

Mirror inversion of quantum states in linear registers

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Transfer of data in linear quantum registers can be significantly simplified with pre-engineered but not dynamically controlled inter-qubit couplings. We show how to implement a mirror inversion of a quantum state of qubits with respect to the centre of the register. Our construction is especially appealing as it requires no dynamical control over individual inter-qubit interactions. If, however, the individual control is available then the mirror inversion operation can be performed on any substring of qubits in the register. In this case a sequence of mirror inversions can efficiently generate any permutation of a quantum state of the involved qubits.

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The network (circuit) model of quantum computation is justifiably the most popular model for investigating both computational power and possible experimental realizations of quantum computers. One of its many appealing features is the reduction of quantum computation to prescribed sequences of elementary operations (quantum logic gates) performed either on individual qubits or on pairs of qubits [1]. However, a tacit assumption that single- and two-qubit operations are much easier to implement than multi-qubit operations, is not always valid. In fact, there are potentially interesting technologies, for example, optical lattices [2], arrays of quantum dots [3–6], or NMR [7, 8], in which joint operations on several qubits are relatively easy whereas addressing individual qubits poses a substantial experimental challenge. Thus it is important to investigate quantum computation with limited control over individual qubits. Here we show that transfer of data in quantum registers can be significantly simplified with pre-engineered but not dynamically controlled inter-qubit couplings.

It is known that quantum computation could in principle be performed by a chain of qubits coupled via the Heisenberg or the XY interactions [9], and that it suffices to control the qubits collectively [10]. Such a chain of qubits represents a quantum register. Further simplifications to this model have been recently introduced by Zhou *et al.* [11] and by Benjamin and Bose [12]. Still, a significant number of elementary operations in the process of computation is delegated to moving around quantum states of individual qubits. We show how to simplify these operations by implementing a mirror inversion of a quantum state with respect to the centre of the chain. More precisely, given a chain of $N + 1$ qubits described by the wavefunction $\Psi(s_0, \dots, s_N)$, where $s_n = 0, 1$ denotes the bit values of the n th qubit, we show how to implement the transformation R

$$R \Psi(s_0, s_1, \dots, s_{N-1}, s_N) = \Psi(s_N, s_{N-1}, \dots, s_1, s_0). \quad (1)$$

Our construction has the advantage that it can be done without applying any dynamical control to the qubits, it only exploits the natural dynamics of the chain governed by a pre-engineered mirror periodic Hamiltonian H such that $\exp(-iTH) = R$ for some time T .

Apart from obvious applications, such as a perfect quantum wire or a ‘data bus’ linking the two opposite ends of the chain studies of periodic and mirror-periodic dynamics of chains of spins with non-homogenous couplings is an interesting subject on its own, with many potential applications outside quantum computation.

Consider $N + 1$ interacting qubits, or spin-1/2 particles, in a quantum register. We choose the Hamiltonian of the system to be of the XY type

$$H = \frac{1}{2} \sum_{x=0}^{N-1} J_x (\sigma_x^{(1)} \cdot \sigma_{x+1}^{(1)} + \sigma_x^{(2)} \cdot \sigma_{x+1}^{(2)}) - \frac{1}{2} \sum_{x=0}^N h_x (\sigma_x^{(3)} - 1), \quad (2)$$

where J_x is the coupling strength between the qubits located at sites x and $x + 1$, and h_x is the ‘Zeeman’ energy of a qubit at site x . Please note that here x labels the position of a qubit in the register, whereas the three Pauli matrices are denoted as $\sigma^{(1)}$, $\sigma^{(2)}$, and $\sigma^{(3)}$.

Now our task is to find the values J_x and h_x for which the Hamiltonian H is mirror periodic. The total z -component of the spin, given by

$$\sigma_{tot}^{(3)} := \sum_{x=0}^N \sigma_x^{(3)} \quad (3)$$

is conserved, i.e., $[\sigma_{tot}^{(3)}, H] = 0$. Hence the Hilbert space of the register decomposes into invariant subspaces, each of which is a distinct eigenspace of the operator $\sigma_{tot}^{(3)}$. The eigenspace with eigenvalue $(2M - N - 1)/2$ corresponds to exactly M qubits having bit value 1. Let us denote this subspace by \mathcal{S}_M .

For convenience of our exposition, we adopt here the standard fermionization technique [13]. We will view the

register as a lattice with $N + 1$ sites, some of which are occupied by indistinguishable and non-interacting, spinless fermions. The bit values 1 and 0 indicate the presence and the absence of the fermion at a given lattice site and the Pauli exclusion principle prevents two or more fermions to occupy the same site. The subspace \mathcal{S}_M corresponds to the M -fermion sector, in which M of the $N + 1$ lattice sites are occupied by fermions. The Jordan-Wigner transformation

$$a_x = \left(\prod_{y < x} \sigma_y^{(3)} \right) \frac{\sigma_x^{(1)} + i\sigma_x^{(2)}}{2}, \quad a_x^\dagger = \left(\prod_{y < x} \sigma_y^{(3)} \right) \frac{\sigma_x^{(1)} - i\sigma_x^{(2)}}{2} \quad (4)$$

allows to rewrite the Hamiltonian (2) in the second quantization form using the fermionic operators a_x and a_x^\dagger ,

$$H = \sum_{x=0}^{N-1} J_x \left(a_x^\dagger a_{x+1} + a_{x+1}^\dagger a_x \right) + \sum_{x=0}^N h_x a_x^\dagger a_x. \quad (5)$$

The Hamiltonian H in (5) describes a set of $N + 1$ non-interacting (or free) fermions which hop between adjacent sites of the lattice, and are subject to a non-uniform magnetic field, denoted by h_x , $x = 0, 1, \dots, N$. Let $|x\rangle$ denote a state in which there is a single fermion at the site x and all other sites are empty. Then the set of states $\{|x\rangle\}$ forms a basis spanning the subspace \mathcal{S}_1 . In this single-particle basis, the Hamiltonian H is represented by the matrix

$$\begin{pmatrix} h_0 & J_0 & 0 & \cdots & 0 \\ J_0 & h_1 & J_1 & \cdots & 0 \\ 0 & J_1 & h_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & J_{N-1} \\ 0 & 0 & 0 & J_{N-1} & h_N \end{pmatrix}. \quad (6)$$

The dynamics of the register is completely determined by the eigenvalues and eigenvectors of the above matrix. Let us denote the energy eigenvalues of the matrix by E_{k_n} , where $k_n = 0, 1, \dots, N$, and the corresponding energy eigenfunction by $\phi_{k_n}(x_n)$ (where $x_n \in \{0, 1, \dots, N\}$). The latter corresponds to a single fermion at the site x_n of the chain. In the M -fermion sector, the energy of M fermions occupying orbitals $0 \leq k_1 < \dots < k_M \leq N$ is then given by

$$E_{k_1, \dots, k_M} = \sum_{i=1}^M E_{k_i} \quad (7)$$

and the corresponding M -particle energy eigenfunction can be written as the Slater determinant

$$\Phi_{k_1, \dots, k_M}(x_1, \dots, x_M) = \frac{1}{\sqrt{M!}} \begin{vmatrix} \phi_{k_1}(x_1) & \cdots & \phi_{k_1}(x_M) \\ \vdots & \ddots & \vdots \\ \phi_{k_M}(x_1) & \cdots & \phi_{k_M}(x_M) \end{vmatrix} \quad (8)$$

The eigenfunction $\Phi_{k_1, \dots, k_M}(x_1, \dots, x_M)$ is completely antisymmetric. Let us now see how this eigenfunction is related to the wavefunction of the quantum register.

In the subspace \mathcal{S}_M , the wavefunction of the register $\Psi(s_0, \dots, s_N)$ can be expressed as $\Psi(x_1, \dots, x_M)$, where x_1, \dots, x_M label the qubits which have bit values equal to 1. Each of the remaining qubits have bit value 0. In other words, the value of $\Psi(x_1, \dots, x_M)$ gives the probability amplitude that the qubits located at the sites x_1, x_2, \dots, x_M represent binary '1' and all other qubits represent binary '0'. Note that the wavefunction $\Psi(x_1, \dots, x_M)$ is symmetric under an interchange of its labels, and is hence bosonic. It can, however, be expressed in terms of the fermionic wavefunctions $\Phi_{k_1, \dots, k_M}(x_1, \dots, x_M)$ in the following manner: In the sector $x_1 < x_2 < \dots < x_M$, the wavefunction of the register corresponding to the energy eigenvalue E_{k_1, \dots, k_M} is set equal to the fermionic eigenfunction $\Phi_{k_1, \dots, k_M}(x_1, \dots, x_M)$:

$$\Psi(x_1, \dots, x_M) \equiv \Psi_{k_1, \dots, k_M}(x_1, \dots, x_M) \quad (9)$$

$$= \Phi_{k_1, \dots, k_M}(x_1, \dots, x_M). \quad (10)$$

In the other sectors the two differ by the sign giving the parity of the permutation required to reshuffle the arguments in increasing order.

The evolution of any single particle wavefunction $\phi(x)$ can be written as

$$\phi(x, t) = \sum_{k=0}^N e^{-itE_k/\hbar} a_k \phi_k(x). \quad (11)$$

A Hamiltonian is defined as *mirror periodic* if it satisfies

$$e^{-iTH} \Phi(x_1, \dots, x_M) = R \Phi(x_1, \dots, x_M) = \Phi(N - x_1, \dots, N - x_M). \quad (12)$$

The mirror periodicity with period T implies periodicity with period $2T$, which in turn implies that for all k the quantity $2TE_k$ is an integer multiple of 2π in units for which $\hbar = 1$ and $\phi_k(N - x) = \pm \phi_k(x)$.

We found two families of mirror periodic Hamiltonians: one (**A**) with linear spectrum and the other (**B**) with quadratic spectrum. An alternative proof of mirror periodicity for the case (**A**), in the single-particle sector, was given by Christandl *et al.* [15]. The proof relied on identifying the Hamiltonian operator with the generator of space rotations and employed group theoretical methods. In this paper we recognize that the mirror periodicity extends to all multi-particle sectors and that it is also shared by another finite quantum chain with eigenfunctions given by Hahn polynomials. Let us now discuss cases (**A**) and (**B**) in detail:

(**A**) The quantum chain with linear spectrum $P(k) = k$ has eigenfunctions $\phi_k(x)$ proportional to Krawtchouk polynomials. This polynomial basis has been used by

Atakishiev *et al.* [14] to construct finite quantum chains admitting periodic solutions.

The Krawtchouk quantum chain which is mirror periodic of period $T = \pi$ has couplings

$$J_x = \sqrt{(x+1)(N-x)} \quad ; \quad h_x = 0, \quad (13)$$

The Krawtchouk polynomials are defined in terms of the hypergeometric functions F as

$$K_k(x, p, N) = {}_2F_1 \left(\begin{matrix} -k, -x \\ -N \end{matrix} \middle| \frac{1}{p} \right) \quad (14)$$

where $k = 0, 1, 2, \dots, N$. The energy eigenfunctions are

$$\phi_k(x) = c_k \sqrt{w(x)} K_k \left(x, \frac{1}{2}, N \right) \quad (15)$$

where c_k is the constant

$$c_k = \sqrt{\frac{(-N)_k}{(-1)^k k!}} \quad (16)$$

and $w(x)$ is the weight function

$$w(x) = \frac{1}{2^N} \binom{N}{x}. \quad (17)$$

The corresponding eigenvalues are $E_k = -k$. In the definitions above we have used the Pochhammer symbol, $(N)_k$ defined as

$$(N)_k = N(N+1) \dots (N+k-1), \quad k = 1, 2, 3, \dots \quad (18)$$

with $(N)_0 = 1$, and the generalized binomial symbol expressed in terms of the Γ function as

$$\binom{N}{x} = \frac{\Gamma(N+1)}{\Gamma(N-x+1)\Gamma(x+1)}. \quad (19)$$

For a more comprehensive description of the Krawtchouk polynomials we refer to [16].

The energy eigenfunctions satisfy the property of reflection symmetry (or antisymmetry):

$$\phi_k(N-x) = (-1)^k \phi_k(x) \quad (20)$$

for all x and all $k = 0, 1, 2, \dots, N$. This follows from the following property of the Krawtchouk polynomials:

$$K_k \left(N-x; \frac{1}{2}, N \right) = (-1)^k K_k \left(x; \frac{1}{2}, N \right), \quad (21)$$

and the fact that the weight function in (17) is symmetric. The phases $(-1)^k$ in (20) perfectly offset the dynamical phases acquired after a time period $T = \pi$, as $\exp(-iTE_k) = (-1)^k$. This shows that the chain defined by the Hamiltonian corresponding to the Krawtchouk polynomials is mirror symmetric with period π .

The dynamics of the Krawtchouk quantum chain of $N+1$ sites is the same as that of a spin $s = N/2$ particle governed by the Hamiltonian $H_s = 2\mathbf{s}_x$. This Hamiltonian acts as follows on the basis vectors $|m\rangle$, $m = -s, \dots, s$:

$$H_s |m\rangle = R(m)|m-1\rangle + L(m)|m+1\rangle,$$

where

$$\begin{aligned} R(m) &= \sqrt{s(s+1) - m(m-1)} \\ L(m) &= \sqrt{s(s+1) - m(m+1)}. \end{aligned}$$

It is possible to establish a relation between H_s and a mirror-periodic Krawtchouk chain of $N+1 = 2s+1$ sites. This is done by identifying the state $|x\rangle$ corresponding to a single particle occupying the site x with the state $|m\rangle$, where $m = s-x$. In this case, $R(m)$ reduces to J_x and $L(m)$ reduces to J_{x-1} , showing that the spin Hamiltonian H_s is equivalent to the mirror periodic Krawtchouk Hamiltonian.

(B) One can use Hahn polynomials to find a family of mirror periodic quantum chains whose period is an integer multiple of π with quadratic spectrum $E_k = k(k+2\alpha+1)$, where α is of the form

$$\alpha = \frac{2p+1}{2q} \quad (22)$$

where p, q are integers with $q \neq 0$. The couplings are

$$J_x = \sqrt{(x+1)(N-x)(\alpha+N-x)(\alpha+x+1)} \quad (23)$$

and the Zeeman terms are given by

$$h_x = \frac{N^2}{2} + (\alpha+1)N - 2 \left(x - \frac{N}{2} \right)^2. \quad (24)$$

This model has eigenfunctions $\phi_k(x)$ given by Hahn polynomials. The Hahn polynomials are defined in terms of the hypergeometric functions F as

$$Q_k(x; \alpha, \beta, N) = {}_3F_2 \left(\begin{matrix} -k, k+\alpha+\beta+1, x \\ \alpha+1, -N \end{matrix} \middle| 1 \right) \quad (25)$$

where $k = 0, 1, 2, \dots, N$. The energy eigenfunctions of the Hamiltonian (2) are given by

$$\phi_k(x) = c_k \sqrt{w(x)} Q_k(x; \alpha, \alpha, N) \quad (26)$$

where c_k is the constant

$$c_k = \sqrt{\frac{(2k+2\alpha+1)(N!)^2}{(k+2\alpha+1)_{N+1} k!(N-k)!}}, \quad (27)$$

and $w(x)$ is the weight function

$$w(x) = \binom{\alpha+x}{x} \binom{\alpha+N-x}{N-x}. \quad (28)$$

For further details on Hahn polynomials see [16].

To show that the $\phi_k(x)$ are either reflection symmetric or anti-symmetric, we notice that

$$Q_k(N-x; \alpha, \alpha, N) = (-1)^k Q_k(x; \alpha, \alpha, N), \quad (29)$$

and that the weight function in (28) is symmetric. Hence, $\phi_k(N-x) = (-1)^k \phi_k(x)$, for all x and all $k = 0, 1, 2, \dots, N$. If α satisfies (22) and $T = q\pi$, the phases $(-1)^k$ perfectly offset the dynamical phases. In fact

$$\exp(-iT E_k) = \exp(-i\pi[q(k^2 + k) + (2p+1)k]) = (-1)^k \quad (30)$$

since $k^2 + k$ is even for all $k = 0, \dots, N$. This shows that the Hahn chain is mirror periodic of period $T = q\pi$.

The Hahn chain Hamiltonian in the special case $q = 1$, i.e. when $\alpha = (2p+1)/2$ is half-integer, is related to atomic Hamiltonians with $\mathbf{L} \cdot \mathbf{S}$ coupling. Consider the Hamiltonian

$$H_{LS} = \mathbf{L} \cdot \mathbf{S} \quad (31)$$

restricted to the sector with fixed total angular momentum L , total spin S and with projections along a fixed axis adding up to zero, i.e. $M = M_L + M_S = 0$. The Hamiltonian in (31) acts as follows on the basis vectors $|M_S\rangle \equiv |L, S; M_L, M_S\rangle$:

$$H_{LS}|M_S\rangle = D|M_S\rangle + R|M_S - 1\rangle + L|M_S + 1\rangle \quad (32)$$

where

$$D \equiv D(M_S) = -M_S^2 \quad (33)$$

$$R \equiv R(M_S) \quad (34)$$

$$= \frac{1}{2} \sqrt{(L+M_S)(L-M_S+1)(S+M_S)(S-M_S+1)}$$

$$L \equiv L(M_S) \quad (35)$$

$$= \frac{1}{2} \sqrt{(L-M_S)(L+M_S+1)(S-M_S)(S+M_S+1)}.$$

Assuming that $S < L$ and that S is a half-integer, it is possible to establish a relation between H_{LS} and a mirror-periodic Hahn chain of $N = 2S$ sites and $\alpha = L - S$. This is done by identifying the state $|x\rangle$ corresponding to a single particle occupying the site x with the state $|M_S\rangle$, where $M_S = S - x$. We find

$$D = -\left(x - \frac{N}{2}\right)^2, \quad (36)$$

$$R = \frac{1}{2} \sqrt{(\alpha + N - x)(\alpha + x + 1)(N - x)(x + 1)}, \quad (37)$$

$$L = \frac{1}{2} \sqrt{(\alpha + x)(\alpha + N - x + 1)x(N - x + 1)}. \quad (38)$$

Hence $R(M_S) = \frac{1}{2} J_x$, $L(M_S) = \frac{1}{2} J_{x-1}$ and $D(M_S) = \frac{1}{2} h_x + \text{const}$, showing that the LS coupling Hamiltonian

is proportional to a mirror periodic Hahn Hamiltonian up to a constant energy shift.

In conclusion, in this Letter we have demonstrated how to simplify transfer of data in quantum registers by implementing a mirror inversion of a quantum state with respect to the centre of the register. Our construction is especially appealing as it requires no dynamical control over individual qubits but only pre-engineered inter-qubit couplings. If, however, the individual control is available then the mirror inversion operation can be performed on any substring of qubits in the register. In this case a sequence of mirror inversions can efficiently generate any permutation of a quantum state of the involved qubits.

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