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Hubbard Model, Conserved Quantities, and Computer Algebra

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The constants of motion of the half-filled four-point Hubbard model with cyclic boundary conditions are given in Wannier and Bloch representation. The total number operator and total spin operator are conserved and spin-reversal symmetry exists. In Wannier representation we have additionally the C_{4v} symmetry and in Bloch representation we have the total momentum operator which is conserved. The anticommutation relations for Fermi operators with spin are implemented using computer algebra. Using computer algebra, all the constants of motion are given. The one-dimensional Hubbard model admits a Lax representation. From the Lax pair we find a new constant of motion.

1. INTRODUCTION

The Hubbard model plays an important role in the modeling of magnetism, charge density waves, and high-T_c superconductivity, since the interaction term of the Hubbard Hamiltonian can be written as

$$n_{i\uparrow}n_{i\downarrow} \equiv \tfrac{1}{4}(1-\alpha_i) + \hat{R}_{iz} + \tfrac{1}{3}(\alpha_i - 1)\,\mathbf{S}_i^2 + \tfrac{1}{3}(\alpha_i + 1)\,\mathbf{R}_i^2$$

Here $\mathbf{S}_i$ are the spin operators

$$\hat{S}_{ix} = \frac{1}{2}(c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow}), \quad \hat{S}_{iy} = \frac{1}{2i}(c_{i\uparrow}^\dagger c_{i\downarrow} - c_{i\downarrow}^\dagger c_{i\uparrow}), \quad \hat{S}_{iz} = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$$

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and $\mathbf{R}_i$ are the quasispin operators

$$\hat{R}_{iz}=\frac{1}{2}(c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}+c_{i\downarrow}c_{i\uparrow}),\ \ \hat{R}_{iy}=\frac{1}{2i}(c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}-c_{i\uparrow}c_{i\downarrow}),\ \ \hat{R}_{iz}=\frac{1}{2}(n_{i\uparrow}+n_{i\downarrow}-1)$$

Both the spin operators and quasi spin operators form a Lie algebra under the commutator.

This decomposition of the interacting part makes it possible to search for magnetism ($\langle \mathbf{S}_i\rangle \neq 0$), charge ordering ($\langle R_{iz}\rangle \neq 0$), or superconduction ($\langle R_{ix}\rangle \neq 0$) in the Hubbard model.

We investigate the constants of motion of a four-point system with cyclic boundary conditions in the Bloch representation and the Wannier representation. We apply computer algebra (Hearn, 1991; Steeb and Lewien, 1992) in this study. The study is limited to the half-filled case, i.e., $N_e = N$ (where N is the number of lattice sites and N_e is the number of electrons) and with total spin in the z direction $S_z = 0$. We also discuss the degeneracy in connection with the von Neumann and Wigner (1929) theorem.

In Wannier representation the Hubbard model is given by

$$\hat{H}=t\sum_{i=1}^{4}\sum_{\sigma}(c_{i+1\sigma}^{\dagger}c_{i\sigma}+c_{i\sigma}^{\dagger}c_{i+1\sigma})+U\sum_{i=1}^{4}n_{i\uparrow}n_{i\downarrow} \tag{1}$$

where $5 \equiv 1$. Thus the hopping integral t only acts for nearest neighbors.

The spectrum of the system can also be found by using the Bloch representation of the Hamiltonian (4), i.e.,

$$\hat{H}=\sum_{k\sigma}\varepsilon(k)c_{k\sigma}^{\dagger}c_{k\sigma}+\frac{U}{4}\sum_{k_1,k_2,k_3,k_4}\delta(k_1-k_2+k_3-k_4)c_{k_1\uparrow}^{\dagger}c_{k_2\uparrow}c_{k_3\downarrow}^{\dagger}c_{k_4\downarrow} \tag{2}$$

where

$$\varepsilon(k)=2t\cos k$$

($ka \rightarrow k$, with a the lattice spacing) and

$$k\in\left\{-\frac{\pi}{2},0,\frac{\pi}{2},\pi \text{ modulo } 2\pi\right\} \tag{3}$$

Computer algebra is a helpful tool in studying Fermi systems. We show how the anticommutation relations can be implemented with computer algebra. Then we give an application to the Hubbard model. In computations two tasks have to be performed. Let $\hat{A}$ be a linear operator expressed as Fermi operators and let $|\phi\rangle$ be a state expressed with Fermi creation operators and the vacuum state $|0\rangle$. Then we have to evaluate the new state $\hat{A}\,|\phi\rangle$, where we have to apply that $c_{j\sigma}\,|0\rangle = 0$. The second task arises in connection with the Heisenberg equation of motion

$$i\hbar \frac{d\hat{A}}{dt} = [\hat{A}, \hat{H}](t)$$

where $\hat{H}$ is the Hamilton operator of the system. This equation describes the time evolution of the linear operator $\hat{A}$. To solve this equation we have to evaluate

$$[\hat{A}, \hat{H}], \quad [\hat{A}, [\hat{A}, \hat{H}]], \ldots$$

If

$$[\hat{A}, \hat{H}] = 0$$

then $\hat{A}$ is called a constant of motion (conserved quantity). Both tasks can be implemented with computer algebra packages. There are several good computer algebra packages available. For our purpose we use REDUCE (Hearn, 1991; Steeb and Lewien, 1992). We can easily implement the anticommutation relation of the Fermi creation and annihilation operators. As an example we consider the four-point Hubbard model with cyclic boundary conditions. We give a higher-order conserved quantity.

2. CONSERVED QUANTITIES

The total number operator is given by

$$\hat{N}_e := \sum_{i=1}^{4} \sum_{\sigma \in \{\uparrow\downarrow\}} n_{i\sigma}$$

with the eigenvalues $N_e = 0, 1, 2, 3, 4$. The total spin operator in the z direction is given by

$$\hat{S}_z := \tfrac{1}{2} \sum_{i=1}^{4} (n_{i\uparrow} - n_{i\downarrow})$$

with the eigenvalues $0, \frac{1}{2}, -\frac{1}{2}, 1, -1, \frac{3}{2}, -\frac{3}{2}, 2, -2$. Since the Hubbard model (1) commutes with $\hat{N}_e$ and $\hat{S}_z$, the spectrum can be calculated in each of the subspaces separately. In the following we consider $N_e = 4$

(so-called half-filled case) and $S_z = 0$. For $N_e = 4$, $S_z = 0$, the dimension of the Hilbert space is given by dim $\mathscr{H} = 36$. A basis is given by

$$\{c_{i\uparrow}^\dagger c_{j\uparrow}^\dagger c_{m\downarrow}^\dagger c_{n\downarrow}^\dagger |0\rangle;\ i<j,\ m<n;\ i=1,2,3; m=1,2,3\}$$

where $c_{j\sigma}|0\rangle = 0$ and $\langle 0|0\rangle = 1$.

Since the Hamilton operator (1) admits C_{4v} symmetry and it is invariant with respect to spin reversal to spin reversal, the solution space can be further decomposed into invariant subspaces. The group C_{4v} admits five classes and therefore five irreducible representations. Four representations, A_1, A_2, A_3, and A_4, are one-dimensional and one, A_5, is two-dimensional. The group-theoretic reduction with the help of the group C_{4v} and spin reversal to the invariant subspaces S_i has been investigated by Villet and Steeb (1990).

The Hamiltonian (2) commutes also with the total momentum operator

$$\hat{P} = \sum_{k\sigma} k n_{k\sigma}$$

where k is given by (3). Obviously the eigenvalues of $\hat{P}$ are given by $-\pi/2$, 0, $\pi/2$, π. Thus the subspaces with a given total momentum are invariant. A basis for given momentum P is then given by

$$\{c_{k_1\uparrow}^\dagger c_{k_2\uparrow}^\dagger c_{k_3\downarrow}^\dagger c_{k_4\downarrow}^\dagger |0\rangle; k_1 \neq k_2, k_3 \neq k_4\}$$

where

$$k_1 + k_2 + k_3 + k_4 = P, \quad \text{modulo } 2\pi$$

Spin reversal symmetry also exists and the solution space is decomposed into subspaces $V_i (i = 1, 2, \ldots, 8)$ with dimensions 4, 4, 4, 6, 4, 4, 3, 7.

It seems that the total momentum operator $\hat{P}$ in the Bloch representation is related to the group C_4, which has four irreducible one-dimensional representations and describes rotation by 90°, 180°, 270°, and 360° = 0°. The operator $\hat{P}$ has four eigenvalues. The question therefore arises of how the symmetries σ_v and σ_d of the C_{4v} symmetry (i.e., reflections in two planes of symmetry) appear in the Bloch representation.

In both the above approaches degeneracy is still found in some of the subspaces.

Von Neumann and Wigner (1929) proved the following theorem: Real symmetric matrices with a multiple eigenvalue form a real algebraic variety of codimension 2 in the space of all real symmetric matrices. This implies the famous noncrossing rule, which asserts that a generic one-parameter family of real symmetric matrices contains no matrix with a multiple eigenvalue. Generic means that if the Hamilton operator admits symmetries, the underlying Hilbert space has to be decomposed into the invariant subspaces.

These degeneracies in the four-point Hubbard model indicate that higher invariants (conserved quantities) may exist.

Recently, Olmedilla and Wadati (1987) have found a Lax pair L_m and M_m for the one-dimensional Hubbard model in the Wannier representation, where m denotes a lattice site and

$$\frac{dL_m}{dt} = M_{m+1} L_m - L_m M_m$$

From the Lax representation we find that besides the constants of motion $\hat{S}_z$ and $\hat{N}_e$ we also find the higher-order conserved quantity

$$\begin{aligned}\hat{C} = \sum_{j=1}^{4} \, &[(c_{j\uparrow}^{\dagger} c_{j-1\uparrow} - c_{j-1\uparrow}^{\dagger} c_{j\uparrow})(n_{j\downarrow} + n_{j-1\downarrow}) \\ &+ (c_{j\downarrow}^{\dagger} c_{j-1\downarrow} - c_{j-1\downarrow}^{\dagger} c_{j\downarrow})(n_{j\uparrow} + n_{j-1\uparrow})] \\ &- \sum_{j=1}^{4} \sum_{\sigma} (c_{j\sigma}^{\dagger} c_{j-1\sigma} - c_{j-1\sigma}^{\dagger} c_{j\sigma})\end{aligned} \tag{4}$$

The calculation that $\hat{C}$ is a constant of motion, i.e., $[\hat{C}, \hat{H}] = 0$, is rather lengthy. The use of computer algebra is helpful. The existence of this higher-order constant of motion is related to the fact that the one-dimensional Hubbard model admits a Lax representation.

3. IMPLEMENTATION

Let us now introduce the Fermi anticommutation relations and their implementation with computer algebra. We consider a family of linear operators on a finite-dimensional vector space V,

$$c_{j\sigma}, \quad c_{j\sigma}^{\dagger}, \quad j = 1, 2, \ldots, N, \quad \sigma \in \{\uparrow, \downarrow\}$$

with

$$[c_{j\sigma}, c_{k\sigma'}]_+ = [c_{j\sigma}^{\dagger}, c_{k\sigma'}^{\dagger}]_+ = 0$$

and

$$[c_{j\sigma}, c^{\dagger}_{k\sigma'}]_+ = \delta_{jk}\delta_{\sigma\sigma'} I$$

where I is the identity operator in the finite-dimensional vector space and $k = 1, 2, \ldots, N$. The indexes j, k are the quantum numbers together with the spin σ. From the relations given above it follows that

$$(c^{\dagger}_{j\sigma})^2 = 0, \qquad (c_{j\sigma})^2 = 0, \qquad j = 1, 2, \ldots, N$$

We also have to introduce an ordering for the spin. We put all spin-up operators on the left-hand side. Furthermore, we have to introduce an ordering for the quantum number (index) j, where $j = 1, 2, \ldots, N$. We set the Fermi operators with the lower quantum number on the left-hand side, i.e., $j_1 \leqslant j_2 \leqslant \cdots \leqslant j_N$. The listing in REDUCE (Version 3.4) is given in the following program:

```
%c1(j): fermi creation operator with spin up;
%c2(j): fermi annihilation operator with spin up;
%d1(j): fermi creation operator with spin down;
%d2(j): fermi annihilation operator with spin down;

operator c1, d1, c2, d2, N, HK, HU, CL;
noncom c1, d1, c2, d2, N, HK, HU, CL;

for all j let c1(j)*c1(j) = 0;
for all j let c2(j)*c2(j) = 0;
for all j let d1(j)*d1(j) = 0;
for all j let d2(j)*d2(j) = 0;

for all j let c2(j)*c1(j) = - c1(j)*c2(j) + 1;
for all j,k such that j neq k let
c2(j)*c1(k) = - c1(k)*c2(j);

for all j let d2(j)*d1(j) = - d1(j)*d2(j) + 1;
for all j,k such that j neq k let
d2(j)*d1(k) = - d1(k)*d2(j);

for all j,k let d1(j)*c1(k) = - c1(k)*d1(j);
for all j,k let d2(j)*c2(k) = - c2(k)*d2(j);
for all j,k let d1(j)*c2(k) = - c2(k)*d1(j);
for all j,k let d2(j)*c1(k) = - c1(k)*d2(j);
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for all j,k such that j leq k let c1(j)*c1(k) = - c1(k)*c1(j);
for all j,k such that j leq k let c2(j)*c2(k) = - c2(k)*c2(j);
for all j,k such that j leq k let d1(j)*d1(k) = - d1(k)*d1(j);
for all j,k such that j leq k let d2(j)*d2(k) = - d2(k)*d2(j);

% HK: kinetic part of four point Hubbard model (10);
HK := t*(c1(2)*c2(1)+c1(3)*c2(2)+c1(4)*c2(3)+c1(1)*c2(4)
    +c1(1)*c2(2)+c1(2)*c2(3)+c1(3)*c2(4)+c1(4)*c2(1)
    +d1(2)*d2(1)+d1(3)*d2(2)+d1(4)*d2(3)+d1(1)*d2(4)
    +d1(1)*d2(2)+d1(2)*d2(3)+d1(3)*d2(4)+d1(4)*d2(1));

% HU: interacting part of four point Hubbard model (10);
HU := U*(c1(1)*c2(1)*d1(1)*d2(1)+c1(2)*c2(2)*d1(2)*d2(2)
     +c1(3)*c2(3)*d1(3)*d2(3)+c1(4)*c2(4)*d1(4)*d2(4));

% N: number operator given by (11)
N := c1(1)*c2(1)+c1(2)*c2(2)+c1(3)*c2(3)+c1(4)*c2(4)
    +d1(1)*d2(1)+d1(2)*d2(2)+d1(3)*d2(3)+d1(4)*d2(4);

% Commutator of HK and N;
r2 := HK*N - N*HK;

%constant of motion given by (14);
CL := (c1(1)*c2(4)-c1(4)*c2(1))*(d1(1)*d2(1)+d1(4)*d2(4))
     +(d1(1)*d2(4)-d1(4)*d2(1))*(c1(1)*c2(1)+c1(4)*c2(4))
     -(c1(1)*c2(4)-c1(4)*c2(1)+d1(1)*d2(4)-d1(4)*d2(1))
     +(c1(2)*c2(1)-c1(1)*c2(2))*(d1(2)*d2(2)+d1(1)*d2(1))
     +(d1(2)*d2(1)-d1(1)*d2(2))*(c1(2)*c2(2)+c1(1)*c2(1))
     -(c1(2)*c2(1)-c1(1)*c2(2)+d1(2)*d2(1)-d1(1)*d2(2))
     +(c1(3)*c2(2)-c1(2)*c2(3))*(d1(3)*d2(3)+d1(2)*d2(2))
     +(d1(3)*d2(2)-d1(2)*d2(3))*(c1(3)*c2(3)+c1(2)*c2(2))
     -(c1(3)*c2(2)-c1(2)*c2(3)+d1(3)*d2(2)-d1(2)*d2(3))
     +(c1(4)*c2(3)-c1(3)*c2(4))*(d1(4)*d2(4)+d1(3)*d2(3))
     +(d1(4)*d2(3)-d1(3)*d2(4))*(c1(4)*c2(4)+c1(3)*c2(3))
     -(c1(4)*c2(3)-c1(3)*c2(4)+d1(4)*d2(3)-d1(3)*d2(4));

%commutators;
r3 := HK*CL - CL*HK;
r4 := HU*CL - CL*HU;
```

Fig. 1. Program: Fermi operators and Hubbard model.

To summarize: We have shown that the Fermi commutation relation can be implemented with the help of computer algebra. Using computer algebra, we have demonstrated that the number operator and the operator $\hat{C}$ given by (4) are constants of motion. We can also easily show that the total momentum operator is a constant of motion of the Hamiltonian (2).

The program has been run on a 486 AT computer under DOS. Finally, we mention that the program given above can be implemented with $C++$ applying object-oriented programming (Steeb *et al.*, 1993).

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