SYMMETRIES OF AN EXTENDED HUBBARD MODEL

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Abstract. An extended Hubbard model with phonons is considered on a $D$-dimensional lattice. The symmetries of the model are studied in various cases. It is shown that for a certain choice of the parameters a superconducting $SU_q(2)$ holds as a true quantum symmetry—but only for $D = 1$.

1. Introduction

In this article we are going to study extensions of the Hubbard model on a $D$-dimensional lattice and their symmetries.

The Hubbard model was originally introduced in [1] and is the simplest model describing systems of itinerant interacting electrons in solid-state physics. Its importance is mainly due to the possibility that it may describe high-temperature superconductivity.

Since the work of Yang and Zhang [2,3] it has been known that the Hubbard model has a $SU(2) \times SU(2))/\mathbb{Z}_2$-symmetry. This symmetry is the product of two separate $SU(2)$ symmetries: a magnetic symmetry, which accounts for the (antiferro-)magnetic properties of the electron system, and a superconductive symmetry, which is supposed to give rise to superconductivity when it is broken.

A. Montorsi and M. Rasetti investigated whether the symmetry of the standard Hubbard model generalizes to a quantum group symmetry of the Hubbard model with phonons. In [4] they claim the existence of a superconductive $SU_q(2)$-quantum group symmetry and a standard magnetic $SU(2)$-symmetry for a Hubbard model with non-local phonon interaction. We were able to verify this symmetry for a particular extension of the Hubbard model, but find it to be restricted to 1-dimensional lattices. Moreover, this Quantum Symmetric Hubbard Model is not the standard Hubbard Model with Phonons.

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2. The Extended Hubbard Model

The Hamiltonian of the extended Hubbard model is given by [4,5]:

\[ H_{Hub} = H_{el}^{(loc)} + H_{ph}^{(loc)} + H_{el-ph}^{(loc)} + H_{(non-loc)} \]  

where

\[ H_{el}^{(loc)} = u \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} \]  

\[ H_{ph}^{(loc)} = \sum_i \left( \frac{\vec{p}_i^2}{2M} + \frac{1}{2} M \omega_i^2 \vec{x}_i^2 \right) \]  

\[ H_{el-ph}^{(loc)} = -\tilde{\lambda} \sum_i (n_{i\uparrow} + n_{i\downarrow}) \vec{x}_i \]  

\[ H_{(non-loc)} = \sum_{\langle i,j \rangle} \sum_{\sigma} T_{ij} a_j^{\dagger \sigma} a_{i\sigma} \]  

with \( T_{ij} = T_{ji}^\dagger \) given by

\[ T_{ij} = te^{-\hbar \zeta \vec{R}_{ij} \cdot \vec{R}_{ij}} \exp \left\{ \zeta \vec{R}_{ij} \cdot (\vec{x}_i - \vec{x}_j) + i \vec{p}_i \cdot (\vec{p}_j - \vec{p}_i) \right\} \]  

In these expressions the Hamiltonian depends on the operators \( a_{i\sigma}, a_{i\sigma}^\dagger, \vec{p}_i, \vec{x}_i \), where \( a_{i\sigma}, a_{i\sigma}^\dagger \) are fermionic annihilation/creation operators for an electron with spin \( \sigma = \{\uparrow, \downarrow\} \) at site \( i \), while \( \vec{p}_i, \vec{x}_i \) are momentum and displacement operators for an ion at site \( i \) with the usual commutation relations.

The Hamiltonian also depends on \( \vec{R}_i \) which gives the rest position of the ion at site \( i \). Note that the expression \( \vec{R}_{ij} \) always has unit modulus and that in the one-dimensional case it just amounts to a sign. \( |\vec{R}_i - \vec{R}_j| \) is the interatomic distance at equilibrium so that it does not depend on \( i, j \). In the following we will explain the various terms composing \( H_{Hub} \):

\( H_{el}^{(loc)} \) is the local electron-electron interaction and is the sum of two terms. The first one, the on-site repulsion \( u \sum_i n_{i\uparrow} n_{i\downarrow} \), is reminiscent of the Coulomb repulsion between the electrons and is determined by the parameter \( u \). The second one, the chemical potential \( -\mu \sum_{i,\sigma} n_{i\sigma} \), shows that the Hamiltonian is written in a grand-canonical formalism; the parameter \( \mu \) fixes the average number of electrons in the lattice.

\( H_{ph}^{(loc)} \) is the kinetic term for the phonons, which are described by a set of decoupled Einstein oscillators, all with the same frequency \( \omega \) and the same mass \( M \).

\( H_{el-ph}^{(loc)} \) is the local phonon-electron interaction term [6,7] with coupling constant \( \tilde{\lambda} \), which at each site gives an attractive force proportional to the number of electrons and to the ion displacement.

The crucial term is the non-local one. It is a hopping amplitude, and gives the probability that an electron can jump from one site to another one. Notice that we have retained only the nearest neighbour terms \( \langle ij \rangle \) and hence assumed negligible overlap between all other atomic orbitals. In the extended model this amplitude depends on the ion displacement and momentum, resulting in a non-local interaction between the phonons and the ions.

Let’s study different special cases of the extended Hubbard model and see which models can be recovered.
2.1 Overview of the different models contained in the extended Hubbard model.

In the following table we give a list of different models contained in the Extended Hubbard Model. A more detailed explanation follows in the remarks.

I) Hubbard Model with: $\zeta = 0$
   a) generic case: $\vec{\lambda} \neq 0, \vec{\kappa} \neq 0$
   b) with local phonon interaction: $\vec{\lambda} \neq 0, \vec{\kappa} = 0$
      $\overset{\text{Lang-Firsov-transform.}}{\implies} \overset{\text{Mean field approx.}}{\implies} \text{c) Standard Hubbard model}$
   c) no local phonon interaction: $\vec{\lambda} = 0, \vec{\kappa} \neq 0$
   d) Standard Hubbard Model plus decoupled Einstein Oscillators: $\vec{\lambda} = 0, \vec{\kappa} = 0$

II) Hubbard model with: $\zeta \neq 0$, but $\vec{\kappa} = 0$
   a) with local phonon interaction: $\vec{\lambda} \neq 0$
   b) no local phonon interaction: $\vec{\lambda} = 0$

III) General case: $\zeta \neq 0, \vec{\lambda} \neq 0, \vec{\kappa} \neq 0$

Remarks

ad I) When $\vec{\kappa} = 0, \zeta = 0$, but $\vec{\lambda} \neq 0$ (case Ib) the Hamiltonian $H_{Hub}$ can be used to describe bipolarons [8], a model in which there is only the local electron-phonon interaction. Notice that equivalently, it is possible to describe the bipolarons with a Hamiltonian of the type $H_{Hub}$ with $\vec{\lambda} = 0$, but $\vec{\kappa} \neq 0$ (case Ic). This can be done by performing a unitary transformation, the Lang-Firsov transformation [9], on $a_{i\sigma}, a_{i\sigma}^\dagger, p_i, x_i$ with a unitary operator

$$U(\vec{\kappa}) \equiv \exp \left( i \vec{\kappa} \cdot \sum_{l,\sigma} \hat{p}_l n_{l\sigma} \right).$$  \hspace{1cm} (7)

Performing a mean-field approximation on the phonon variables (when $\vec{\lambda} = 0$), one recovers the standard Hubbard model.

ad II) When $\vec{\kappa} = 0$ the Hamiltonian $H_{Hub}$ describes the Hubbard model with phonons added. To see this, remember that the hopping amplitude in (5) is originally defined by Hubbard [1] as

$$T_{ij} = \int d^3r \, \Psi^* (\vec{r} - \vec{R}_i - \vec{x}_i) \left( -\frac{\hbar^2 \nabla^2}{2m} \right) \Psi (\vec{r} - \vec{R}_j - \vec{x}_j).$$  \hspace{1cm} (8)

where $\Psi (\vec{r} - \vec{R}_i)$ is the Wannier electron wave function. $T_{ij}$ is a function only of $\vec{a}_{ij} \equiv (\vec{R}_i + \vec{x}_i) - (\vec{R}_j + \vec{x}_j)$. We approximate the Wannier electron functions with atomic orbitals, which show an asymptotic exponential decay $\Psi (\vec{r}) \sim e^{-\zeta |\vec{r}|}$ and find

$$\nabla_{\vec{a}_{ij}} T (\vec{a}_{ij}) = \int d^3r \, \zeta \frac{(\vec{r} - \vec{a}_{ij})}{|\vec{r} - \vec{a}_{ij}|} \Psi^* (\vec{r} - \vec{a}_{ij}) \frac{\hbar^2 \nabla^2}{2m} \Psi (\vec{r}).$$  \hspace{1cm} (9)

Because of the rapid exponential decay of $\Psi (\vec{r})$, we can neglect $\vec{r}$ in $|\vec{r} - \vec{a}_{ij}|$ so that [10]

$$\nabla_{\vec{a}_{ij}} T (\vec{a}_{ij}) = -\zeta \frac{\vec{a}_{ij}}{|\vec{a}_{ij}|} T (\vec{a}_{ij})$$  \hspace{1cm} (10)

which integrates to $T (\vec{a}_{ij}) = T_0 e^{-\zeta |\vec{a}_{ij}|}$. 

\[ |\vec{a}_{ij}| = |\vec{R}_i - \vec{R}_j + \vec{x}_i - \vec{x}_j| \text{ can be approximated by } |\vec{x}_i - \vec{x}_j| \ll |\vec{R}_i - \vec{R}_j| \text{ such that } [5] \]

\[ T_{ij} = t \exp \left( -\zeta \frac{|\vec{R}_i - \vec{R}_j|}{|\vec{x}_i - \vec{x}_j|} \right) \]  

(11)

with a new constant \( t = T_0 \exp(-\zeta |\vec{R}_i - \vec{R}_j|) \).

3. Symmetries of the Extended Hubbard Model

None of the terms added to Hubbard model affect the magnetic \( SU(2) \)-symmetry. Hence, in the sequel we shall only be concerned with the supercondutive symmetry of the model. Denote the Jimbo-Drinfel’d generators of \( U_q(su(2)) \) with \( X^\pm, H \). They satisfy the following commutation relations (see e.g. [11]):

\[
[H, X^{(\pm)}] = \pm 2X^{(\pm)}, \quad [X^+, X^-] = \frac{q^H - q^{-H}}{q - q^{-1}}
\]  

(12)

3.1 Local commutation relations

**Definition Local representation of the superconductive \( U_q(su(2)) \) at each site \( l \) [4]:**

\[
\rho_s(X^+) \equiv K_l^{(+)} = e^{-i\vec{\Phi} \cdot \vec{p}_l} a_l^\dagger a_l^\uparrow
\]  

(13)

\[
\rho_s(X^-) \equiv K_l^{(-)} = e^{i\vec{\Phi} \cdot \vec{p}_l} a_l a_l^\uparrow = (K_l^{(+)})^\dagger
\]  

(14)

\[
\rho_s(H) \equiv 2K_l^{(z)} = n_l^\uparrow + n_l^\downarrow - 1
\]  

(15)

The parameter \( \vec{\Phi} \) appearing in (13),(14) does not affect the \( U_q(su(2)) \)-commutation relations, and for the moment it should be regarded as a free variable, which will be determined by the commutation relations with the Hamiltonian. \( \vec{\Phi} \) can be interpreted as the parameter of a Lang-Firsov transformation [9] of the fermionic operators.

**Theorem 1. The local part of the Hamiltonian commutes with the local generators**

\[
\left[ K_l^{(+), H^{(loc)}} \right] = \left[ K_l^{(-), H^{(loc)}} \right] = \left[ K_l^{(z), H^{(loc)}} \right] = 0
\]  

(16)

if and only if the following conditions are satisfied:

\[
\Phi = \frac{2\vec{\lambda}}{\hbar M \omega^2},
\]  

(17)

\[
\mu = \frac{u}{2} - \frac{1}{4} \omega^2 H^2 \Phi^2 = \frac{u}{2} - \frac{\vec{\lambda}^2}{4M \omega^2}.
\]  

(18)

3.2 Global commutation relations

Switching signs on \( \rho_s(X^\pm) \) gives again a representation of \( U_q(su(2)) \). It is necessary to consider both representations, i.e.

\[
\rho_s^\pm(X^+) = \pm \rho_s(X^+), \quad \rho_s^\pm(X^-) = \pm \rho_s(X^-), \quad \rho_s^\pm(H) = \rho_s(H),
\]  

(19)

if the convention is chosen that fermionic operators at different sites anticommute. For each lattice site \( l \) a sign \( \sigma(l) \in \{1, -1\} \) and the associated representation \( \rho_s^{(l)} \) will be determined by the symmetry. The local commutation relations are not affected by this choice.

Further, it is necessary to fix some ordering of the lattice sites to be able to define a tensor product and hence to construct a global symmetry.
Definition: Global representation of the superconductive $U_q(su(2))$ [4]:

$$K^{(+)} = \bigotimes_l \rho^\sigma(l)(\Delta(N-1)(X^+)) = \sum_l \sigma(l) \prod_{r<l} e^{\alpha K^{(+)}_r} K^{(+)}_l \prod_{r>l} e^{-\alpha^* K^{(+)}_r}, \quad (20)$$

$$K^{(-)} = \bigotimes_l \rho^\sigma(l)(\Delta(N-1)(X^-)) = \sum_l \sigma(l) \prod_{r<l} e^{\alpha^* K^{(-)}_r} K^{(-)}_l \prod_{r>l} e^{-\alpha K^{(-)}_r}, \quad (21)$$

$$K^{(z)} = \bigotimes_l \rho^\sigma(l)(\Delta(N-1)(H)) = \sum_l K^{(z)}_l, \quad (22)$$

$\Delta$ is the coproduct of $U_q(su(2))$ (see e.g. [11]), $\alpha = \ln(q)$ is the deformation parameter, $N$ is the number of lattice sites.

Theorem 2. The non-local part of the Hamiltonian commutes with the global generators

$$\left[ K^{(+)} , H^{(non-loc)} \right] = \left[ K^{(-)} , H^{(non-loc)} \right] = \left[ K^{(z)} , H^{(non-loc)} \right] = 0 \quad (23)$$

if and only if the following conditions are satisfied for $i, j$ nearest neighbours:

$$\sigma(i) = -\sigma(j), \quad (24)$$

$$2\bar{\kappa} = \bar{\Phi}, \quad (25)$$

$$\text{Re} \alpha = -\bar{R}_{ij} \cdot \bar{\Phi} \bar{\zeta} \hbar, \quad (26)$$

$$\prod_{i<r<j} e^{\alpha K^{(z)}_r} = \prod_{i<r<j} e^{-\alpha^* K^{(z)}_r}. \quad (27)$$

Remarks to Theorem 2: Eq. (24) imposes that nearest neighbours must have opposite signs. This gives a restriction on the possible lattices, e.g. a triangular lattice is inconsistent with our conventions.

Eq. (25) fixes the parameter $\bar{\Phi}$ of (13),(14) and relates it to the parameter $\bar{\kappa}$ appearing in the Hamiltonian $H_{Hubb}$ (6). As $\bar{\kappa}$ can be interpreted as the parameter of a Lang-Firsov transformation on the Hamiltonian, while $\bar{\Phi}$ can be interpreted as the parameter of a Lang-Firsov transformation on the generators of the symmetry, eq. (25) can be interpreted as a consistency relation, requiring the same transformation to be done on the Hamiltonian and on the generators.

Eq. (26) determines the real part of the deformation parameter $\alpha$ of the quantum group. In order for such equation to make sense it is necessary to choose a lexicographic ordering of the lattice sites, so that the sign of the term $\bar{R}_{ij}$ does not depend on the particular couple $i, j$. Notice that there is no restriction on the imaginary part of the deformation parameter; we can safely choose it to be real.

Eq. (27) is trivially satisfied if $\alpha = 0$; it is a strong condition in the case $\alpha \neq 0$: It then implies for nearest neighbours $i < j$ that there cannot be a site $r$ in between them, i.e. with $i < r < j$. However, such a condition requires that the lattice on which the Hubbard model is defined is one-dimensional, and that a ordering of sites is chosen in which the sites are numbered from left to right in increasing or decreasing order.

Proof. (Sketch) The (undeformed) generator $K^{(z)}$ commutes with $H^{(non-loc)}$ given by (5) as in the classical ($q = 1$) case.
We still have to calculate
\[ K^{(+)} , H^{(\text{non-loc})} = \]
\[ t \sum_{i<j} e^{-\hbar \zeta \vec{R}_{ij}} \left\{ \left( a_{i \uparrow}^\dagger a_{i \downarrow}^\dagger a_{j \downarrow} a_{j \uparrow} + a_{i \downarrow}^\dagger a_{i \uparrow}^\dagger a_{j \uparrow} a_{j \downarrow} \right) \times \left[ Z_{ij} \left( 2 \cosh \left( \frac{1}{2} \vec{R}_{ij} \cdot \vec{\Phi} \zeta \hbar \right) - 2 \cosh \left( \frac{1}{2} \vec{R}_{ij} \cdot \vec{\Phi} \zeta \hbar + \frac{1}{2} \alpha \right) \right) \right. \]
\[ + Z_{ji} \left( 2 \cosh \left( \frac{1}{2} \vec{R}_{ij} \cdot \vec{\Phi} \zeta \hbar \right) - 2 \cosh \left( \frac{1}{2} \vec{R}_{ij} \cdot \vec{\Phi} \zeta \hbar + \frac{1}{2} \alpha \right) \right) \right] \]
\[ + \left( a_{i \uparrow}^\dagger a_{i \downarrow}^\dagger a_{j \downarrow}^\dagger a_{j \uparrow} + a_{i \downarrow}^\dagger a_{i \uparrow}^\dagger a_{j \uparrow}^\dagger a_{j \downarrow} \right) e^{\hbar \zeta \vec{R}_{ij} \cdot \vec{\Phi} \zeta \hbar} \left[ Z_{ij} \left( e^{\frac{1}{2} \alpha \ast} - 1 \right) + Z_{ji} \left( e^{-\frac{1}{2} \alpha \ast} - 1 \right) \right] \]
\[ + \left( a_{i \uparrow}^\dagger a_{i \downarrow}^\dagger a_{j \downarrow} + a_{i \downarrow}^\dagger a_{i \uparrow}^\dagger a_{j \uparrow} \right) e^{-\frac{1}{2} \vec{R}_{ij} \cdot \vec{\Phi} \zeta \hbar} \left[ Z_{ij} \left( e^{\frac{1}{2} \alpha \ast} - 1 \right) + Z_{ji} \left( e^{-\frac{1}{2} \alpha \ast} - 1 \right) \right] \]
\[ + \left( a_{i \uparrow}^\dagger a_{j \downarrow}^\dagger - a_{i \downarrow}^\dagger a_{j \uparrow}^\dagger \right) \left[ Z_{ij} e^{\hbar \zeta \vec{R}_{ij} \cdot \vec{\Phi} \zeta \hbar} + Z_{ji} e^{-\hbar \zeta \vec{R}_{ij} \cdot \vec{\Phi} \zeta \hbar} \right] \right\} \]
\[ + \sum_{l} \sum_{i<j<i<j} \sigma(l) e^{-\hbar \zeta \vec{R}_{ij} \cdot \vec{\Phi} \zeta \hbar} \prod_{r<l,r \neq i} e^{\alpha K_{r}^{(z)}} \prod_{r<l,r \neq j} e^{-\alpha \ast K_{r}^{(z)}} \times \left[ e^{\alpha K_{i}^{(z)}} e^{-\alpha \ast K_{i}^{(z)}} , e^{i \vec{\zeta} \cdot (\vec{\Phi} \zeta \hbar)} \prod_{r<i,r \neq j} e^{\alpha K_{r}^{(z)}} \prod_{r<i,r \neq j} e^{-\alpha \ast K_{r}^{(z)}} \right]. \]
\[ \text{(28)} \]

The sums containing different numbers of fermionic operators are linearly independent and must all vanish separately. (We have fixed a normal ordering for the fermionic operators.) Studying the term containing \( a_{i \uparrow}^\dagger a_{j \uparrow}^\dagger - a_{i \downarrow}^\dagger a_{j \downarrow}^\dagger \), the conditions (24)-(27) are obtained. It turns out that the same conditions guarantee that also the others sums vanish.

### 3.3 Summary

| **Classical Symmetry** | **Quantum Symmetry** |
|------------------------|-----------------------|
| \( \alpha = 0 \)       | \( \alpha \neq 0, q = \exp(\alpha) \) |
| \( D \) arbitrary      | \( D = 1 \) |
| Id), IIb): \( SU(2)_s \)-symmetry; \( \mu = \frac{u}{2} \) | III): \( SU_q(2)_s \)-symmetry; \( R \alpha = 2 \kappa \hbar \) |
| Ina): \( SU(2)_s \)-symmetry; \( \mu = u/2 - \hbar^2 \kappa^2 \omega^2 \); \( \bar{\lambda} = \hbar M \omega^2 \bar{\kappa} \) | \( \mu = u/2 - \hbar^2 \kappa^2 \omega^2 \); \( \bar{\lambda} = \hbar M \omega^2 \bar{\kappa} \) |
| Ib), Ic), IIa): no symmetry | |

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Remark: After choosing an appropriate ordering of the lattice sites for model III in the 1-dimensional case, we have set $\kappa \equiv -\vec{R}_{ij} \cdot \vec{\kappa}$. The models Ib), Ic) and IIa) have no symmetry, because the condition $2\vec{\kappa} = \frac{2\vec{\lambda}}{\hbar M \omega}$ is not satisfied.

4. Discussion

The standard Hubbard model Id) (with decoupled Einstein oscillators) and the Hubbard model IIb) without local phonon interaction ($\vec{\lambda} = 0$) have a superconductive $SU(2)_s$ symmetry at “half-filling” $\mu = u/2$. Two other models Ia), III) with local phonon interaction ($\lambda \neq 0$) have superconducting symmetries $SU(2)_s$ and $SU_q(2)_s$ respectively at $\mu = u/2 - \hbar^2 \kappa^2 M \omega^2$. It is well known [9] that a Lang-Firsov transformation can be performed on the model Ia), shifting the parameters and thereby eliminating the local phonon interaction $\vec{\lambda}$. The resulting Hamiltonian has a $SU(2)_s$-symmetry at “half-filling” $\mu = u/2$. It turns out that a Lang-Firsov transformation with the unitary operator (7) can also be used to eliminate the local electron-phonon interaction term from the Extended Hubbard Model. The parameters are shifted according to

$$\vec{\lambda} \to \vec{\lambda} - M \omega^2 \hbar \vec{\kappa}, \quad u \to u - 2\hbar \vec{\lambda} \cdot \vec{\kappa} + M \omega^2 \hbar^2 \vec{\kappa}^2, \quad \mu \to \mu + \hbar \vec{\lambda} \cdot \vec{\kappa} - 1/2 M \omega^2 \hbar^2 \vec{\kappa}^2$$

and the hopping term $H_{el-ph}^{(non-loca)}$ becomes

$$t \sum_{(i<j),\sigma} e^{i\vec{R}_{ij} \cdot (\vec{\xi}_i - \vec{\xi}_j)} q^{\frac{j}{2}} a_{j\sigma}^\dagger a_{i\sigma} \left(1 + (q^{\frac{-j}{2}} - 1)n_{i,-\sigma}\right) \left(1 + (q^{\frac{j}{2}} - 1)n_{j,-\sigma}\right) + h.c.$$ (30)

The resulting Hamiltonian has a superconducting $SU_q(2)_s$ quantum symmetry at “half filling” $\mu = u/2$ (!) with $\vec{\lambda} = 0$ and only for $D = 1$.

It is even possible to eliminate all phonon terms from this Quantum Symmetric Hamiltonian by a mean field approximation [8,9] without breaking the quantum symmetry. More precisely one performs a thermal average over $H_{ph}$-eigenstates and assumes uncorrelated Einstein oscillators (note that $\vec{\lambda} = 0$ !). The exponential in the hopping term is then approximated by a temperature-dependent constant.

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