Hamilton Operators, Discrete Symmetries, Brute Force and SymbolicC++

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Abstract To find the discrete symmetries of a Hamilton operator $\hat{H}$ is of central importance in quantum theory. Here we describe and implement a brute force method to determine the discrete symmetries given by permutation matrices for Hamilton operators acting in a finite-dimensional Hilbert space. Spin and Fermi systems are considered as examples. A computer algebra implementation in SymbolicC++ is provided.

1 Introduction

In quantum mechanics the system is described by a self-adjoint (Hamilton) operator $\hat{H}$ acting in a Hilbert space $\mathcal{H}$. Here we consider the finite dimensional Hilbert space $\mathbb{C}^n$ where $\hat{H}$ is a hermitian matrix [1, 2, 3, 4, 5]. One of the main tasks is to find the $n \times n$ unitary matrices U such that $U^*\hat{H}U = \hat{H}$, where $U^* = U^{-1}$. The $n \times n$ unitary matrices form the compact Lie group $U(n)$. Note that if $U^*\hat{H}U = \hat{H}$ and $V^*\hat{H}V = \hat{H}$ then $(UV)^*\hat{H}(UV) = \hat{H}$, where $(UV)^* \equiv V^*U^*$. Thus the set of matrices that keep $\hat{H}$ invariant form a group themselves [6].

An important finite subgroup of the group $U(n)$ are the $n \times n$ permutation matrices. The number of $n \times n$ permutation matrices is $n!$. For a given hermitian $n \times n$ matrix $\hat{H}$ we want to find all the $n \times n$ permutation matrices P such that

$$P^T\hat{H}P = \hat{H}$$

where $P^{-1} = P^T$. These permutation matrices form a subgroup of all $n \times n$ permutation matrices. Obviously the $n \times n$ identity matrix I_n satisfies $I_n\hat{H}I_n = \hat{H}$.

Here we describe and implement in SymbolicC++ a brute force method to find these permutation matrices.

After this finite group has been found one determines the conjugacy classes. Now for a finite group G the number of conjugacy classes is equivalent to the number of non-equivalent irreducible matrix representations. From the conjugacy classes and the permutation matrices we can construct projection matrices to decompose the Hilbert space into invariant sub Hilbert spaces [6]. For example, if the permutation matrix P satisfies $P^2 = I_n$, then $\Pi_1 = (I_n + P)/2$, $\Pi_2 = (I_n - P)/2$ are projection matrices (with $\Pi_1\Pi_2 = 0$) which can be utilized to decompose the Hilbert space $\mathbb{C}^n$ into invariant subspaces.

2 Examples

We consider four examples: two Fermi systems and two spin systems.

Example 1. Let $c_j^\dagger$, c_j ($j = 1, 2, 3$) be Fermi creation and annihilation operators, respectively. Consider the Hamilton operator

$$\hat{H} = t(c_1^\dagger c_2 + c_2^\dagger c_1 + c_2^\dagger c_3 + c_3^\dagger c_2 + c_1^\dagger c_3 + c_3^\dagger c_1) + k_1 c_1^\dagger c_1 + k_2 c_2^\dagger c_2 + k_3 c_3^\dagger c_3$$

and the number operator $\hat{N} = c_1^\dagger c_1 + c_2^\dagger c_2 + c_3^\dagger c_3$. Then $[\hat{H}, \hat{N}] = 0$. Since $[\hat{H}, \hat{N}] = 0$ we find $\hat{N}$ is a constant of motion, i.e. the total number of Fermi particles remains constant in the sense that if $|n\rangle$ is an eigenstate of the number operator $\hat{N}$ with eigenvalue n at time 0, then $|n\rangle(t) = e^{-i\hat{H}t/\hbar}|n\rangle$ remains an eigenstate of $\hat{N}$ with eigenvalue n for all times. Given a basis with two Fermi particles

$$c_1^\dagger c_2^\dagger |\mathbf{0}\rangle, \quad c_1^\dagger c_3^\dagger |\mathbf{0}\rangle, \quad c_2^\dagger c_3^\dagger |\mathbf{0}\rangle .$$

Then we find the matrix representation of $\hat{H}$

$$\hat{H} = \begin{pmatrix} k_1 + k_2 & t & -t \\ t & k_1 + k_3 & t \\ -t & t & k_2 + k_3 \end{pmatrix} .$$

The matrix representation of $\hat{N}$ is the diagonal matrix $2I_3$, where I_3 is the 3×3 identity matrix. For $k_1 \neq k_2$, $k_1 \neq k_3$, $k_2 \neq k_3$ no non-trivial symmetry is found. Also for $k_1 \neq k_2$, $k_1 \neq k_3$, $k_2 = k_3$ no non-trivial symmetry is found. For $k = k_1 = k_2 = k_3$ we obtain the permutation matrix

$$P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} .$$

Thus using the projection matrices $\Pi_1 = (I_3 - P)/2$, $\Pi_2 = (I_3 - P)/2$ the Hilbert space $\mathbb{C}^3$ can be decomposed into invariant subspaces. For the case $k = k_1 = k_2 = k_3$ we find the eigenvalues $2k - 2t$ and $2k + t$ (twice).

Example 2. Consider the Hamilton operator (two-point Hubbard model)

$$\hat{H} = t(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow} + c_{2\uparrow}^\dagger c_{1\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow})$$

where $n_{j\uparrow} := c_{j\uparrow}^\dagger c_{j\uparrow}$, $n_{j\downarrow} := c_{j\downarrow}^\dagger c_{j\downarrow}$. The operators $c_{j\uparrow}^\dagger, c_{j\downarrow}^\dagger, c_{j\uparrow}, c_{j\downarrow}$ are Fermi operators. The Hubbard Hamilton operator commutes with the total number operator $\hat{N}$ and the total spin operator $\hat{S}_z$ where

$$\hat{N} := \sum_{j=1}^{2}(c_{j\uparrow}^\dagger c_{j\uparrow} + c_{j\downarrow}^\dagger c_{j\downarrow}), \qquad \hat{S}_z := \frac{1}{2}\sum_{j=1}^{2}(c_{j\uparrow}^\dagger c_{j\uparrow} - c_{j\downarrow}^\dagger c_{j\downarrow}) \,.$$

We consider the subspace with two particles $N = 2$ and total spin $S_z = 0$. A basis in this four dimensional Hilbert space is given by

$$c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger|\mathbf{0}\rangle, \quad c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger|\mathbf{0}\rangle, \quad c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger|\mathbf{0}\rangle, \quad c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger|\mathbf{0}\rangle \,.$$

We find the matrix representation of $\hat{H}$ for this basis. Using the Fermi anti-commutation relations and $c_{j\uparrow}|\mathbf{0}\rangle = 0$, $c_{j\downarrow}|\mathbf{0}\rangle = 0$ for $j = 1, 2$ we obtain the matrix representation of $\hat{H}$ with the given basis

$$H = \begin{pmatrix} U & t & t & 0 \\ t & 0 & 0 & t \\ t & 0 & 0 & t \\ 0 & t & t & U \end{pmatrix} .$$

We find the four permutation matrices $P_0 = I_4 = I_2 \star I_2 = I_2 \otimes I_2$,

$$P_1 = I_2 \star \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad P_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \star I_2, \quad P_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \star \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

where we define the star product $\star$ of the two 2×2 matrices A, B as [6]

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \star \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} := \begin{pmatrix} a_{11} & 0 & 0 & a_{12} \\ 0 & b_{11} & b_{12} & 0 \\ 0 & b_{21} & b_{22} & 0 \\ a_{21} & 0 & 0 & a_{22} \end{pmatrix} .$$

We note that the star product of two 2×2 permutation matrices is a 4×4 permutation matrix. Here P_1 is the swap gate. The four permutation matrices P_0, P_1,

P_2, P_3 form a commutative group with $P_j^2 = I_4$ for $j = 0, 1, 2, 3$. If P is an $n \times n$ permutation matrix with $P^2 = I_n$ then

$$\Pi_1 = \frac{1}{2}(I_n + P), \qquad \Pi_2 = \frac{1}{2}(I_n - P)$$

are projection matrices with $\Pi_1 \Pi_2 = 0_n$, where 0_n is the $n \times n$ zero matrix. Using the permutation matrices P_0 and P_3 (which form a subgroup) these projection operators can now be used to find the invariant subspaces

$$\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \right\}, \quad \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \right\}.$$

These four vectors (after normalization) are known in quantum computing as the Bell basis [1, 2, 3, 4, 5]. This leads to the two invariant sub Hilbert spaces

$$\left\{ \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle + c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle), \quad \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle + c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle) \right\}$$

$$\left\{ \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle - c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle), \quad \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle - c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle) \right\}.$$

Example 3. Let σ_1, σ_2, σ_3 be the Pauli spin matrices

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Consider the Hamilton operators [7]

$$\hat{H} = \hbar\omega_1 \sigma_3 \otimes I_2 + \hbar\omega_2 I_2 \otimes \sigma_1 + \epsilon(\sigma_3 \otimes \sigma_1)$$

$$\hat{K} = \hbar\omega_1 \sigma_3 \otimes I_2 + \hbar\omega_2 I_2 \otimes \sigma_1 + \epsilon(\sigma_1 \otimes \sigma_3)$$

where for the second Hamilton operator $\hat{K}$ the interaction term is swapped around, i.e. $\sigma_3 \otimes \sigma_1 \to \sigma_1 \otimes \sigma_3$. This provides symmetry breaking. For the Hamilton operator $\hat{H}$ we find the symmetries (permutation matrices)

$$P_0 = I_4, \quad P_1 = I_2 \oplus \sigma_1, \quad P_2 = \sigma_1 \oplus I_2, \quad P_3 = \sigma_1 \oplus \sigma_1$$

where $\oplus$ denotes the direct sum. The four matrices form a commutative group under matrix multiplication. All satisfy $P_j^2 = I_4$. Thus we can use the projection matrices $\Pi_1 = (I_4 + P_j)/2$, $\Pi_2 = (I_4 - P_j)/2$ to decompose the Hilbert space into two invariant subspaces. On the other hand for the Hamilton operator $\hat{K}$ we only find the identity matrix $P_0 = I_4$, i.e. no non-trivial symmetry is admitted.

Example 4. Consider the Hamilton operator for triple spin interaction

$$\hat{H} = \sigma_1 \otimes \sigma_2 \otimes \sigma_3 \,.$$

The eigenvalues of this hermitian and unitary 8×8 matrix are $+1$ (four-fold degenerate) and -1 (four-fold degenerate). Owing to this degeneracy one expects a "large" number of symmetries. Applying the SymbolicC++ code we find 24 permutation matrices listed $P_0, P_1, \ldots, P_{23}$ with $P_0 = I_8$. They form a non-commutative group under matrix multiplication and are a subgroup of the group of 8×8 permutation matrices. We note that the Kronecker product $\otimes$ and the direct sum $\oplus$ of two permutation matrices is again a permutation matrix [8]. Now we can list the ones with $P_j^2 = I_8$. We have

$$\begin{aligned}
P_1 &= I_2 \oplus \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) \oplus I_2 \\
P_2 &= (I_2 \star \sigma_1) \oplus (\sigma_1 \star I_2) \\
P_5 &= I_2 \otimes I_2 \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \sigma_1 \otimes I_2 \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\
P_6 &= (\sigma_1 \star I_2) \oplus (I_2 \star \sigma_1) \\
P_8 &= I_2 \otimes \sigma_1 \otimes \sigma_1 \\
P_{13} &= I_2 \otimes I_2 \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \sigma_1 \otimes I_2 \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\
P_{15} &= \sigma_1 \otimes I_2 \otimes I_2 \\
P_{23} &= \sigma_1 \otimes \sigma_1 \otimes \sigma_1 \,.
\end{aligned}$$

The other ones can be found by multiplication of these permutation matrices, for example $P_3 = P_1 P_2$ etc. Thus the 24 matrices form a subgroup of the permutation group of 8×8 matrices.

Another spin Hamilton operator studied is [9]

$$\hat{H} = a \sum_{j=1}^{4} \sigma_3(j)\sigma_3(j+1) + b \sum_{j=1}^{4} \sigma_1(j)$$

with cyclic boundary conditions, i.e. $\sigma_3(5) \equiv \sigma_3(1)$. Here a, b are real constants and σ_1, σ_2 and σ_3 are the Pauli matrices. Thus the underlying Hilbert space is

$\mathbb{C}^{16}$. Recall that

$$\sigma_k(1) = \sigma_k \otimes I_2 \otimes I_2 \otimes I_2, \qquad \sigma_k(2) = I_2 \otimes \sigma_k \otimes I_2 \otimes I_2$$

$$\sigma_k(3) = I_2 \otimes I_2 \otimes \sigma_k \otimes I_2, \qquad \sigma_k(4) = I_2 \otimes I_2 \otimes I_2 \otimes \sigma_k$$

where $k = 1, 2, 3$. We obtain the symmetric 16×16 matrix for $\hat{H}$

$$\begin{pmatrix}
4a & b & b & 0 & b & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
b & 0 & 0 & b & 0 & b & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 \\
b & 0 & 0 & b & 0 & 0 & b & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 \\
0 & b & b & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 \\
b & 0 & 0 & 0 & 0 & b & b & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 \\
0 & b & 0 & 0 & b & -4a & 0 & b & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 \\
0 & 0 & b & 0 & b & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & b & 0 \\
0 & 0 & 0 & b & 0 & b & b & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b \\
b & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b & b & 0 & b & 0 & 0 & 0 \\
0 & b & 0 & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & b & 0 & b & 0 & 0 \\
0 & 0 & b & 0 & 0 & 0 & 0 & 0 & b & 0 & -4a & b & 0 & 0 & b & 0 \\
0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & b & b & 0 & 0 & 0 & 0 & b \\
0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & b & b & 0 \\
0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & 0 & b & 0 & 0 & b \\
0 & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & b & 0 & 0 & b \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & b & b & 4a
\end{pmatrix}.$$

The Hamilton operator $\hat{H}$ admits the C_{4v} symmetry group. The order of this non-commutative group is 8. One finds the following set of eight symmetries [9]

$$E : (1,2,3,4) \to (1,2,3,4) \qquad C_2 : (1,2,3,4) \to (3,4,1,2)$$

$$C_4 : (1,2,3,4) \to (2,3,4,1) \qquad C_4^3 : (1,2,3,4) \to (4,1,2,3)$$

$$\sigma_v : (1,2,3,4) \to (2,1,4,3) \qquad \sigma_v' : (1,2,3,4) \to (4,3,2,1)$$

$$\sigma_d : (1,2,3,4) \to (1,4,3,2) \qquad \sigma_d' : (1,2,3,4) \to (3,2,1,4)$$

which form a group isomorphic to C_{4v}. The symmetries can be found by calculating the 16×16 permutation matrices such that $\hat{H} = P^T \hat{H} P$.

3 Code Description

Algorithms for finding all permutations of a sequence of objects are described by Knuth [10]. For a given n the permutation matrices are generated with the following algorithm. The algorithm implements the nested loops

For $j_0 = 0, 1, \ldots, n-1$ do
For $j_1 = 0, 1, \ldots, n-1$ do

$\ddots$

For $j_{n-1} = 0, 1, \ldots, n-1$ do
If $j_0 \neq j_1 \neq \cdots \neq j_{n-1}$ then
use the permutation $(0, 1, 2, \ldots, n-1) \to (j_0, j_1, j_2, \ldots, j_{n-1})$.
End loop

$\vdots$

End loop
End loop

Algorithm to find all permutation matrices.

1. Create an array $(j_0, j_1, \ldots, j_{n-1})$ of loop variables.
2. Initialize $j_k := -1$ for $k = 0, 1, \ldots, n-1$.
3. Initialize the loop variable index i to $i := 0$.
4. While $i \geq 0$
   (a) *Iterate.*
   Set $j_i := j_i + 1$.
   (b) *Termination condition.*
   If $j_i = n$ terminate this loop:
      i. Set $j_i := -1$.
      ii. *Exit the nested loop.*
      Set $i := i - 1$.
      iii. Goto 4.
   (c) If $j_k = j_i$ for some $k \in \{0, 1, \ldots, i-1\}$ then goto 4.
   (d) *Enter the next nested loop.*
   Set $i := i + 1$.
   (e) *Innermost loop completes.*
   If $i = n$ then use the permutation $(0, 1, 2, \ldots, n-1) \to (j_0, j_1, j_2, \ldots, j_{n-1})$ i.e. the permutation matrix P is given by

$$(P)_{uv} = \begin{cases} 1 & \text{if } v = j_u \\ 0 & \text{otherwise} \end{cases} .$$

The SymbolicC++ program [11] utilizes the vector class of the Standard Template Library. The Hamilton operator refers to example 2 in the text (two point Hubbard model).

```
// permutation.cpp

#include <iostream>
#include <vector>
#include "symbolicc++.h"
using namespace std;

int total;
Symbolic H;

void commutes(const Symbolic &P)
{
 if(P*H==H*P) cout << "P[" << total++ << "] = " << P << endl;
}

void find_perm(int n,void (*use)(const Symbolic&))
{
 int i, k;
 Symbolic P;
 vector<int> j(n,-1);

 i = 0; j[0] = -1;
 while(i >= 0)
 {
  if(++j[i]==n) { j[i--] = -1; continue; }
  if(i < 0) break;
  for(k=0;k<i;++k) if(j[k]==j[i]) break;
  if(k!=i) continue;
  ++i;
  if(i==n)
  {
  P = 0*Symbolic("",n,n);
  for(k=0;k<n;k++) P(k,j[k]) = 1;
  use(P);
  --i;
  }
 }
}

int main(void)
{
 using SymbolicConstant::i;
 Symbolic sqrt2 = sqrt(Symbolic(2));
```

```
 Symbolic U("U"); Symbolic t("t");
 H = ((U,t,t,Symbolic(0)),(t,Symbolic(0),Symbolic(0),t),
      (t,Symbolic(0),Symbolic(0),t),(Symbolic(0),t,t,U));
 cout << "H = " << H << endl;
 total = 0;
 find_perm(H.rows(),commutes);
 return 0;
}
```

A Maxima implementation is available from the authors.

4 Conclusion

We applied a brute force method to find all possible permutation matrices that provide symmetries for given Hamilton operators in a finite dimensional Hilbert space. With growing size of the Hamilton operators matrix representation finding the permutation matrices becomes very time-consuming. A more efficient approach would be to find only the generators of the group of permutation matrices that provide symmetries for a given Hamilton operator. Another open question is how this method can be extended to find other classes of symmetries.

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