 vars2 m1 m2 = ptensor-mat dims vars2 vars1 m2
  m1
  ⟨proof⟩

```

Key property: associativity of tensor product

```

lemma ind-in-set-mono:
  fixes a b :: nat and A :: nat set
  assumes a ∈ A b ∈ A a < b
  shows ind-in-set A a < ind-in-set A b
  ⟨proof⟩

```

```

lemma ind-in-set-inj:
  fixes a b :: nat and A :: nat set
  assumes a ∈ A b ∈ A ind-in-set A a = ind-in-set A b
  shows a = b
  ⟨proof⟩

lemma ind-in-set-mono2:
  fixes a b :: nat and A :: nat set
  assumes a ∈ A b ∈ A ind-in-set A a < ind-in-set A b
  shows a < b
  ⟨proof⟩

lemma ind-in-set-bij-betw:
  fixes A B :: nat set
  assumes B ⊆ A c ∈ B
  shows bij-betw (ind-in-set A) {i ∈ B. i < c} {i ∈ ind-in-set A ‘ B. i < ind-in-set
A c}
  ⟨proof⟩

lemma ind-in-set-assoc:
  fixes A B C :: nat set
  assumes C ⊆ B B ⊆ A
  shows ind-in-set (ind-in-set A ‘ B) ‘ (ind-in-set A ‘ C) = ind-in-set B ‘ C
  ⟨proof⟩

lemma nths-reencode-eq3:
  fixes A B C :: nat set
  assumes C ⊆ B B ⊆ A
  shows nths (nthxs xs (ind-in-set A ‘ B)) (ind-in-set B ‘ C) = nthxs xs (ind-in-set
A ‘ C)
  ⟨proof⟩

lemma nths-assoc-three-A:
  fixes A B C :: nat set
  assumes A ∩ B = {}
  and (A ∪ B) ∩ C = {}
  shows nths (nthxs xs (ind-in-set (A ∪ B ∪ C) ‘ (A ∪ B))) (ind-in-set (A ∪ B) ‘
A)
  = nthxs xs (ind-in-set (A ∪ B ∪ C) ‘ A)
  ⟨proof⟩

lemma nths-assoc-three-B:
  fixes A B C :: nat set
  assumes A ∩ B = {}
  and (A ∪ B) ∩ C = {}
  shows nths (nthxs xs (ind-in-set (A ∪ B ∪ C) ‘ (A ∪ B))) (ind-in-set (A ∪ B) ‘
B)
  = nths (nthxs xs (ind-in-set (A ∪ B ∪ C) ‘ (B ∪ C))) (ind-in-set (B ∪ C) ‘
C)

```

$B)$
 $\langle proof \rangle$

lemma *nths-assoc-three-C*:

fixes $A B C :: \text{nat set}$
 assumes $A \cap B = \{\}$
 and $(A \cup B) \cap C = \{\}$
 shows $\text{nths}(\text{nths}(\text{xs}(\text{ind-in-set}(A \cup B \cup C) \cdot (B \cup C)))) (\text{ind-in-set}(B \cup C) \cdot C)$
 $= \text{nths}(\text{xs}(\text{ind-in-set}(A \cup B \cup C) \cdot C))$
 $\langle proof \rangle$

lemma *valid-index-ind-in-set*:

assumes $is \triangleleft \text{nths dims } A \ B \subseteq A$
 shows $\text{nths}(\text{is}(\text{ind-in-set } A \cdot B)) \triangleleft \text{nths dims } B$
 $\langle proof \rangle$

lemma *ind-in-set-id*:

fixes $A :: \text{nat set}$
 assumes *finite A*
 shows $\text{ind-in-set } A \cdot A = \{0..< \text{card } A\}$
 $\langle proof \rangle$

lemma *nths-complement-ind-in-set*:

fixes $A B :: \text{nat set}$
 assumes $A \cap B = \{\}$
 card $(A \cup B) = \text{length } xs$
 shows $\text{nths}(\text{xs}(-\text{ind-in-set}(A \cup B) \cdot A)) = \text{nths}(\text{xs}(\text{ind-in-set}(A \cup B) \cdot B))$
 $\langle proof \rangle$

lemma *ind-in-set-inj'*:

fixes $A B :: \text{nat set}$
 assumes $B \subseteq A$
 shows $\text{inj-on}(\text{ind-in-set } A) B$
 $\langle proof \rangle$

lemma *ind-in-set-less*:

fixes $x :: \text{nat}$ **and** $A :: \text{nat set}$
 assumes *finite A* $x \in A$
 shows $\text{ind-in-set } A \ x < \text{card } A$
 $\langle proof \rangle$

lemma *ptensor-mat-assoc*:

assumes $\text{vars1} \cap \text{vars2} = \{\}$
 and $(\text{vars1} \cup \text{vars2}) \cap \text{vars3} = \{\}$
 and $\text{vars1} \cup \text{vars2} \cup \text{vars3} \subseteq \{0..< \text{length dims}\}$
 shows $\text{ptensor-mat dims}(\text{vars1} \cup \text{vars2}) \text{ vars3} (\text{ptensor-mat dims}(\text{vars1} \text{ vars2}) \text{ m1 m2}) \text{ m3} =$
 $\text{ptensor-mat dims}(\text{vars1} (\text{vars2} \cup \text{vars3})) \text{ m1} (\text{ptensor-mat dims}(\text{vars2} \text{ vars3}) \text{ m2})$

$m2\ m3)$
 $\langle proof \rangle$

Some simple consequences of associativity

```
lemma pmat-extension-assoc:
  assumes vars1 ∩ vars2 = {}
  and (vars1 ∪ vars2) ∩ vars3 = {}
  and vars1 ∪ vars2 ∪ vars3 ⊆ {0..< length dims}
  shows pmat-extension dims vars1 (vars2 ∪ vars3) m =
    pmat-extension dims (vars1 ∪ vars2) vars3 (pmat-extension dims vars1
  vars2 m)
  ⟨proof⟩
end
```

4.6 Commands on subset of variables

```
context state-sig
begin
```

```
definition Utrans-P :: nat set ⇒ complex mat ⇒ com where
  Utrans-P vars U = Utrans (mat-extension dims vars U)
```

```
lemma well-com-Utrans-P:
  assumes U ∈ carrier-mat (prod-list (nths dims vars)) (prod-list (nths dims vars))
  and unitary U
  shows well-com (Utrans-P vars U)
⟨proof⟩
```

```
definition Measure-P :: nat set ⇒ nat ⇒ (nat ⇒ complex mat) ⇒ com list ⇒ com where
  Measure-P vars n Ps Cs = Measure n (λn. mat-extension dims vars (Ps n)) Cs
```

```
definition While-P :: nat set ⇒ complex mat ⇒ complex mat ⇒ com ⇒ com
where
  While-P vars M0 M1 C = While (λn.
    if n = 0 then mat-extension dims vars M0
    else if n = 1 then mat-extension dims vars M1
    else undefined) C
end
```

```
end
```

5 Standard gates

```
theory Gates
  imports Complex-Matrix
begin
```

Pauli matrices

```
definition sigma-x :: complex mat where
  sigma-x = mat-of-rows-list 2 [[0, 1], [1, 0]]
```

```
definition sigma-y :: complex mat where
  sigma-y = mat-of-rows-list 2 [[0, -i], [i, 0]]
```

```
definition sigma-z :: complex mat where
  sigma-z = mat-of-rows-list 2 [[1, 0], [0, -1]]
```

Hadamard matrices

```
definition hadamard :: complex mat where
  hadamard = mat 2 2 (λ(i, j). if (i = 0 ∨ j = 0) then 1 / csqrt 2 else -1 / sqrt 2)
```

```
lemma hadamard-dim:
  hadamard ∈ carrier-mat 2 2
  ⟨proof⟩
```

```
lemma hermitian-hadamard:
  hermitian hadamard
  ⟨proof⟩
```

```
lemma csqrt-2-sq:
  complex-of-real (sqrt 2) * complex-of-real (sqrt 2) = 2
  ⟨proof⟩
```

```
lemma sum-le-2:
  ⋀(f::nat⇒complex). sum f {0..<2} = f 0 + f 1
  ⟨proof⟩
```

```
lemma unitary-hadamard:
  unitary hadamard
  ⟨proof⟩
```

The matrix [0 0 .. 0 1 1 0 .. 0 0 0 1 .. 0 0 0 0 .. 1 0] implements
i := i + 1 in the last variable.

```
definition mat-incr :: nat ⇒ complex mat where
  mat-incr n = mat n n (λ(i,j). if i = 0 then (if j = n - 1 then 1 else 0) else (if i = j + 1 then 1 else 0))
```

```
lemma mat-incr-dim:
  mat-incr n ∈ carrier-mat n n
  ⟨proof⟩
```

```
lemma adjoint-mat-incr:
  adjoint (mat-incr n) = mat n n (λ(i,j). if j = 0 then (if i = n - 1 then 1 else 0) else (if j = i + 1 then 1 else 0))
  ⟨proof⟩
```

```

lemma mat-incr-mult-adjoint-mat-incr:
  shows mat-incr n * (adjoint (mat-incr n)) = 1_m n
  ⟨proof⟩

lemma unitary-mat-incr:
  unitary (mat-incr n)
  ⟨proof⟩

end

```

6 Partial and total correctness

```

theory Quantum-Hoare
  imports Quantum-Program
begin

context state-sig
begin

definition density-states :: state set where
  density-states = { $\varrho \in \text{carrier-mat } d \text{ } d$ . partial-density-operator  $\varrho$ }

lemma denote-density-states:
   $\varrho \in \text{density-states} \implies \text{well-com } S \implies \text{denote } S \varrho \in \text{density-states}$ 
  ⟨proof⟩

definition is-quantum-predicate :: complex mat  $\Rightarrow$  bool where
  is-quantum-predicate  $P \longleftrightarrow P \in \text{carrier-mat } d \text{ } d \wedge \text{positive } P \wedge P \leq_L 1_m \text{ } d$ 

lemma trace-measurement2:
  assumes  $m: \text{measurement } n \geq M \text{ and } dA: A \in \text{carrier-mat } n \text{ } n$ 
  shows  $\text{trace } ((M \text{ } 0) * A * \text{adjoint } (M \text{ } 0)) + \text{trace } ((M \text{ } 1) * A * \text{adjoint } (M \text{ } 1)) = \text{trace } A$ 
  ⟨proof⟩

lemma qp-close-under-unitary-operator:
  fixes  $U \text{ } P :: \text{complex mat}$ 
  assumes  $dU: U \in \text{carrier-mat } d \text{ } d$ 
  and  $u: \text{unitary } U$ 
  and  $qp: \text{is-quantum-predicate } P$ 
  shows  $\text{is-quantum-predicate } (\text{adjoint } U * P * U)$ 
  ⟨proof⟩

lemma qps-after-measure-is-qp:
  assumes  $m: \text{measurement } d \text{ } n \text{ } M \text{ and } qpk: \bigwedge k. k < n \implies \text{is-quantum-predicate } (P \text{ } k)$ 
  shows  $\text{is-quantum-predicate } (\text{matrix-sum } d \text{ } (\lambda k. \text{adjoint } (M \text{ } k) * P \text{ } k * M \text{ } k) \text{ } n)$ 
  ⟨proof⟩

```

definition hoare-total-correct :: complex mat \Rightarrow com \Rightarrow complex mat \Rightarrow bool $(\langle \models_t \{(1-)\} / (-) / \{(1-)\} \rangle 50)$ **where**
 $\models_t \{P\} S \{Q\} \longleftrightarrow (\forall \varrho \in \text{density-states}. \text{trace}(P * \varrho) \leq \text{trace}(Q * \text{denote } S \varrho))$

definition hoare-partial-correct :: complex mat \Rightarrow com \Rightarrow complex mat \Rightarrow bool
 $(\langle \models_p \{(1-)\} / (-) / \{(1-)\} \rangle 50)$ **where**
 $\models_p \{P\} S \{Q\} \longleftrightarrow (\forall \varrho \in \text{density-states}. \text{trace}(P * \varrho) \leq \text{trace}(Q * \text{denote } S \varrho) + (\text{trace } \varrho - \text{trace}(\text{denote } S \varrho)))$

lemma total-implies-partial:
assumes S: well-com S
and total: $\models_t \{P\} S \{Q\}$
shows $\models_p \{P\} S \{Q\}$
 $\langle \text{proof} \rangle$

lemma predicate-prob-positive:
assumes $\theta_m d d \leq_L P$
and $\varrho \in \text{density-states}$
shows $\theta \leq \text{trace}(P * \varrho)$
 $\langle \text{proof} \rangle$

lemma total-pre-zero:
assumes S: well-com S
and Q: is-quantum-predicate Q
shows $\models_t \{\theta_m d d\} S \{Q\}$
 $\langle \text{proof} \rangle$

lemma partial-post-identity:
assumes S: well-com S
and P: is-quantum-predicate P
shows $\models_p \{P\} S \{1_m d\}$
 $\langle \text{proof} \rangle$

6.1 Weakest liberal preconditions

definition is-weakest-liberal-precondition :: complex mat \Rightarrow com \Rightarrow complex mat \Rightarrow bool **where**
 $\text{is-weakest-liberal-precondition } W S P \longleftrightarrow$
 $\text{is-quantum-predicate } W \wedge \models_p \{W\} S \{P\} \wedge (\forall Q. \text{is-quantum-predicate } Q \longrightarrow$
 $\models_p \{Q\} S \{P\} \longrightarrow Q \leq_L W)$

definition wlp-measure :: nat \Rightarrow (nat \Rightarrow complex mat) \Rightarrow ((complex mat \Rightarrow complex mat) list) \Rightarrow complex mat \Rightarrow complex mat **where**
 $wlp\text{-measure } n M WS P = \text{matrix-sum } d (\lambda k. \text{adjoint } (M k) * ((WS!k) P) * (M k)) n$

```

fun wlp-while-n :: complex mat  $\Rightarrow$  complex mat  $\Rightarrow$  (complex mat  $\Rightarrow$  complex mat)
 $\Rightarrow$  nat  $\Rightarrow$  complex mat  $\Rightarrow$  complex mat where
  wlp-while-n M0 M1 WS 0 P =  $1_m$  d
  | wlp-while-n M0 M1 WS (Suc n) P = adjoint M0 * P * M0 + adjoint M1 * (WS
    (wlp-while-n M0 M1 WS n P)) * M1

lemma measurement2-leq-one-mat:
  assumes dP:  $P \in \text{carrier-mat } d$  and dQ:  $Q \in \text{carrier-mat } d$ 
  and leP:  $P \leq_L 1_m$  d and leQ:  $Q \leq_L 1_m$  d and m: measurement d 2 M
  shows (adjoint (M 0) * P * (M 0) + adjoint (M 1) * Q * (M 1))  $\leq_L 1_m$  d
  ⟨proof⟩

lemma wlp-while-n-close:
  assumes close:  $\bigwedge P. \text{is-quantum-predicate } P \implies \text{is-quantum-predicate } (\text{WS } P)$ 
  and m: measurement d 2 M and qpP: is-quantum-predicate P
  shows is-quantum-predicate (wlp-while-n (M 0) (M 1) WS k P)
  ⟨proof⟩

lemma wlp-while-n-mono:
  assumes  $\bigwedge P. \text{is-quantum-predicate } P \implies \text{is-quantum-predicate } (\text{WS } P)$ 
  and  $\bigwedge P Q. \text{is-quantum-predicate } P \implies \text{is-quantum-predicate } Q \implies P \leq_L Q$ 
   $\implies \text{WS } P \leq_L \text{WS } Q$ 
  and measurement d 2 M
  and is-quantum-predicate P
  and is-quantum-predicate Q
  and  $P \leq_L Q$ 
  shows (wlp-while-n (M 0) (M 1) WS k P)  $\leq_L$  (wlp-while-n (M 0) (M 1) WS k Q)
  ⟨proof⟩

definition wlp-while :: complex mat  $\Rightarrow$  complex mat  $\Rightarrow$  (complex mat  $\Rightarrow$  complex mat)
 $\Rightarrow$  complex mat  $\Rightarrow$  complex mat where
  wlp-while M0 M1 WS P = (THE Q. limit-mat ( $\lambda n.$  wlp-while-n M0 M1 WS n P) Q d)

lemma wlp-while-exists:
  assumes  $\bigwedge P. \text{is-quantum-predicate } P \implies \text{is-quantum-predicate } (\text{WS } P)$ 
  and  $\bigwedge P Q. \text{is-quantum-predicate } P \implies \text{is-quantum-predicate } Q \implies P \leq_L Q$ 
   $\implies \text{WS } P \leq_L \text{WS } Q$ 
  and m: measurement d 2 M
  and qpP: is-quantum-predicate P
  shows is-quantum-predicate (wlp-while (M 0) (M 1) WS P)
   $\wedge$  ( $\forall n.$  (wlp-while (M 0) (M 1) WS P)  $\leq_L$  (wlp-while-n (M 0) (M 1) WS n P))
   $\wedge$  ( $\forall W'.$  ( $\forall n.$   $W' \leq_L (\text{wlp-while-n } (M 0) (M 1) \text{ WS } n \text{ P}) \implies W' \leq_L$ 
    (wlp-while (M 0) (M 1) WS P)))
   $\wedge$  limit-mat ( $\lambda n.$  wlp-while-n (M 0) (M 1) WS n P) (wlp-while (M 0) (M 1) WS P) d

```

$\langle proof \rangle$

lemma *wlp-while-mono*:

assumes $\bigwedge P. \text{is-quantum-predicate } P \implies \text{is-quantum-predicate} (\text{WS } P)$
and $\bigwedge P Q. \text{is-quantum-predicate } P \implies \text{is-quantum-predicate } Q \implies P \leq_L Q$
 $\implies \text{WS } P \leq_L \text{WS } Q$
and measurement $d \neq M$
and *is-quantum-predicate* P
and *is-quantum-predicate* Q
and $P \leq_L Q$
shows *wlp-while* ($M 0$) ($M 1$) $\text{WS } P \leq_L \text{wlp-while} (M 0) (M 1) \text{ WS } Q$

$\langle proof \rangle$

fun *wlp* :: *com* \Rightarrow *complex mat* \Rightarrow *complex mat* **where**

$wlp \text{ SKIP } P = P$
 $| wlp (Utrans U) P = \text{adjoint } U * P * U$
 $| wlp (\text{Seq } S1 S2) P = wlp S1 (wlp S2 P)$
 $| wlp (\text{Measure } n M S) P = \text{wlp-measure } n M (\text{map } wlp S) P$
 $| wlp (\text{While } M S) P = \text{wlp-while} (M 0) (M 1) (wlp S) P$

lemma *wlp-measure-expand-m*:

assumes $m: m \leq n$ **and** $wc: \text{well-com} (\text{Measure } n M S)$
shows $wlp (\text{Measure } m M S) P = \text{matrix-sum } d (\lambda k. \text{adjoint} (M k) * (wlp (S!k) P) * (M k)) m$
 $\langle proof \rangle$

lemma *wlp-measure-expand*:

assumes $wc: \text{well-com} (\text{Measure } n M S)$
shows $wlp (\text{Measure } n M S) P = \text{matrix-sum } d (\lambda k. \text{adjoint} (M k) * (wlp (S!k) P) * (M k)) n$
 $\langle proof \rangle$

lemma *wlp-mono-and-close*:

shows *well-com* $S \implies \text{is-quantum-predicate } P \implies \text{is-quantum-predicate } Q \implies P \leq_L Q$
 $\implies \text{is-quantum-predicate} (\text{wlp } S P) \wedge \text{wlp } S P \leq_L \text{wlp } S Q$
 $\langle proof \rangle$

lemma *wlp-close*:

assumes $wc: \text{well-com } S$ **and** $qp: \text{is-quantum-predicate } P$
shows *is-quantum-predicate* ($\text{wlp } S P$)
 $\langle proof \rangle$

lemma *wlp-soundness*:

well-com $S \implies$
 $(\bigwedge P. (\text{is-quantum-predicate } P \implies$
 $(\forall \varrho \in \text{density-states}. \text{trace} (\text{wlp } S P * \varrho) = \text{trace} (P * (\text{denote } S \varrho)) + \text{trace}$
 $\varrho - \text{trace} (\text{denote } S \varrho))))$
 $\langle proof \rangle$

lemma *denote-while-split*:

assumes *wc*: well-com (*While M S*) **and** *dsr*: $\varrho \in \text{density-states}$

shows *denote* (*While M S*) $\varrho = (M 0) * \varrho * \text{adjoint}(M 0) + \text{denote}(\text{While } M S)$ (*denote S* ($M 1 * \varrho * \text{adjoint}(M 1)$))
(proof)

lemma *wlp-while-split*:

assumes *wc*: well-com (*While M S*) **and** *qpP*: is-quantum-predicate *P*

shows *wlp* (*While M S*) $P = \text{adjoint}(M 0) * P * (M 0) + \text{adjoint}(M 1) * (\text{wlp } S (\text{wlp } (\text{While } M S) P)) * (M 1)$
(proof)

lemma *wlp-is-weakest-liberal-precondition*:

assumes well-com *S* **and** is-quantum-predicate *P*

shows is-weakest-liberal-precondition (*wlp S P*) *S P*

(proof)

6.2 Hoare triples for partial correctness

inductive *hoare-partial* :: complex mat \Rightarrow com \Rightarrow complex mat \Rightarrow bool (\vdash_p ($\{(1)\}/(-)/\{(1)\}$), 50) **where**

- is-quantum-predicate P* $\Rightarrow \vdash_p \{P\} \text{ SKIP } \{P\}$
- | *is-quantum-predicate P* $\Rightarrow \vdash_p \{\text{adjoint } U * P * U\} \text{ Utrans } U \{P\}$
- | *is-quantum-predicate P* $\Rightarrow \text{is-quantum-predicate } Q \Rightarrow \text{is-quantum-predicate } R$
 \Rightarrow
 - $\vdash_p \{P\} S1 \{Q\} \Rightarrow \vdash_p \{Q\} S2 \{R\} \Rightarrow$
 - $\vdash_p \{P\} \text{ Seq } S1 S2 \{R\}$
- | $(\bigwedge k. k < n \Rightarrow \text{is-quantum-predicate } (P k)) \Rightarrow \text{is-quantum-predicate } Q \Rightarrow$
 $(\bigwedge k. k < n \Rightarrow \vdash_p \{P k\} S ! k \{Q\}) \Rightarrow$
 $\vdash_p \{\text{matrix-sum } d (\lambda k. \text{adjoint}(M k) * P k * M k) n\} \text{ Measure } n M S \{Q\}$
- | *is-quantum-predicate P* $\Rightarrow \text{is-quantum-predicate } Q \Rightarrow$
 $\vdash_p \{Q\} S \{\text{adjoint}(M 0) * P * M 0 + \text{adjoint}(M 1) * Q * M 1\} \Rightarrow$
 $\vdash_p \{\text{adjoint}(M 0) * P * M 0 + \text{adjoint}(M 1) * Q * M 1\} \text{ While } M S \{P\}$
- | *is-quantum-predicate P* $\Rightarrow \text{is-quantum-predicate } Q \Rightarrow \text{is-quantum-predicate } P'$
 $\Rightarrow \text{is-quantum-predicate } Q' \Rightarrow$
 $P \leq_L P' \Rightarrow \vdash_p \{P'\} S \{Q'\} \Rightarrow Q' \leq_L Q \Rightarrow \vdash_p \{P\} S \{Q\}$

theorem *hoare-partial-sound*:

$\vdash_p \{P\} S \{Q\} \Rightarrow \text{well-com } S \Rightarrow \models_p \{P\} S \{Q\}$

(proof)

lemma *wlp-complete*:

well-com S $\Rightarrow \text{is-quantum-predicate } P \Rightarrow \vdash_p \{\text{wlp } S P\} S \{P\}$

(proof)

theorem *hoare-partial-complete*:

$\models_p \{P\} S \{Q\} \Rightarrow \text{well-com } S \Rightarrow \text{is-quantum-predicate } P \Rightarrow \text{is-quantum-predicate } Q \Rightarrow \vdash_p \{P\} S \{Q\}$

$\langle proof \rangle$

6.3 Consequences of completeness

```

lemma hoare-patial-seq-assoc-sem:
  shows  $\models_p \{A\} (S1 ;; S2) ;; S3 \{B\} \longleftrightarrow \models_p \{A\} S1 ; (S2 ;; S3) \{B\}$ 
   $\langle proof \rangle$ 

lemma hoare-patial-seq-assoc:
  assumes well-com S1 and well-com S2 and well-com S3
    and is-quantum-predicate A and is-quantum-predicate B
  shows  $\vdash_p \{A\} (S1 ;; S2) ;; S3 \{B\} \longleftrightarrow \vdash_p \{A\} S1 ; (S2 ;; S3) \{B\}$ 
   $\langle proof \rangle$ 

end

end

```

7 Grover's algorithm

```

theory Grover
  imports Partial-State Gates Quantum-Hoare
begin

```

7.1 Basic definitions

```

locale grover-state =
  fixes n :: nat
    and f :: nat  $\Rightarrow$  bool
  assumes n:  $n > 1$ 
    and dimM:  $\text{card } \{i. i < (2::nat) \wedge n \wedge f i\} > 0$ 
       $\text{card } \{i. i < (2::nat) \wedge n \wedge f i\} < (2::nat) \wedge n$ 
begin

  definition N where
     $N = (2::nat) \wedge n$ 

  definition M where
     $M = \text{card } \{i. i < N \wedge f i\}$ 

lemma N-ge-0 [simp]:  $0 < N$   $\langle proof \rangle$ 

lemma M-ge-0 [simp]:  $0 < M$   $\langle proof \rangle$ 

lemma M-neq-0 [simp]:  $M \neq 0$   $\langle proof \rangle$ 

lemma M-le-N [simp]:  $M < N$   $\langle proof \rangle$ 

lemma M-not-ge-N [simp]:  $\neg M \geq N$   $\langle proof \rangle$ 

```

definition $\psi :: \text{complex vec where}$
 $\psi = \text{Matrix.vec } N (\lambda i. 1 / \text{sqrt } N)$

lemma $\psi\text{-dim [simp]}:$

$\psi \in \text{carrier-vec } N$
 $\text{dim-vec } \psi = N$
 $\langle \text{proof} \rangle$

lemma $\psi\text{-eval:}$

$i < N \implies \psi \$ i = 1 / \text{sqrt } N$
 $\langle \text{proof} \rangle$

lemma $\psi\text{-inner:}$

$\text{inner-prod } \psi \psi = 1$
 $\langle \text{proof} \rangle$

lemma $\psi\text{-norm:}$

$\text{vec-norm } \psi = 1$
 $\langle \text{proof} \rangle$

definition $\alpha :: \text{complex vec where}$

$\alpha = \text{Matrix.vec } N (\lambda i. \text{if } i \text{ then } 0 \text{ else } 1 / \text{sqrt } (N - M))$

lemma $\alpha\text{-dim [simp]}:$

$\alpha \in \text{carrier-vec } N$
 $\text{dim-vec } \alpha = N$
 $\langle \text{proof} \rangle$

lemma $\alpha\text{-eval:}$

$i < N \implies \alpha \$ i = (\text{if } i \text{ then } 0 \text{ else } 1 / \text{sqrt } (N - M))$
 $\langle \text{proof} \rangle$

lemma $\alpha\text{-inner:}$

$\text{inner-prod } \alpha \alpha = 1$
 $\langle \text{proof} \rangle$

definition $\beta :: \text{complex vec where}$

$\beta = \text{Matrix.vec } N (\lambda i. \text{if } i \text{ then } 1 / \text{sqrt } M \text{ else } 0)$

lemma $\beta\text{-dim [simp]}:$

$\beta \in \text{carrier-vec } N$
 $\text{dim-vec } \beta = N$
 $\langle \text{proof} \rangle$

lemma $\beta\text{-eval:}$

$i < N \implies \beta \$ i = (\text{if } i \text{ then } 1 / \text{sqrt } M \text{ else } 0)$
 $\langle \text{proof} \rangle$

```

lemma β-inner:
  inner-prod β β = 1
  ⟨proof⟩

lemma alpha-beta-orth:
  inner-prod α β = 0
  ⟨proof⟩

lemma beta-alpha-orth:
  inner-prod β α = 0
  ⟨proof⟩

definition θ :: real where
  θ = 2 * arccos (sqrt ((N - M) / N))

lemma cos-theta-div-2:
  cos (θ / 2) = sqrt ((N - M) / N)
  ⟨proof⟩

lemma sin-theta-div-2:
  sin (θ / 2) = sqrt (M / N)
  ⟨proof⟩

lemma θ-neq-0:
  θ ≠ 0
  ⟨proof⟩

abbreviation ccos where ccos φ ≡ complex-of-real (cos φ)
abbreviation csin where csin φ ≡ complex-of-real (sin φ)

lemma ψ-eq:
  ψ = ccos (θ / 2) ·v α + csin (θ / 2) ·v β
  ⟨proof⟩

lemma psi-inner-alpha:
  inner-prod ψ α = ccos (θ / 2)
  ⟨proof⟩

lemma psi-inner-beta:
  inner-prod ψ β = csin (θ / 2)
  ⟨proof⟩

definition alpha-l :: nat ⇒ complex where
  alpha-l l = ccos ((l + 1 / 2) * θ)

lemma alpha-l-real:
  alpha-l l ∈ Reals
  ⟨proof⟩

```

```

lemma conj-alpha-l:
  conjugate (alpha-l l) = alpha-l l
  ⟨proof⟩

definition beta-l :: nat ⇒ complex where
  beta-l l = csin ((l + 1 / 2) * θ)

lemma beta-l-real:
  beta-l l ∈ Reals
  ⟨proof⟩

lemma conj-beta-l:
  conjugate (beta-l l) = beta-l l
  ⟨proof⟩

lemma csin-ccos-squared-add:
  ccos (a::real) * ccos a + csin a * csin a = 1
  ⟨proof⟩

lemma alpha-l-beta-l-add-norm:
  alpha-l l * alpha-l l + beta-l l * beta-l l = 1
  ⟨proof⟩

definition psi-l where
  psi-l l = (alpha-l l) ·v α + (beta-l l) ·v β

lemma psi-l-dim:
  psi-l l ∈ carrier-vec N
  ⟨proof⟩

lemma inner-psi-l:
  inner-prod (psi-l l) (psi-l l) = 1
  ⟨proof⟩

abbreviation proj :: complex vec ⇒ complex mat where
  proj v ≡ outer-prod v v

definition psi'-l where
  psi'-l l = (alpha-l l) ·v α - (beta-l l) ·v β

lemma psi'-l-dim:
  psi'-l l ∈ carrier-vec N
  ⟨proof⟩

definition proj-psi'-l where
  proj-psi'-l l = proj (psi'-l l)

lemma proj-psi'-dim:
  proj-psi'-l l ∈ carrier-mat N N

```

$\langle proof \rangle$

lemma *psi-inner-psi'-l*:

$$inner\text{-}prod \psi (\psi' \cdot l) = (alpha \cdot l * ccos (\vartheta / 2) - beta \cdot l * csin (\vartheta / 2))$$
 $\langle proof \rangle$

lemma *double-ccos-square*:

$$2 * ccos (a::real) * ccos a = ccos (2 * a) + 1$$
 $\langle proof \rangle$

lemma *double-csin-square*:

$$2 * csin (a::real) * csin a = 1 - ccos (2 * a)$$
 $\langle proof \rangle$

lemma *csin-double*:

$$2 * csin (a::real) * ccos a = csin(2 * a)$$
 $\langle proof \rangle$

lemma *ccos-add*:

$$ccos (x + y) = ccos x * ccos y - csin x * csin y$$
 $\langle proof \rangle$

lemma *alpha-l-Suc-l-derive*:

$$\begin{aligned} & 2 * (alpha \cdot l * ccos (\vartheta / 2) - beta \cdot l * csin (\vartheta / 2)) * ccos (\vartheta / 2) - alpha \cdot l \\ &= alpha \cdot l (l + 1) \\ & \quad (\text{is } ?lhs = ?rhs) \end{aligned}$$
 $\langle proof \rangle$

lemma *csin-add*:

$$csin (x + y) = ccos x * csin y + csin x * ccos y$$
 $\langle proof \rangle$

lemma *beta-l-Suc-l-derive*:

$$\begin{aligned} & 2 * (alpha \cdot l * ccos (\vartheta / 2) - beta \cdot l * csin (\vartheta / 2)) * csin (\vartheta / 2) + beta \cdot l \\ &= beta \cdot l (l + 1) \\ & \quad (\text{is } ?lhs = ?rhs) \end{aligned}$$
 $\langle proof \rangle$

lemma *psi-l-Suc-l-derive*:

$$\begin{aligned} & 2 * (alpha \cdot l * ccos (\vartheta / 2) - beta \cdot l * csin (\vartheta / 2)) \cdot_v \psi - psi' \cdot l = psi \cdot l (l \\ &+ 1) \\ & \quad (\text{is } ?lhs = ?rhs) \end{aligned}$$
 $\langle proof \rangle$

7.2 Grover operator

Oracle O

definition *proj-O* :: complex mat **where**

$$proj\text{-}O = mat N N (\lambda(i, j). if i = j then (if f i then 1 else 0) else 0)$$

```

lemma proj-O-dim:
  proj-O ∈ carrier-mat N N
  ⟨proof⟩

lemma proj-O-mult-alpha:
  proj-O *v α = zero-vec N
  ⟨proof⟩

lemma proj-O-mult-beta:
  proj-O *v β = β
  ⟨proof⟩

definition mat-O :: complex mat where
  mat-O = mat N N (λ(i,j). if i = j then (if i then -1 else 1) else 0)

lemma mat-O-dim:
  mat-O ∈ carrier-mat N N
  ⟨proof⟩

lemma mat-O-mult-alpha:
  mat-O *v α = α
  ⟨proof⟩

lemma mat-O-mult-beta:
  mat-O *v β = - β
  ⟨proof⟩

lemma hermitian-mat-O:
  hermitian mat-O
  ⟨proof⟩

lemma unitary-mat-O:
  unitary mat-O
  ⟨proof⟩

definition mat-Ph :: complex mat where
  mat-Ph = mat N N (λ(i,j). if i = j then if i = 0 then 1 else -1 else 0)

lemma hermitian-mat-Ph:
  hermitian mat-Ph
  ⟨proof⟩

lemma unitary-mat-Ph:
  unitary mat-Ph
  ⟨proof⟩

definition mat-G' :: complex mat where
  mat-G' = mat N N (λ(i,j). if i = j then 2 / N - 1 else 2 / N)

```

Geometrically, the Grover operator G is a rotation

```
definition mat-G :: complex mat where
  mat-G = mat-G' * mat-O
end
```

7.3 State of Grover's algorithm

The dimensions are [2, 2, ..., 2, n]. We work with a very special case as in the paper

```
locale grover-state-sig = grover-state + state-sig +
  fixes R :: nat
  fixes K :: nat
  assumes dims-def: dims = replicate n 2 @ [K]
  assumes R: R = pi / (2 * θ) - 1 / 2
  assumes K: K > R

begin

lemma K-gt-0:
  K > 0
  ⟨proof⟩

  Bits q0 to q_(n-1)

definition vars1 :: nat set where
  vars1 = {0 ..< n}

  Bit r

definition vars2 :: nat set where
  vars2 = {n}

lemma length-dims:
  length dims = n + 1
  ⟨proof⟩

lemma dims-nth-lt-n:
  l < n ==> nth dims l = 2
  ⟨proof⟩

lemma nths-Suc-n-dims:
  nths dims {0 ..<(Suc n)} = dims
  ⟨proof⟩

interpretation ps2-P: partial-state2 dims vars1 vars2
  ⟨proof⟩

interpretation ps-P: partial-state ps2-P.dims0 ps2-P.vars1'⟨proof⟩
```

```

abbreviation tensor-P where
  tensor-P A B  $\equiv$  ps2-P.ptensor-mat A B

lemma tensor-P-dim:
  tensor-P A B  $\in$  carrier-mat d d
   $\langle proof \rangle$ 

lemma dims-nths-le-n:
  assumes l  $\leq n$ 
  shows nths dims {0..<l} = replicate l 2
   $\langle proof \rangle$ 

lemma dims-nths-one-lt-n:
  assumes l < n
  shows nths dims {l} = [2]
   $\langle proof \rangle$ 

lemma dims-vars1:
  nths dims vars1 = replicate n 2
   $\langle proof \rangle$ 

lemma nths-rep-2-n:
  nths (replicate n 2) {n} = []
   $\langle proof \rangle$ 

lemma dims-vars2:
  nths dims vars2 = [K]
   $\langle proof \rangle$ 

lemma d-vars1:
  prod-list (nths dims vars1) = N
   $\langle proof \rangle$ 

lemma ps2-P-dims0:
  ps2-P.dims0 = dims
   $\langle proof \rangle$ 

lemma ps2-P-vars1':
  ps2-P.vars1' = vars1
   $\langle proof \rangle$ 

lemma ps2-P-d0:
  ps2-P.d0 = d
   $\langle proof \rangle$ 

lemma ps2-P-d1:
  ps2-P.d1 = N
   $\langle proof \rangle$ 

```

```

lemma ps2-P-d2:
  ps2-P.d2 = K
  ⟨proof⟩

lemma ps-P-d:
  ps-P.d = d
  ⟨proof⟩

lemma ps-P-d1:
  ps-P.d1 = N
  ⟨proof⟩

lemma ps-P-d2:
  ps-P.d2 = K
  ⟨proof⟩

lemma nths-uminus-vars1:
  nths dims (− vars1) = nths dims vars2
  ⟨proof⟩

lemma tensor-P-mult:
  assumes m1 ∈ carrier-mat (2^n) (2^n)
  and m2 ∈ carrier-mat (2^n) (2^n)
  and m3 ∈ carrier-mat K K
  and m4 ∈ carrier-mat K K
  shows (tensor-P m1 m3) * (tensor-P m2 m4) = tensor-P (m1 * m2) (m3 *
  m4)
  ⟨proof⟩

lemma mat-ext-vars1:
  shows mat-extension dims vars1 A = tensor-P A (1_m K)
  ⟨proof⟩

lemma Utrans-P-is-tensor-P1:
  Utrans-P vars1 A = Utrans (tensor-P A (1_m K))
  ⟨proof⟩

lemma nths-dims-uminus-vars2:
  nths dims (−vars2) = nths dims vars1
  ⟨proof⟩

lemma mat-ext-vars2:
  assumes A ∈ carrier-mat K K
  shows mat-extension dims vars2 A = tensor-P (1_m N) A
  ⟨proof⟩

lemma Utrans-P-is-tensor-P2:
  assumes A ∈ carrier-mat K K
  shows Utrans-P vars2 A = Utrans (tensor-P (1_m N) A)
  ⟨proof⟩

```

$\langle proof \rangle$

7.4 Grover's algorithm

Apply hadamard operator to first n variables

```

definition hadamard-on-i :: nat  $\Rightarrow$  complex mat where
  hadamard-on-i i = pmat-extension dims {i} (vars1 - {i}) hadamard
declare hadamard-on-i-def [simp]

fun hadamard-n :: nat  $\Rightarrow$  com where
  hadamard-n 0 = SKIP
  | hadamard-n (Suc i) = hadamard-n i ;; Utrans (tensor-P (hadamard-on-i i) (1_m K))

  Body of the loop

definition D :: com where
  D = Utrans-P vars1 mat-O ;;
    hadamard-n n ;;
    Utrans-P vars1 mat-Ph ;;
    hadamard-n n ;;
    Utrans-P vars2 (mat-incr K)

lemma unitary-ex-mat-O:
  unitary (tensor-P mat-O (1_m K))
  ⟨proof⟩

lemma unitary-ex-mat-Ph:
  unitary (tensor-P mat-Ph (1_m K))
  ⟨proof⟩

lemma unitary-hadamard-on-i:
  assumes k < n
  shows unitary (hadamard-on-i k)
  ⟨proof⟩

lemma unitary-exhadamard-on-i:
  assumes k < n
  shows unitary (tensor-P (hadamard-on-i k) (1_m K))
  ⟨proof⟩

lemma hadamard-on-i-dim:
  assumes k < n
  shows hadamard-on-i k  $\in$  carrier-mat N N
  ⟨proof⟩

lemma well-com-hadamard-k:
  k  $\leq$  n  $\implies$  well-com (hadamard-n k)
  ⟨proof⟩

```

```

lemma well-com-hadamard-n:
  well-com (hadamard-n n)
  ⟨proof⟩

lemma well-com-mat-O:
  well-com (Utrans-P vars1 mat-O)
  ⟨proof⟩

lemma well-com-mat-Ph:
  well-com (Utrans-P vars1 mat-Ph)
  ⟨proof⟩

lemma unitary-exmat-incr:
  unitary (tensor-P (1_m N) (mat-incr K))
  ⟨proof⟩

lemma well-com-mat-incr:
  well-com (Utrans-P vars2 (mat-incr K))
  ⟨proof⟩

lemma well-com-D: well-com D
  ⟨proof⟩

  Test at while loop

definition M0 :: complex mat where
  M0 = mat K K (λ(i,j). if i = j ∧ i ≥ R then 1 else 0)

lemma hermitian-M0:
  hermitian M0
  ⟨proof⟩

lemma M0-dim:
  M0 ∈ carrier-mat K K
  ⟨proof⟩

lemma M0-mult-M0:
  M0 * M0 = M0
  ⟨proof⟩

definition M1 :: complex mat where
  M1 = mat K K (λ(i,j). if i = j ∧ i < R then 1 else 0)

lemma M1-dim:
  M1 ∈ carrier-mat K K
  ⟨proof⟩

lemma hermitian-M1:
  hermitian M1
  ⟨proof⟩

```

lemma *M1-mult-M1*:

*M1 * M1 = M1*

{proof}

lemma *M1-add-M0*:

M1 + M0 = 1_m K

{proof}

Test at the end

definition *testN :: nat ⇒ complex mat* **where**

testN k = mat N N (λ(i,j). if i = k ∧ j = k then 1 else 0)

lemma *hermitian-testN*:

hermitian (testN k)

{proof}

lemma *testN-mult-testN*:

*testN k * testN k = testN k*

{proof}

lemma *testN-dim*:

testN k ∈ carrier-mat N N

{proof}

definition *test-fst-k :: nat ⇒ complex mat* **where**

test-fst-k k = mat N N (λ(i, j). if (i = j ∧ i < k) then 1 else 0)

lemma *sum-test-k*:

assumes *m ≤ N*

shows *matrix-sum N (λk. testN k) m = test-fst-k m*

{proof}

lemma *test-fst-kN*:

test-fst-k N = 1_m N

{proof}

lemma *matrix-sum-tensor-P1*:

(λk. k < m ⇒ g k ∈ carrier-mat N N) ⇒ (A ∈ carrier-mat K K) ⇒

matrix-sum d (λk. tensor-P (g k) A) m = tensor-P (matrix-sum N g m) A

{proof}

Grover's algorithm. Assume we start in the zero state

definition *Grover :: com* **where**

Grover = hadamard-n n ;;

While-P vars2 M0 M1 D ;;

Measure-P vars1 N testN (replicate N SKIP)

lemma *well-com-if*:

well-com (*Measure-P vars1 N testN (replicate N SKIP)*)
(proof)

lemma *well-com-while*:
well-com (*While-P vars2 M0 M1 D*)
(proof)

lemma *well-com-Grover*:
well-com Grover
(proof)

7.5 Correctness

Pre-condition: assume in the zero state

definition *ket-pre* :: *complex vec* **where**
ket-pre = Matrix.vec N (λk. if k = 0 then 1 else 0)

lemma *ket-pre-dim*:
ket-pre ∈ carrier-vec N *(proof)*

definition *pre* :: *complex mat* **where**
pre = proj ket-pre

lemma *pre-dim*:
pre ∈ carrier-mat N N
(proof)

lemma *norm-pre*:
inner-prod ket-pre ket-pre = 1
(proof)

lemma *pre-trace*:
trace pre = 1
(proof)

lemma *positive-pre*:
positive pre
(proof)

lemma *pre-le-one*:
pre ≤L 1m N
(proof)

Post-condition: should be in a state i with f i = 1

definition *post* :: *complex mat* **where**
post = mat N N (λ(i, j). if (i = j ∧ f i) then 1 else 0)

lemma *post-dim*:
post ∈ carrier-mat N N

$\langle proof \rangle$

lemma hermitian-post:
hermitian post
 $\langle proof \rangle$

Hoare triples of initialization

definition ket-zero :: complex vec **where**
ket-zero = Matrix.vec 2 ($\lambda k. \text{if } k = 0 \text{ then } 1 \text{ else } 0$)

lemma ket-zero-dim:
ket-zero \in carrier-vec 2 $\langle proof \rangle$

definition proj-zero **where**
proj-zero = proj ket-zero

definition ket-one **where**
ket-one = Matrix.vec 2 ($\lambda k. \text{if } k = 1 \text{ then } 1 \text{ else } 0$)

definition proj-one **where**
proj-one = proj ket-one

definition ket-plus **where**
ket-plus = Matrix.vec 2 ($\lambda k. 1 / \text{csqrt } 2$)

lemma ket-plus-dim:
ket-plus \in carrier-vec 2 $\langle proof \rangle$

lemma ket-plus-eval [simp]:
 $i < 2 \implies \text{ket-plus } \$ i = 1 / \text{csqrt } 2$
 $\langle proof \rangle$

lemma csqrt-2-sq [simp]:
complex-of-real ($\sqrt{2}$) * complex-of-real ($\sqrt{2}$) = 2
 $\langle proof \rangle$

lemma ket-plus-tensor-n:
partial-state.tensor-vec [2, 2] {0} ket-plus ket-plus = Matrix.vec 4 ($\lambda k. 1 / 2$)
 $\langle proof \rangle$

definition proj-plus **where**
proj-plus = proj ket-plus

lemma hadamard-on-zero:
hadamard *_v ket-zero = ket-plus
 $\langle proof \rangle$

fun exH-k :: nat \Rightarrow complex mat **where**
exH-k 0 = hadamard-on-i 0

```

| exH-k (Suc k) = exH-k k * hadamard-on-i (Suc k)

fun H-k :: nat  $\Rightarrow$  complex mat where
  H-k 0 = hadamard
| H-k (Suc k) = ptensor-mat dims {0..<(Suc k)} {(Suc k)} (H-k k) hadamard

lemma H-k-dim:
   $k < n \implies H-k k \in \text{carrier-mat} (2^{\wedge}(\text{Suc } k)) (2^{\wedge}(\text{Suc } k))$ 
  ⟨proof⟩

lemma exH-k-eq-H-k:
   $k < n \implies \text{exH-k } k = \text{pmat-extension dims } \{0..<(\text{Suc } k)\} \{(Suc k)..<n\} (\text{H-k } k)$ 
  ⟨proof⟩

lemma mult-exH-k-left:
  assumes Suc k < n
  shows hadamard-on-i (Suc k) * exH-k k = exH-k (Suc k)
  ⟨proof⟩

lemma exH-eq-H:
  exH-k (n - 1) = H-k (n - 1)
  ⟨proof⟩

fun ket-zero-k :: nat  $\Rightarrow$  complex vec where
  ket-zero-k 0 = ket-zero
| ket-zero-k (Suc k) = ptensor-vec dims {0..<(Suc k)} {(Suc k)} (ket-zero-k k)
ket-zero

lemma ket-zero-k-dim:
  assumes k < n
  shows ket-zero-k k  $\in$  carrier-vec (2^{\wedge}(Suc k))
  ⟨proof⟩

fun ket-plus-k where
  ket-plus-k 0 = ket-plus
| ket-plus-k (Suc k) = ptensor-vec dims {0..<(Suc k)} {(Suc k)} (ket-plus-k k)
ket-plus

lemma ket-plus-k-dim:
  assumes k < n
  shows ket-plus-k k  $\in$  carrier-vec (2^{\wedge}(Suc k))
  ⟨proof⟩

lemma H-k-ket-zero-k:
   $k < n \implies (H-k k) *_v (\text{ket-zero-k } k) = (\text{ket-plus-k } k)$ 
  ⟨proof⟩

```

```

lemma encode1-replicate-2:
  partial-state.encode1 (replicate (Suc k) 2) {0..} i = i mod (2 ^ k)
  ⟨proof⟩

lemma encode2-replicate-2:
  assumes i < 2 ^ Suc k
  shows partial-state.encode2 (replicate (Suc k) 2) {0..} i = i div (2 ^ k)
  ⟨proof⟩

lemma ket-zero-k-decode:
  k < n ==> ket-zero-k k = Matrix.vec (2^(Suc k)) (λk. if k = 0 then 1 else 0)
  ⟨proof⟩

lemma ket-plus-k-decode:
  k < n ==> ket-plus-k k = Matrix.vec (2^(Suc k)) (λl. 1 / csqrt (2^(Suc k)))
  ⟨proof⟩

lemma exH-k-mult-pre-is-psi:
  exH-k (n - 1) *v ket-pre = ψ
  ⟨proof⟩

definition ket-k :: nat ⇒ complex vec where
  ket-k x = Matrix.vec K (λk. if k = x then 1 else 0)

lemma ket-k-dim:
  ket-k k ∈ carrier-vec K
  ⟨proof⟩

lemma mat-incr-mult-ket-k:
  k < K ==> (mat-incr K) *v (ket-k k) = (ket-k ((k + 1) mod K))
  ⟨proof⟩

definition proj-k where
  proj-k x = proj (ket-k x)

lemma proj-k-dim:
  proj-k k ∈ carrier-mat K K
  ⟨proof⟩

lemma norm-ket-k-lt-K:
  k < K ==> inner-prod (ket-k k) (ket-k k) = 1
  ⟨proof⟩

lemma norm-ket-k-ge-K:
  k ≥ K ==> inner-prod (ket-k k) (ket-k k) = 0
  ⟨proof⟩

lemma norm-ket-k:
  inner-prod (ket-k k) (ket-k k) ≤ 1

```

```

⟨proof⟩

lemma proj-k-mat:
  assumes k < K
  shows proj-k k = mat K K (λ(i, j). if (i = j ∧ i = k) then 1 else 0)
  ⟨proof⟩

lemma positive-proj-k:
  positive (proj-k k)
  ⟨proof⟩

lemma proj-k-le-one:
  (proj-k k) ≤L 1m K
  ⟨proof⟩

definition proj-psi where
  proj-psi = proj ψ

lemma proj-psi-dim:
  proj-psi ∈ carrier-mat N N
  ⟨proof⟩

lemma norm-psi:
  inner-prod ψ ψ = 1
  ⟨proof⟩

lemma proj-psi-mat:
  proj-psi = mat N N (λk. 1 / N)
  ⟨proof⟩

lemma hermitian-proj-psi:
  hermitian proj-psi
  ⟨proof⟩

lemma hermitian-exproj-psi:
  hermitian (tensor-P proj-psi (1m K))
  ⟨proof⟩

lemma proj-psi-is-projection:
  proj-psi * proj-psi = proj-psi
  ⟨proof⟩

lemma proj-psi-trace:
  trace (proj-psi) = 1
  ⟨proof⟩

lemma positive-proj-psi:
  positive (proj-psi)
  ⟨proof⟩

```

```

lemma proj-psi-le-one:
  (proj-psi) ≤L 1m N
  ⟨proof⟩

lemma hermitian-hadamard-on-k:
  assumes k < n
  shows hermitian (hadamard-on-i k)
  ⟨proof⟩

lemma hermitian-H-k:
  k < n ⇒ hermitian (H-k k)
  ⟨proof⟩

lemma unitary-H-k:
  k < n ⇒ unitary (H-k k)
  ⟨proof⟩

lemma exH-k-dim:
  shows k < n ⇒ exH-k k ∈ carrier-mat N N
  ⟨proof⟩

lemma exH-n-dim:
  shows exH-k (n - 1) ∈ carrier-mat N N
  ⟨proof⟩

lemma unitary-exH-k:
  shows k < n ⇒ unitary (exH-k k)
  ⟨proof⟩

lemma hermitian-exH-n:
  hermitian (exH-k (n - 1))
  ⟨proof⟩

lemma exH-k-mult-psi-is-pre:
  exH-k (n - 1) *v ψ = ket-pre
  ⟨proof⟩

fun exexH-k :: nat ⇒ complex mat where
  exexH-k k = tensor-P (exH-k k) (1m K)

lemma unitary-exexH-k:
  k < n ⇒ unitary (exexH-k k)
  ⟨proof⟩

lemma exexH-k-dim:
  k < n ⇒ exexH-k k ∈ carrier-mat d d
  ⟨proof⟩

```

```

lemma hoare-seq-utrans:
  fixes  $P :: \text{complex mat}$ 
  assumes unitary  $U1$  and unitary  $U2$  and is-quantum-predicate  $P$ 
    and  $dU1: U1 \in \text{carrier-mat } d$   $d$  and  $dU2: U2 \in \text{carrier-mat } d$   $d$ 
  shows
     $\vdash_p \{ \text{adjoint} (U2 * U1) * P * (U2 * U1) \}$ 
     $\text{Utrans } U1;; \text{Utrans } U2$ 
     $\{P\}$ 
   $\langle \text{proof} \rangle$ 

lemma qp-close-after-exexH-k:
  fixes  $P :: \text{complex mat}$ 
  assumes is-quantum-predicate  $P$ 
  shows  $k < n \implies \text{is-quantum-predicate} (\text{adjoint} (\text{exexH-}k \ k) * P * \text{exexH-}k \ k)$ 
   $\langle \text{proof} \rangle$ 

lemma hoare-hadamard-n:
  fixes  $P :: \text{complex mat}$ 
  shows is-quantum-predicate  $P \implies k < n \implies$ 
     $\vdash_p \{ \text{adjoint} (\text{exexH-}k \ k) * P * \text{exexH-}k \ k \}$ 
     $\text{hadamard-}n \ (\text{Suc } k)$ 
     $\{P\}$ 
   $\langle \text{proof} \rangle$ 

lemma qp-pre:
  is-quantum-predicate ( $\text{tensor-}P \text{ pre } (\text{proj-}k \ 0)$ )
   $\langle \text{proof} \rangle$ 

lemma qp-init-post:
  is-quantum-predicate ( $\text{tensor-}P \text{ proj-}\psi \ (\text{proj-}k \ 0)$ )
   $\langle \text{proof} \rangle$ 

lemma tensor-P-adjoint-left-right:
  assumes  $m1 \in \text{carrier-mat } N \ N$  and  $m2 \in \text{carrier-mat } K \ K$  and  $m3 \in \text{carrier-mat } N \ N$  and  $m4 \in \text{carrier-mat } K \ K$ 
  shows  $\text{adjoint} (\text{tensor-}P \ m1 \ m2) * \text{tensor-}P \ m3 \ m4 * \text{tensor-}P \ m1 \ m2 = \text{tensor-}P \ (\text{adjoint } m1 * m3 * m1) \ (\text{adjoint } m2 * m4 * m2)$ 
   $\langle \text{proof} \rangle$ 

abbreviation exH-n where
   $\text{exH-}n \equiv \text{exH-}k \ (n - 1)$ 

lemma hoare-triple-init:
   $\vdash_p \{ \text{tensor-}P \text{ pre } (\text{proj-}k \ 0) \}$ 
   $\text{hadamard-}n \ n$ 
   $\{ \text{tensor-}P \text{ proj-}\psi \ (\text{proj-}k \ 0) \}$ 

```

$\langle proof \rangle$

Hoare triples of while loop

definition proj-psi-l **where**
proj-psi-l l = proj (psi-l l)

lemma positive-psi-l:
 $k < K \implies$ positive (proj-psi-l k)
 $\langle proof \rangle$

lemma hermitian-proj-psi-l:
 $k < K \implies$ hermitian (proj-psi-l k)
 $\langle proof \rangle$

definition P' **where**
 $P' = \text{tensor-}P (\text{proj-psi-l } R) (\text{proj-}k R)$

lemma proj-psi-l-dim:
proj-psi-l l \in carrier-mat N N
 $\langle proof \rangle$

definition Q :: complex mat **where**
 $Q = \text{matrix-sum } d (\lambda l. \text{tensor-}P (\text{proj-psi-l } l) (\text{proj-}k l)) R$

lemma psi-l-le-id:
shows proj-psi-l l $\leq_L 1_m$ N
 $\langle proof \rangle$

lemma positive-proj-psi-l:
shows positive (proj-psi-l l)
 $\langle proof \rangle$

definition proj-fst-k :: nat \Rightarrow complex mat **where**
proj-fst-k k = mat K K ($\lambda(i, j). \text{if } (i = j \wedge i < k) \text{ then } 1 \text{ else } 0$)

lemma hermitian-proj-fst-k:
adjoint (proj-fst-k k) = proj-fst-k k
 $\langle proof \rangle$

lemma proj-fst-k-is-projection:
proj-fst-k k * proj-fst-k k = proj-fst-k k
 $\langle proof \rangle$

lemma positive-proj-fst-k:
positive (proj-fst-k k)
 $\langle proof \rangle$

lemma proj-fst-k-le-one:
proj-fst-k k $\leq_L 1_m$ K

$\langle proof \rangle$

lemma *sum-proj-k*:
 assumes $m \leq K$
 shows *matrix-sum* $K (\lambda k. proj\text{-}k k) m = proj\text{-}fst\text{-}k m$
 $\langle proof \rangle$

lemma *proj-psi-proj-k-le-expo-j-k*:
 shows *tensor-P* $(proj\text{-}psi\text{-}l k) (proj\text{-}k l) \leq_L tensor\text{-}P (1_m N) (proj\text{-}k l)$
 $\langle proof \rangle$

definition $Q1 :: complex\ mat$ **where**
$$Q1 = matrix\text{-}sum d (\lambda l. tensor\text{-}P (proj\text{-}psi'\text{-}l l) (proj\text{-}k l)) R$$

lemma *tensor-P-left-right-partial1*:
 assumes $m1 \in carrier\text{-}mat N N$ **and** $m2 \in carrier\text{-}mat N N$ **and** $m3 \in carrier\text{-}mat K K$ **and** $m4 \in carrier\text{-}mat N N$
 shows *tensor-P* $m1 (1_m K) * tensor\text{-}P m2 m3 * tensor\text{-}P m4 (1_m K) = tensor\text{-}P (m1 * m2 * m4) m3$
 $\langle proof \rangle$

lemma *tensor-P-left-right-partial2*:
 assumes $m1 \in carrier\text{-}mat K K$ **and** $m2 \in carrier\text{-}mat K K$ **and** $m3 \in carrier\text{-}mat N N$ **and** $m4 \in carrier\text{-}mat K K$
 shows *tensor-P* $(1_m N) m1 * tensor\text{-}P m3 m2 * tensor\text{-}P (1_m N) m4 = tensor\text{-}P m3 (m1 * m2 * m4)$
 $\langle proof \rangle$

lemma *matrix-sum-mult-left-right*:
 fixes $A B :: complex\ mat$
 assumes $dg: (\bigwedge k. k < l \implies g k \in carrier\text{-}mat m m)$
 and $dA: A \in carrier\text{-}mat m m$ **and** $dB: B \in carrier\text{-}mat m m$
 shows *matrix-sum* $m (\lambda k. A * g k * B) l = A * matrix\text{-}sum m g l * B$
 $\langle proof \rangle$

lemma *mat-O-split*:
$$mat\text{-}O = 1_m N - 2 \cdot_m proj\text{-}O$$

 $\langle proof \rangle$

lemma *mat-O-mult-psi'-l*:
$$mat\text{-}O *_v (psi'\text{-}l l) = psi\text{-}l l$$

 $\langle proof \rangle$

lemma *mat-O-times-Q1*:
 adjoint $(tensor\text{-}P mat\text{-}O (1_m K)) * Q1 * (tensor\text{-}P mat\text{-}O (1_m K)) = Q$
 $\langle proof \rangle$

definition $Q2$ **where**
$$Q2 = matrix\text{-}sum d (\lambda l. tensor\text{-}P (proj\text{-}psi\text{-}l (l + 1)) (proj\text{-}k l)) R$$

lemma *Q2-dim*:

$Q2 \in \text{carrier-mat } d \ d$
 $\langle \text{proof} \rangle$

lemma *Q2-le-one*:

$Q2 \leq_L 1_m \ d$
 $\langle \text{proof} \rangle$

lemma *qp-Q2*:

is-quantum-predicate Q2
 $\langle \text{proof} \rangle$

lemma *pre-mat*:

$\text{pre} = \text{mat } N \ N \ (\lambda(i, j). \text{ if } i = j \wedge i = 0 \text{ then } 1 \text{ else } 0)$
 $\langle \text{proof} \rangle$

lemma *mat-Ph-split*:

$\text{mat-Ph} = 2 \cdot_m \text{pre} - 1_m \ N$
 $\langle \text{proof} \rangle$

lemma *H-Ph-H*:

$\text{exexH-k } (n-1) * \text{tensor-P mat-Ph } (1_m \ K) * \text{exexH-k } (n - 1) = 2 \cdot_m \text{tensor-P proj-psi } (1_m \ K) - 1_m \ d$
 $\langle \text{proof} \rangle$

lemma *hermitian-proj-psi-minus-1*:

$\text{hermitian } (2 \cdot_m \text{proj-psi} - 1_m \ N)$
 $\langle \text{proof} \rangle$

lemma *unitary-proj-psi-minus-1*:

$\text{unitary } (2 \cdot_m \text{proj-psi} - 1_m \ N)$
 $\langle \text{proof} \rangle$

lemma *proj-psi-minus-1-mult-psi'-l*:

$(2 \cdot_m \text{proj-psi} - 1_m \ N) *_v \text{psi}'-l \ l = \text{psi}-l \ (l + 1)$
 $\langle \text{proof} \rangle$

lemma *proj-psi-minus-1-mult-psi-Suc-l*:

$(2 \cdot_m \text{proj-psi} - 1_m \ N) *_v \text{psi}-l \ (l + 1) = \text{psi}'-l \ l$
 $\langle \text{proof} \rangle$

lemma *exproj-psi-minus-1-tensor*:

$(2 \cdot_m \text{tensor-P proj-psi } (1_m \ K)) - 1_m \ d = \text{tensor-P } (2 \cdot_m \text{proj-psi} - (1_m \ N))$
 $(1_m \ K)$
 $\langle \text{proof} \rangle$

lemma *unitary-exproj-psi-minus-1*:

$\text{unitary } (2 \cdot_m \text{tensor-P proj-psi } (1_m \ K) - 1_m \ d)$

$\langle proof \rangle$

lemma *proj-psi-minus-1-Q2*:
adjoint $(2 \cdot_m \text{tensor-}P \text{ proj-}psi (1_m K) - 1_m d) * Q2 * (2 \cdot_m \text{tensor-}P \text{ proj-}psi (1_m K) - 1_m d) = Q1$
 $\langle proof \rangle$

lemma *qp-Q1*:
is-quantum-predicate *Q1*
 $\langle proof \rangle$

lemma *qp-Q*:
is-quantum-predicate *Q*
 $\langle proof \rangle$

lemma *hoare-triple-D1*:

$\vdash_p \{Q\}$
*Utrans-*P* vars1 mat-*O**
 $\{Q1\}$
 $\langle proof \rangle$

lemma *hoare-triple-D2*:

$\vdash_p \{Q1\}$
*hadamard-*n* n ;;*
*Utrans-*P* vars1 mat-*Ph* ;;*
*hadamard-*n* n*
 $\{Q2\}$
 $\langle proof \rangle$

definition *exM0* **where**
 $exM0 = \text{tensor-}P (1_m N) M0$

lemma *M0-mult-ket-k-R*:
 $M0 *_v \text{ket-}k R = \text{ket-}k R$
 $\langle proof \rangle$

lemma *exP0-P'*:
adjoint $exM0 * P' * exM0 = P'$
 $\langle proof \rangle$

definition *exM1* **where**
 $exM1 = \text{tensor-}P (1_m N) M1$

lemma *M1-mult-ket-k*:
assumes $k < R$
shows $M1 *_v \text{ket-}k k = \text{ket-}k k$
 $\langle proof \rangle$

lemma $\text{exP1-}Q$:
 $\text{adjoint exM1 * Q * exM1} = Q$
 $\langle \text{proof} \rangle$

lemma $\text{qp-}P'$:
 $\text{is-quantum-predicate } P'$
 $\langle \text{proof} \rangle$

lemma P' -add- Q :
 $P' + Q = \text{matrix-sum } d (\lambda l. \text{tensor-}P (\text{proj-psi-}l) (\text{proj-}k l)) (R + 1)$
 $\langle \text{proof} \rangle$

lemma positive- Qk :
 $\text{positive} (\text{tensor-}P (\text{proj-psi-}l) (\text{proj-}k l))$
 $\langle \text{proof} \rangle$

lemma P' - Q -dim:
 $P' + Q \in \text{carrier-mat } d$
 $\langle \text{proof} \rangle$

lemma P' -add- Q -le-one:
 $P' + Q \leq_L 1_m$
 d
 $\langle \text{proof} \rangle$

lemma $\text{qp-}P'$ - Q :
 $\text{is-quantum-predicate } (P' + Q)$
 $\langle \text{proof} \rangle$

lemma $Q2$ -leq-lemma:
 $\text{tensor-}P (1_m N) (\text{mat-incr } K) * Q2 * \text{adjoint} (\text{tensor-}P (1_m N) (\text{mat-incr } K))$
 $\leq_L P' + Q$
 $\langle \text{proof} \rangle$

lemma $Q2$ -leq:
 $Q2 \leq_L \text{adjoint} (\text{tensor-}P (1_m N) (\text{mat-incr } K)) * (P' + Q) * \text{tensor-}P (1_m N)$
 $(\text{mat-incr } K)$
 $\langle \text{proof} \rangle$

lemma hoare-triple-D3:
 $\vdash_p \{Q2\}$
 $\text{Utrans-}P \text{ vars2 } (\text{mat-incr } K)$
 $\{\text{adjoint exM0 * P' * exM0} + \text{adjoint exM1 * Q * exM1}\}$
 $\langle \text{proof} \rangle$

lemma qp-D3-post:
 $\text{is-quantum-predicate } (\text{adjoint exM0 * P' * exM0} + \text{adjoint exM1 * Q * exM1})$
 $\langle \text{proof} \rangle$

lemma hoare-triple-D:

$$\vdash_p \{Q\} D \{ \text{adjoint } exM0 * P' * exM0 + \text{adjoint } exM1 * Q * exM1 \}$$

$\langle proof \rangle$

lemma psi-is-psi-l0:

$$\psi = \text{psi-l } 0$$

$\langle proof \rangle$

lemma proj-psi-is-proj-psi-l0:

$$\text{proj-psi} = \text{proj-psi-l } 0$$

$\langle proof \rangle$

lemma lowner-le-Q:

$$\text{tensor-}P \text{ proj-psi } (\text{proj-k } 0) \leq_L \text{adjoint } exM0 * P' * exM0 + \text{adjoint } exM1 * Q * exM1$$

$\langle proof \rangle$

lemma hoare-triple-while:

$$\vdash_p \{ \text{adjoint } exM0 * P' * exM0 + \text{adjoint } exM1 * Q * exM1 \} \text{ While-}P \text{ vars2 } M0 M1 D \{ P' \}$$

$\langle proof \rangle$

lemma R-and-a-half-theta:

$$(R + 1/2) * \vartheta = pi / 2$$

$\langle proof \rangle$

lemma psi-lR-is-beta:

$$\text{psi-l } R = \beta$$

$\langle proof \rangle$

lemma post-mult-beta:

$$\text{post} *_v \beta = \beta$$

$\langle proof \rangle$

lemma post-mult-post:

$$\text{post} * \text{post} = \text{post}$$

$\langle proof \rangle$

lemma post-mult-proj-psi-lR:

$$\text{post} * \text{proj-psi-l } R = \text{proj-psi-l } R$$

$\langle proof \rangle$

lemma proj-psi-lR-mult-post:

```

proj-psi-l R * post = proj-psi-l R
<proof>

lemma proj-psi-lR-mult-proj-psi-lR:
proj-psi-l R * proj-psi-l R = proj-psi-l R
<proof>

lemma proj-psi-lR-le-post:
proj-psi-l R ≤L post
<proof>

lemma P'-le-post-R:
P' ≤L (tensor-P post (proj-k R))
<proof>

lemma positive-post:
positive post
<proof>

lemma lowner-le-P':
P' ≤L tensor-P post (1m K)
<proof>

lemma post-mult-testNk:
assumes f k
shows post * (testN k) = testN k
<proof>

lemma post-mult-testNk-neg:
assumes ¬ f k
shows post * testN k = 0m N N
<proof>

lemma testN-post1:
f k ⇒ adjoint (testN k) * post * testN k = testN k
<proof>

lemma testN-post2:
¬ f k ⇒ adjoint (testN k) * post * testN k = 0m N N
<proof>

definition post-fst-k :: nat ⇒ complex mat where
post-fst-k k = mat N N (λ(i, j). if (i = j ∧ f i ∧ i < k) then 1 else 0)

lemma post-fst-kN:
post-fst-k N = post
<proof>

lemma post-fst-k-Suc:

```

$f i \implies \text{post-fst-}k (\text{Suc } i) = \text{testN } i + \text{post-fst-}k i$
 $\langle \text{proof} \rangle$

lemma $\text{post-fst-}k\text{-Suc-neg}:$
 $\neg f i \implies \text{post-fst-}k (\text{Suc } i) = \text{post-fst-}k i$
 $\langle \text{proof} \rangle$

lemma $\text{testN-sum}:$
 $\text{matrix-sum } N (\lambda k. \text{adjoint} (\text{testN } k) * \text{post} * \text{testN } k) N = \text{post}$
 $\langle \text{proof} \rangle$

lemma $\text{tensor-P-testN-sum}:$
 $\text{matrix-sum } d (\lambda k. \text{adjoint} (\text{tensor-P } (\text{testN } k) (1_m K)) * \text{tensor-P post } (1_m K)$
 $* \text{tensor-P } (\text{testN } k) (1_m K)) N =$
 $\text{tensor-P post } (1_m K)$
 $\langle \text{proof} \rangle$

lemma $\text{post-le-one}:$
 $\text{post} \leq_L 1_m N$
 $\langle \text{proof} \rangle$

lemma $\text{qp-post}:$
 $\text{is-quantum-predicate } (\text{tensor-P post } (1_m K))$
 $\langle \text{proof} \rangle$

lemma $\text{hoare-triple-if}:$
 $\vdash_p \{\text{tensor-P post } (1_m K)\}$
 $\text{Measure-P vars1 } N \text{ testN } (\text{replicate } N \text{ SKIP})$
 $\{\text{tensor-P post } (1_m K)\}$
 $\langle \text{proof} \rangle$

theorem $\text{grover-partial-deduct}:$
 $\vdash_p \{\text{tensor-P pre } (\text{proj-}k 0)\}$
 Grover
 $\{\text{tensor-P post } (1_m K)\}$
 $\langle \text{proof} \rangle$

theorem $\text{grover-partial-correct}:$
 $\models_p \{\text{tensor-P pre } (\text{proj-}k 0)\}$
 Grover
 $\{\text{tensor-P post } (1_m K)\}$
 $\langle \text{proof} \rangle$
end

end

References

- [1] M. Ying. Floyd–Hoare logic for quantum programs. *ACM Transactions on Programming Languages and Systems*, 33(6):19:1–19:49, 2011.