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On quantum groups in the Hubbard model with phonons

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Abstract. The correct Hamiltonian for an extended Hubbard model with quantum group symmetry as introduced by Montorsi and Rasetti is derived for a D-dimensional lattice. It is shown that the superconducting $SU_q(2)$ holds as a true quantum symmetry only for $D = 1$ and that terms of higher order in the fermionic operators are needed in addition to phonons. A discussion of quantum symmetries in general is given in a formalism that should be readily accessible to non-Hopf algebraists.

1. Introduction

The Hubbard model is the simplest description of itinerant interacting electron systems. In this article we will study generalizations of it on a D-dimensional lattice. The Hamiltonian of the standard Hubbard model is given by [1]

$$H_{\mathrm{Hub}} = H_{\mathrm{el}}^{(\mathrm{non-loc})} + H_{\mathrm{el}}^{(\mathrm{loc})} \tag{1.1}$$

where

$$H_{\mathrm{el}}^{(\mathrm{non-loc})} = -t \sum_{\langle i,j\rangle,\sigma} b_{i\sigma}^{\dagger} b_{j\sigma} \tag{1.2}$$

$$H_{\mathrm{el}}^{(\mathrm{loc})} = u \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma}. \tag{1.3}$$

The one-dimensional model has been solved in [2]. It is well known that the Hubbard model has a $(SU(2) \times SU(2))/\mathbb{Z}_2$ symmetry [3, 4]. This symmetry is the product of two separate $SU(2)$ symmetries: a magnetic and a superconductive one.

Montorsi and Rasetti [5] have introduced a very interesting generalization of the Hubbard model by adding phonons. It turns out that the symmetry of the standard Hubbard model is sometimes a special case of a more general quantum group symmetry. More precisely, while the 'magnetic' $SU(2)$ symmetry is left unchanged, Montorsi and Rasetti claimed that the generators of a 'superconductive' $SU_q(2)$ quantum group commute with their extended Hamiltonian. We were able to verify this symmetry for an extended Hubbard model on a one-dimensional lattice†, while we found unsurmountable obstructions in the higher dimensional case. As we will show this is essentially due to ordering problems. Our task in this article is twofold: we will address quantum symmetries in general and we will carefully re-examine the Hubbard model with phonons, deriving each term on physical grounds to obtain the correct Hamiltonian.

† The Hamiltonian in [5] is given *explicitly* only in the one-dimensional case.

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2. Quantum symmetries in quantum mechanics

The role of symmetries in quantum mechanics cannot be underestimated. Some models (harmonic oscillator, hydrogen atom) were in fact first solved relying only on symmetries. Symmetries, especially infinite dimensional ones, serve to provide the constants of motion that are central to integrable models.

It is interesting to see what happens when the usual notion of symmetry is relaxed and transformations given by a Hopf algebra (quantum group) are considered.

To simplify the discussion we will use a formalism that avoids direct reference to Hopf algebraic methods. As given data we take a $*$-Hopf algebra $\mathcal{U}$, its dual Hopf algebra $\mathcal{U}^*$ and a $*$-algebra $\mathcal{A}$ generated by quantum mechanical operators that act on a Hilbert space $\mathcal{H}$. The generators of quantum symmetry transformations exist in $\mathcal{U}$. Here we typically have a one or more parameter deformation of the universal enveloping algebra of a Lie algebra in mind. The elements of the dual Hopf algebra $\mathcal{U}^*$ play the role of functions on the quantum group. The only difference to the classical case is that these functions no longer commute.

2.1. Unitary representation

The elements of $\mathcal{U}$ should act on $\mathcal{H}$. We need a unitary representation ρ on $\mathcal{H}$ that realizes $\mathcal{U}$ in the operator algebra $\mathcal{A}$. Such a representation shall be a linear $*$-preserving map

$$\rho : \mathcal{U} \to \mathcal{A} \qquad \rho(x) : \mathcal{H} \to \mathcal{H} \qquad \rho(x)^\dagger = \rho(x^*) \tag{2.1}$$

that is also an algebra homomorphism†

$$\rho(xy) = \rho(x)\rho(y). \tag{2.2}$$

Here is an example:

Magnetic and superconductive $SU_{(q)}(2)$. The algebra of $SU_q(2)$ is generated by X^+, $X^- = (X^+)^*$ and $H = H^*$ with deformed commutation relations

$$[H, X^\pm] = \pm 2X^\pm \qquad [X^+, X^-] = \frac{q^H - q^{-H}}{q - q^{-1}} \qquad q \in \mathbb{R}\backslash\{0\}. \tag{2.3}$$

As can be checked by direct computation this algebra has the same representation by 2×2 matrices as the undeformed $SU(2)$, namely

$$X^+ \mapsto \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad X^- \mapsto \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad H \mapsto \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.4}$$

From this matrix representation we can find a unitary representation of the algebra (2.3) by creation and annihilation operators using the following simple observation:

Let $c_i^\dagger$, c_i be fermionic or bosonic creation and annihilation operators and m_{ij}, n_{ij} numerical matrices with the same (finite) index set as the $c^\dagger$, c, then $[c^\dagger \cdot m \cdot c, c^\dagger \cdot n \cdot c] = c^\dagger \cdot [m; n] \cdot c$.

If we take for instance $c_i^\dagger \in \{b_\uparrow^\dagger, b_\downarrow^\dagger\}$ and $c_i \in \{b_\uparrow, b_\downarrow\}$ and the matrices from (2.4) we find the generators of the 'magnetic' $SU(2)$:

$$\rho_m(X^+) = {b_\uparrow}^\dagger b_\downarrow \qquad \rho_m(X^-) = {b_\downarrow}^\dagger b_\uparrow \qquad \rho_m(H) = ({b_\uparrow}^\dagger b_\uparrow - {b_\downarrow}^\dagger b_\downarrow). \tag{2.5}$$

Switching ${b_\downarrow}^\dagger \leftrightarrow b_\downarrow$ does not change the algebra of the $c^\dagger$, c (the $b^\dagger$, b are fermionic!) but gives another unitary representation—the 'superconductive' $SU_{(q)}(2)$:

$$\rho_s(X^+) = {b_\uparrow}^\dagger {b_\downarrow}^\dagger \qquad \rho_s(X^-) = b_\downarrow b_\uparrow \qquad \rho_s(H) = ({b_\uparrow}^\dagger b_\uparrow + {b_\downarrow}^\dagger b_\downarrow - 1). \tag{2.6}$$

† *Remark.* $\rho(x)\rho(y) = \rho(z) \Leftrightarrow \rho(z) = \rho(xy) \Leftarrow z = xy$, but *not*: '$\Rightarrow z = xy$'.

(These expressions hold also for $q \neq 1$ because $[\rho_{m/s}(H)]^3 = \rho_{m/s}(H)$.) These generators implement both (local) $SU(2)$ and (local) $SU_q(2)$ for a *single lattice site*. When we deal with generators that act on the *whole lattice* the 'q' reappears and consequently (global) $SU(2)$ and (global) $SU_q(2)$ no longer coincide.

Note. In the following we will not write the symbol 'ρ' explicitly; its presence is implied by context.

2.2. Transformation of states and operators

The key to a simple description of quantum symmetries is the canonical element of $\mathcal{U} \otimes \mathcal{U}^*$ sometimes also called the 'universal T' [6]

$$\mathcal{C} \equiv \sum_i e_i \otimes f^i \in \mathcal{U} \otimes \mathcal{U}^*. \tag{2.7}$$

Here e_i and f^i are (formal) dual linear bases of $\mathcal{U}$ and $\mathcal{U}^*$ respectively. Everything else we need to know about $\mathcal{C}$ here is that it is invertible and unitary:

$$\mathcal{C}^* \equiv \sum_i e_i^* \otimes f^{i*} = \mathcal{C}^{-1}. \tag{2.8}$$

States $|\psi\rangle \in \mathcal{H}$ corresponding to a single site† transform via multiplication by $\mathcal{C}$:

$$|\psi\rangle \mapsto \mathcal{C}|\psi\rangle. \tag{2.9}$$

Operators $\mathcal{O} \in \mathcal{A}$ consequently transform by conjugation

$$\mathcal{O} \mapsto \mathcal{C}\mathcal{O}\mathcal{C}^{-1} = \mathcal{C}\mathcal{O}\mathcal{C}^*. \tag{2.10}$$

States and operators can have full quantum symmetries, i.e. they can be invariant under all of $\mathcal{U}$. This is the case if respectively:

$$\begin{aligned} &\mathcal{C}|\psi\rangle = 1 \cdot |\psi\rangle \\ &\mathcal{C}\mathcal{O}\mathcal{C}^{-1} = \mathcal{O} \cdot 1 \end{aligned} \qquad \text{(conditions for } \textit{full} \text{ symmetry)}. \tag{2.11}$$

When we deal with a lattice, there is a $\mathcal{C}_i$ for each of its sites i. Transformations of several sites (the whole lattice), i.e. of states $|\psi^{(N)}\rangle \in \mathcal{H}^{\otimes N}$ and operators $\mathcal{O}^{(N)} \in \mathcal{A}^{\otimes N}$, are also possible. These are performed with products (in the function part) of the $\mathcal{C}_i$,

$$\mathcal{C}^{(N)} = \mathcal{C}_1\mathcal{C}_2 \ldots \mathcal{C}_N \equiv \sum_{i_1,i_2,\ldots,i_N} e_{i_1} \otimes e_{i_2} \otimes \ldots \otimes e_{i_N} \otimes f^{i_1} f^{i_2} \ldots f^{i_N} \tag{2.12}$$

so that

$$|\psi^{(N)}\rangle \mapsto \mathcal{C}^{(N)}|\psi^{(N)}\rangle \qquad \mathcal{O}^{(N)} \mapsto \mathcal{C}^{(N)}\mathcal{O}^{(N)}(\mathcal{C}^{(N)})^{-1} \tag{2.13}$$

with $(\mathcal{C}^{(N)})^{-1} = \mathcal{C}_N^{-1}\mathcal{C}_{N-1}^{-1} \ldots \mathcal{C}_1^{-1}$. Note that the order of the $\mathcal{C}_i$ in $\mathcal{C}^{(N)}$ is important because the f^i (in the function part of $\mathcal{C}$) are not commutative by assumption for a quantum group.

2.3. Full quantum symmetry

In the following sections we will be interested in quantum symmetries of the Hamiltonian. A Hamiltonian $h \in \mathcal{A}$ has a full 'local' symmetry under $\mathcal{U}$ (at site i) if

$$\mathcal{C}_i h \mathcal{C}_i^{-1} = h \cdot 1. \tag{2.14}$$

It consequently has a full 'global' symmetry under $\mathcal{U}$ (on the whole lattice) if

$$\mathcal{C}^{(N)} h (\mathcal{C}^{(N)})^{-1} = \mathcal{C}_1\mathcal{C}_2 \ldots \mathcal{C}_N h \mathcal{C}_N^{-1}\mathcal{C}_{N-1}^{-1} \ldots \mathcal{C}_1^{-1} = h \cdot 1. \tag{2.15}$$

† Statements for 'single sites' and 'multiple sites' of a lattice obviously apply also to a broader context of tensor products of states—for instance to single/multi-particle states.

In this formalism it is very easy to see that both conditions can also be expressed in terms of commutators, namely

$$[\mathcal{C}_i, h] = 0 \qquad \text{and} \qquad [\mathcal{C}^{(N)}, h] = 0 \tag{2.16}$$

respectively.

2.4. Specified transformations

Often it is important to describe transformations given by specific elements of the Hopf algebra $\mathcal{U}$. So far the transformations were unspecific; their result still contained a part in $\mathcal{U}^*$, i.e. a 'function on the quantum group'; for example

$$\mathcal{C}|\psi\rangle \equiv \sum_i \rho(e_i)|\psi\rangle \otimes f^i \in \mathcal{H} \otimes \mathcal{U}^* \qquad \text{and similarly} \qquad \mathcal{C}\mathcal{O}\mathcal{C}^{-1} \in \mathcal{A} \otimes \mathcal{U}^*. \tag{2.17}$$

A transformation specified by an element $\kappa \in \mathcal{U}$ is obtained by evaluating these function parts on κ; this operation will be denoted by '$|_\kappa$'. (You may think of it as 'plugging-in' of the transformation parameters.) The action (denoted by '$\triangleright$') of κ on a state $|\psi\rangle$ is then given by

$$\kappa \triangleright |\psi\rangle = \mathcal{C}|_\kappa \, |\psi\rangle = \kappa|\psi\rangle \equiv \rho(\kappa)|\psi\rangle \tag{2.18}$$

simply because $\mathcal{C}$—being the canonical element—satisfies $\mathcal{C}|_\kappa = \sum_i e_i \cdot f^i(\kappa) = \kappa$ by definition. Similarly

$$\kappa \triangleright \mathcal{O} = \mathcal{C}\mathcal{O}\mathcal{C}^{-1}|_\kappa \tag{2.19}$$

$$\kappa \triangleright |\psi^{(N)}\rangle = \mathcal{C}^{(N)}|_\kappa |\psi^{(N)}\rangle \tag{2.20}$$

$$\kappa \triangleright \mathcal{O}^{(N)} = \mathcal{C}^{(N)}\mathcal{O}^{(N)}(\mathcal{C}^{(N)})^{-1}|_\kappa. \tag{2.21}$$

The result of contracting the function part of $\mathcal{C}^{(N)} = \mathcal{C}_1\mathcal{C}_2 \ldots \mathcal{C}_N$ with κ gives a prescription (denoted by $\Delta^{(N-1)}(\kappa)$ and called the $(N-1)$-fold coproduct†) how to distribute κ over several tensor factors:

$$\mathcal{C}^{(N)}|_\kappa = \Delta^{(N-1)}(\kappa) \in \mathcal{U}^{\otimes N}. \tag{2.22}$$

It is clear that there cannot be one simple rule for all of $\mathcal{U}$—not even in the classical case; $\Delta(\kappa) = \kappa \otimes 1 + 1 \otimes \kappa$ for instance holds only for 'infinitesimal' κ. The added difference of the quantum case is that then $\Delta(\kappa)$ will in general be not symmetric.

† The coproduct Δ did not enter the formalism as additional input here; it rather follows from Hopf algebra axioms that

$$\mathcal{C}_1\mathcal{C}_2|_\kappa \equiv \sum_{i,j} e_i \otimes e_j \otimes (f^i f^j)(\kappa) = \sum_k \Delta(e_k) \otimes f^k(\kappa) = \Delta(\kappa)$$

$$\mathcal{C}_1\mathcal{C}_2\mathcal{C}_3|_\kappa = (\Delta \otimes id)\Delta(\kappa) = (id \otimes \Delta)\Delta(\kappa) =: \Delta^{(2)}(\kappa)$$

$$\vdots$$

$$\mathcal{C}_1\mathcal{C}_2 \ldots \mathcal{C}_N|_\kappa = \Delta^{(N-1)}(\kappa).$$

The coproducts of a given Hopf algebra are part of the defining relations. Here are the coproducts for the generators of the algebra (2.3):

$$\Delta(H) = H \otimes 1 + 1 \otimes H \qquad \Delta(X^\pm) = X^\pm \otimes q^{-H/2} + q^{H/2} \otimes X^\pm.$$

Coproducts of other elements can be computed from this using the fact that Δ is an algebra homomorphism. The other objects that constitute a Hopf algebra are the antipode S and the co-unit ϵ. They enter our formalism via $\mathcal{C}^{-1}|_\kappa = S(\kappa)$ and $1|_\kappa = \epsilon(\kappa)$. Note that $\epsilon(\kappa)$ is a number. Let $\Delta(\kappa) \equiv \kappa_{(1)} \otimes \kappa_{(2)}$; then $\mathcal{C}\mathcal{O}\mathcal{C}^{-1}|_\kappa = \sum_{i,j} \rho(e_i)\mathcal{O}\rho(Se_j) \otimes (f^i f^j)(\kappa) = \rho(\kappa_{(1)})\mathcal{O}\rho(S\kappa_{(2)})$. This action and Hopf expressions corresponding to equations (2.20)–(2.21) are discussed in [7], for example.

2.5. Partial quantum symmetry

The full quantum symmetries (2.14) and (2.15) are equivalent to

$$\mathcal{C}_i h \mathcal{C}_i^{-1}|_\kappa = h \cdot 1_\kappa \ \forall \kappa \in \mathcal{U} \qquad \text{and} \qquad \mathcal{C}^{(N)} h (\mathcal{C}^{(N)})^{-1}|_\kappa = h \cdot 1_\kappa \ \forall \kappa \in \mathcal{U} \tag{2.23}$$

respectively. We have seen that these full symmetries could be expressed in terms of commutators. As a further illustration of the formalism we will briefly study the case where κ does not range over all of $\mathcal{U}$ but only over a subset $\mathcal{P} \subset \mathcal{U}$. The question is: when is

$$\mathcal{C} h \mathcal{C}^{-1}|_\kappa = h \cdot 1|_\kappa \qquad \forall \kappa \in \mathcal{P} \qquad (\textit{partial} \text{ quantum symmetry}) \tag{2.24}$$

equivalent to

$$[\mathcal{C}, h]|_\kappa = 0 \qquad \forall \kappa \in \mathcal{P} \tag{2.25}$$

for an arbitrary Hamiltonian h? A sufficient condition is easily seen to be

$$A\mathcal{C}|_\kappa = 0 \Leftrightarrow A \cdot 1|_\kappa = 0 \qquad \forall \kappa \in \mathcal{P} \tag{2.26}$$

for all operators A ($\in \mathcal{A} \otimes \mathcal{U}^*$). This can be translated into a condition on the coproducts of elements in $\mathcal{P}$:

$$\Delta(\mathcal{P}) \subset \mathcal{P} \otimes \mathcal{U}. \tag{2.27}$$

3. A generalized Hubbard model

Following [5] we will retain the local electron term (1.3), and add to it the standard Hamiltonian for the phonons and a phonon–electron interaction term

$$H_{\text{Hub}} = H_{\text{el}}^{(\text{loc})} + H_{\text{ph}} + H_{\text{el-ph}}. \tag{3.1}$$

We suppose that the phonons are described by a set of decoupled Einstein oscillators with the same frequency ω

$$H_{\text{ph}} = \sum_i \left(\frac{\boldsymbol{p}_i^2}{2M} + \tfrac{1}{2} M \omega^2 \boldsymbol{y}_i^2 \right) \tag{3.2}$$

where $\boldsymbol{p}_i$ and $\boldsymbol{y}_i$ obey canonical commutation relations as usual. The expression for the phonon–electron term is the one given by Hubbard [1]

$$H_{\text{el-ph}} = \sum_{ij} \sum_\sigma \int \mathrm{d}^D r \, \Psi^*(\boldsymbol{r} - \boldsymbol{R}_i) \left(-\frac{\hbar^2 \nabla^2}{2m} + V(\boldsymbol{r}, \{\boldsymbol{R}_l\}) \right) \Psi(\boldsymbol{r} - \boldsymbol{R}_j) b_{j\sigma}^\dagger b_{i\sigma} \tag{3.3}$$

where $\Psi(\boldsymbol{r} - \boldsymbol{R}_i)$ is the Wannier electron wavefunction centred around the ion at $\boldsymbol{R}_i$, while $b_{j\sigma}^\dagger$, $b_{i\sigma}$ are fermionic creation and annihilation operators. (In this context the Wannier functions will be approximated by atomic orbitals.) To take account of the ion oscillations around their equilibrium positions, the arguments of the Wannier functions and of the potential V in the integral must be shifted:

$$\boldsymbol{R}_k \to \boldsymbol{R}_k + \boldsymbol{y}_k \qquad (k = i, j, l).$$

The term obtained from the potential V in (3.3) has a significant contribution only for $i = j = l$ (i.e. neglecting all $\boldsymbol{R}_l$ with $l \neq i$ in V) and results by linear variation in a local electron–phonon interaction term [8, 9]

$$H_{\text{el-ph}}^{(\text{loc})} = -\boldsymbol{\lambda} \cdot \sum_i (n_{i\uparrow} + n_{i\downarrow}) \boldsymbol{y}_i \tag{3.4}$$

and a term that contributes to μ in (1.3). The non-local electron–phonon interaction term is crucial in the approach of Montorsi and Rasetti. We would like to give a derivation leading

directly to the exponential form, which is necessary for the quantum symmetry. (See [10] for the derivation of a linear approximation.)

We shall retain only the nearest-neighbour terms $\langle ij\rangle$ in the kinetic energy term of (3.3); this assumes negligible overlap between all other atomic orbitals:

$$H_{\text{el}-\text{ph}}^{(\text{non-loc})} = \sum_{\langle i,j\rangle} T_{ij} b_{j\sigma}^{\dagger} b_{i\sigma} \tag{3.5}$$

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

$$T_{ij} = \int \mathrm{d}^D r\, \Psi^*(\boldsymbol{r} - \boldsymbol{R}_i - \boldsymbol{y}_i) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \Psi(\boldsymbol{r} - \boldsymbol{R}_j - \boldsymbol{y}_j). \tag{3.6}$$

Assuming that Ψ has finite support, it is possible to shift the integration variable

$$\boldsymbol{r} \to \boldsymbol{r} - \boldsymbol{R}_j - \boldsymbol{y}_j.$$

With this substitution T_{ij} becomes a function only of $\boldsymbol{a}_{ij} \equiv (\boldsymbol{R}_i + \boldsymbol{y}_i) - (\boldsymbol{R}_j + \boldsymbol{y}_j)$:

$$T_{ij} = \int \mathrm{d}^D r\, \Psi^*(\boldsymbol{r} - \boldsymbol{a}_{ij}) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \Psi(\boldsymbol{r}) = T(\boldsymbol{a}_{ij}). \tag{3.7}$$

The atomic orbitals show an asymptotic exponential decay

$$\Psi(\boldsymbol{r}) \sim \mathrm{e}^{-\zeta|\boldsymbol{r}|} \tag{3.8}$$

and we have hence (approximately)

$$\nabla_{\boldsymbol{a}_{ij}} T(\boldsymbol{a}_{ij}) = \int \mathrm{d}^D r\, \zeta \frac{(\boldsymbol{r} - \boldsymbol{a}_{ij})}{|\boldsymbol{r} - \boldsymbol{a}_{ij}|} \Psi^*(\boldsymbol{r} - \boldsymbol{a}_{ij}) \frac{\hbar^2\nabla^2}{2m} \Psi(\boldsymbol{r}). \tag{3.9}$$

Again, due to the rapid exponential decay of $\Psi(\boldsymbol{r})$, we can neglect $\boldsymbol{r}$ in $|\boldsymbol{r} - \boldsymbol{a}_{ij}|$ so that

$$\nabla_{\boldsymbol{a}_{ij}} T(\boldsymbol{a}_{ij}) = -\zeta \frac{\boldsymbol{a}_{ij}}{|\boldsymbol{a}_{ij}|} T(\boldsymbol{a}_{ij}) \tag{3.10}$$

which integrates to

$$T(\boldsymbol{a}_{ij}) = T_0 \mathrm{e}^{-\zeta|\boldsymbol{a}_{ij}|}. \tag{3.11}$$

$|\boldsymbol{a}_{ij}| = |\boldsymbol{R}_i - \boldsymbol{R}_j + \boldsymbol{y}_i - \boldsymbol{y}_j|$ can be expanded using $|\boldsymbol{y}_i - \boldsymbol{y}_j| \ll |\boldsymbol{R}_i - \boldsymbol{R}_j|$ such that finally

$$T_{ij} = t \exp\left(-\zeta \frac{(\boldsymbol{R}_i - \boldsymbol{R}_j)}{|\boldsymbol{R}_i - \boldsymbol{R}_j|} (\boldsymbol{y}_i - \boldsymbol{y}_j)\right) \tag{3.12}$$

with a new constant $t = T_0 \exp(-\zeta|\boldsymbol{R}_i - \boldsymbol{R}_j|)$. Note that the term

$$\boldsymbol{R}_{ij} \equiv -\frac{(\boldsymbol{R}_i - \boldsymbol{R}_j)}{|\boldsymbol{R}_i - \boldsymbol{R}_j|}$$

always has the same module and that in the one-dimensional case it just amounts to a sign. $|\boldsymbol{R}_i - \boldsymbol{R}_j|$ is the interatomic distance at equilibrium so that it does not depend on i, j. The complete non-local electron–phonon interaction term in the Hamiltonian is

$$H_{\text{el}-\text{ph}}^{(\text{non-loc})} = t \sum_{\langle i,j\rangle} \sum_{\sigma} \exp\{\zeta \boldsymbol{R}_{ij} \cdot (\boldsymbol{y}_i - \boldsymbol{y}_j)\} b_{j\sigma}^{\dagger} b_{i\sigma} \tag{3.13}$$

and the full Hamiltonian of the Hubbard model with phonons is

$$\begin{aligned} H_{\text{Hub}} = {} & u \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} + \sum_i \left(\frac{\boldsymbol{p}_i^2}{2M} + \frac{1}{2} M\omega^2 \boldsymbol{y}_i^2\right) - \boldsymbol{\lambda} \cdot \sum_i (n_{i\uparrow} + n_{i\downarrow}) \boldsymbol{y}_i \\ & + \left(t \sum_{\langle i<j\rangle} \sum_{\sigma} \exp\{\zeta \boldsymbol{R}_{ij} \cdot (\boldsymbol{y}_i - \boldsymbol{y}_j)\} b_{j\sigma}^{\dagger} b_{i\sigma} + \text{HC}\right). \end{aligned} \tag{3.14}$$

The Hamiltonian considered in [5] is formally obtained (in the one-dimensional case—see the remark below) from (3.14) by a similarity transformation (half of a Lang–Firsov transformation [11]) on the fermionic operators $b^\dagger_{j\sigma}$ and $b_{i\sigma}$ only:

$$a_{i\sigma} \equiv U(\boldsymbol{\kappa}) b_{i\sigma} U^{-1}(\boldsymbol{\kappa}) \tag{3.15}$$

$$a^\dagger_{j\sigma} \equiv U(\boldsymbol{\kappa}) b^\dagger_{j\sigma} U^{-1}(\boldsymbol{\kappa}) \tag{3.16}$$

with a unitary operator

$$U(\boldsymbol{\beta}) \equiv \exp\left(\mathrm{i}\boldsymbol{\beta} \cdot \sum_{l,\sigma} \boldsymbol{p}_l n_{l\sigma}\right) \tag{3.17}$$

that commutes with the generators of *magnetic* $SU(2)$ and depends on a set of constant parameters β^k, $k = 1, \ldots, D$. While this transformation does not change the number operators $n_{l\uparrow}$ and $n_{l\downarrow}$, it results in an exponential factor in $\boldsymbol{p}_i - \boldsymbol{p}_j$ for

$$b^\dagger_{j\sigma} b_{i\sigma} = \exp[\mathrm{i}\boldsymbol{\kappa} \cdot (\boldsymbol{p}_i - \boldsymbol{p}_j)] a^\dagger_{j\sigma} a_{i\sigma} \tag{3.18}$$

so that the hopping term is now given by

$$H^{(\text{non-loc})}_{\text{el}-\text{ph}} = t \sum_{\langle i<j\rangle} \sum_{\sigma} \exp\{\zeta \boldsymbol{R}_{ij} \cdot (\boldsymbol{y}_i - \boldsymbol{y}_j)\} \exp\{\mathrm{i}\boldsymbol{\kappa} \cdot (\boldsymbol{p}_i - \boldsymbol{p}_j)\} a^\dagger_{j\sigma} a_{i\sigma} + \text{HC} \tag{3.19}$$

or, combining the exponentials,

$$H^{(\text{non-loc})}_{\text{el}-\text{ph}} = t \sum_{\langle i<j\rangle} \sum_{\sigma} \exp[-\hbar\zeta \boldsymbol{R}_{ij} \cdot \boldsymbol{\kappa}] \exp\{\zeta \boldsymbol{R}_{ij} \cdot (\boldsymbol{y}_i - \boldsymbol{y}_j) + \mathrm{i}\boldsymbol{\kappa} \cdot (\boldsymbol{p}_i - \boldsymbol{p}_j)\} a^\dagger_{j\sigma} a_{i\sigma} + \text{HC}. \tag{3.20}$$

Remark. Note that while the $\boldsymbol{y}_i$ commute with $b^\dagger_{i\sigma}$, $b_{i\sigma}$, they do not commute with the new fermionic creation and annihilation operators $a^\dagger_{i\sigma}$, $a_{i\sigma}$ as defined in (3.15), (3.16). The authors of [5], however, assumed commutativity between the fermionic operators and coordinates of the ions. In order to be able to connect to their work we will formally replace the $\boldsymbol{y}_i$ in H_{Hub} with new coordinates $\boldsymbol{x}_i$ that do commute with the $a^\dagger_{i\sigma}$, $a_{i\sigma}$. (The $\boldsymbol{x}_i$ will hence no longer commute with the $b^\dagger_{i\sigma}$, $b_{i\sigma}$.) This will of course modify the Hamiltonian. The Hamiltonian that we *will* work with in the next section is:

$$H = H^{(\text{loc})} + H^{(\text{non-loc})} \tag{3.21}$$

with

$$H^{(\text{loc})} = u \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} + \sum_i \left(\frac{\boldsymbol{p}_i^2}{2M} + \frac{1}{2} M\omega^2 \boldsymbol{x}_i^2\right) - \boldsymbol{\lambda} \cdot \sum_i (n_{i\uparrow} + n_{i\downarrow}) \boldsymbol{x}_i \tag{3.22}$$

$$H^{(\text{non-loc})} = t \sum_{\langle i<j\rangle} \sum_{\sigma} \exp\{\zeta \boldsymbol{R}_{ij} \cdot (\boldsymbol{x}_i - \boldsymbol{x}_j)\} \exp\{\mathrm{i}\boldsymbol{\kappa} \cdot (\boldsymbol{p}_i - \boldsymbol{p}_j)\} a^\dagger_{j\sigma} a_{i\sigma} + \text{HC}. \tag{3.23}$$

The relation of this Hamiltonian with the one of the Hubbard model with phonons (3.14) will be discussed in section 5. The fact that H_{Hub} and H are inequivalent can, for instance, be seen by noting that the expression

$$\tilde{T}_{ij} = t \exp\{\zeta \boldsymbol{R}_{ij} \cdot (\boldsymbol{x}_i - \boldsymbol{x}_j)\} \exp\{\mathrm{i}\boldsymbol{\kappa} \cdot (\boldsymbol{p}_i - \boldsymbol{p}_j)\}$$

for the hopping amplitude in (3.23) does not satisfy the condition $\tilde{T}_{ji} = \tilde{T}^\dagger_{ij}$ so that $\sum_{\langle i,j\rangle} \tilde{T}_{ij} a^\dagger_{j\sigma} a_{i\sigma}$ is no longer Hermitean.

4. Superconductive $U_q su(2)$

The local superconductive $U_q(su(2))$ is given by

$$\rho_s(X^+) = K_l^{(+)} = b_{l\uparrow}^\dagger b_{l\downarrow}^\dagger = \exp(-\mathrm{i}\boldsymbol{\Phi}\cdot\boldsymbol{p}_l) a_{l\uparrow}^\dagger a_{l\downarrow}^\dagger \tag{4.1}$$

$$\rho_s(X^-) = K_l^{(-)} = b_{l\downarrow} b_{l\uparrow} = \exp(\mathrm{i}\boldsymbol{\Phi}\cdot\boldsymbol{p}_l) a_{l\downarrow} a_{l\uparrow} = (K_l^{(+)})^\dagger \tag{4.2}$$

$$\rho_s(H) = 2K_l^{(z)} = n_{l\uparrow} + n_{l\downarrow} - 1. \tag{4.3}$$

These are the generators for transformations of an individual lattice site l, as defined in (2.6). They are expressed in terms of the operators $b_{l\sigma}, b_{l\sigma}^\dagger$. In order to compute the commutation relations with Hamiltonian (3.21) it is necessary to express them in terms of operators $a_{l\sigma}, a_{l\sigma}^\dagger$ as introduced in (3.15) and (3.16). The parameter $\boldsymbol{\beta}$ appearing in (3.17), on which the transformation depends, is chosen here to be $\boldsymbol{\Phi}/2$ and, for the moment, it should be regarded as a free parameter which will be determined by the commutation relations. We will see later (4.33) that consistently with the choice $\boldsymbol{\beta} = \boldsymbol{\kappa}$ made in equations (3.15) and (3.16), the commutation relations will require $\boldsymbol{\Phi} = 2\boldsymbol{\kappa}$. (Notice that $n_{l\sigma} = a_{l\sigma}^\dagger a_{l\sigma} = b_{l\sigma}^\dagger b_{l\sigma}$.)

To describe the symmetries of the Hubbard model with phonons it is necessary to consider two distinct representations of the superconductive $U_q(su(2))$ for different lattice sites. One (ρ_s^+) is equal to ρ_s, the other (ρ_s^-) differs from ρ_s by a minus sign on the generators $X^\pm$:

$$\rho_s^\pm(X^+) = \pm\rho_s(X^+) \qquad \rho_s^\pm(X^-) = \pm\rho_s(X^-) \qquad \rho_s^\pm(H) = \rho_s(H). \tag{4.4}$$

For each lattice site l a sign $\sigma(l) \in \{1, -1\}$ is chosen and the representation ρ_s^+ or ρ_s^- is associated to it depending on whether $\sigma(l) = 1$ or $\sigma(l) = -1$ respectively. The local commutation relations are not affected by this choice. The sign will, however, be crucial for the global commutation relations. Hence, for the moment we will not specify a rule for assigning a representation to a given site, but we will see later (4.29) that sites corresponding to nearest neighbours must have opposite representations ρ^+ and ρ^-. This is exactly what happens in the classical case [3]. For orthogonal (square) lattices a choice of the sign which implements this condition is

$$\sigma(l) = (-1)^{\|l\|} \tag{4.5}$$

where $\|l\| = \sum_{n=1}^D l_n$ is the length of the index l which labels the site l.

For the moment we will choose an arbitrary ordering of the lattice sites. Choosing an ordering is necessary to be able to define a tensor product and hence to construct a global symmetry. According to the definition of the coproduct in $U_q(su(2))$ (see equation (2.22) and footnote on p 848)

$$\Delta(X^+) = \mathrm{e}^{\frac{1}{2}\alpha H} \otimes X^+ + X^+ \otimes \mathrm{e}^{-\frac{1}{2}\alpha^* H} \tag{4.6}$$

$$\Delta(X^-) = \mathrm{e}^{\frac{1}{2}\alpha^* H} \otimes X^- + X^- \otimes \mathrm{e}^{-\frac{1}{2}\alpha H} = (\Delta(X^+))^\dagger \tag{4.7}$$

$$\Delta(H) = H \otimes 1 + 1 \otimes H \tag{4.8}$$

where the deformation parameter is chosen to be $q = \mathrm{e}^\alpha$ and α is a complex parameter to be determined by the commutation relations and through the representations $\rho_s^\pm$ we obtain the generators of global superconductive $U_q(su(2))$

$$K^{(+)} = \bigotimes_l \rho_s^{\sigma(l)}(\Delta^{(N-1)}(X^+)) \tag{4.9}$$

$$K^{(-)} = \bigotimes_l \rho_s^{\sigma(l)}(\Delta^{(N-1)}(X^-)) = (K^{(+)})^\dagger \tag{4.10}$$

$$K^{(z)} = \bigotimes_l \rho_s^{\sigma(l)}(\Delta^{(N-1)}(H)) \tag{4.11}$$

where N is the number of lattice sites. Using (4.6)–(4.8) these generators are computed to be

$$K^{(+)} = \sum_l \sigma(l) \prod_{r<l} \exp(\alpha K_r^{(z)}) K_l^{(+)} \prod_{r>l} \exp(-\alpha^* K_r^{(z)}) \tag{4.12}$$

$$K^{(-)} = \sum_l \sigma(l) \prod_{r<l} \exp(\alpha^* K_r^{(z)}) K_l^{(-)} \prod_{r>l} \exp(-\alpha K_r^{(z)}) = (K^{(+)})^\dagger \tag{4.13}$$

and

$$K^{(z)} = \sum_l K_l^{(z)}. \tag{4.14}$$

4.1. Local commutation relations

The local part of the Hamiltonian commutes with the local generators

$$[K_l^{(+)}, H^{(\mathrm{loc})}] = [K_l^{(-)}, H^{(\mathrm{loc})}] = [K_l^{(z)}, H^{(\mathrm{loc})}] = 0 \tag{4.15}$$

if the following conditions hold

$$\boldsymbol{\Phi} = \frac{2\boldsymbol{\lambda}}{\hbar M \omega^2} \tag{4.16}$$

$$\mu = \frac{u}{2} - \frac{1}{4} M\omega^2 \hbar^2 \Phi^2 = \frac{u}{2} - \frac{\boldsymbol{\lambda}^2}{M\omega^2}. \tag{4.17}$$

4.2. Global commutation relations

The fact that $K^{(z)}$ commutes with $H^{(\text{non-loc})}$ given by (3.23) is immediate. We must calculate

$$[K^{(+)}, H^{(\text{non-loc})}] = \Bigg[\sum_l \sigma(l) \prod_{r<l} \exp(\alpha K_r^{(z)}) K_j^{(+)} \prod_{r>l} \exp(-\alpha^* K_r^{(z)}),$$
$$t \sum_{\langle i<j \rangle} \sum_\sigma \exp[\zeta \boldsymbol{R}_{ij} \cdot (\boldsymbol{x}_i - \boldsymbol{x}_j)] \exp[\mathrm{i}\boldsymbol{\kappa} \cdot (\boldsymbol{p}_i - \boldsymbol{p}_j)] a_{j\sigma}^\dagger a_{i\sigma} \Bigg]. \tag{4.18}$$

It can be seen that

$$[\exp(-\mathrm{i}\boldsymbol{\Phi} \cdot \boldsymbol{p}_l), \exp[\zeta \boldsymbol{R}_{ij} \cdot (\boldsymbol{x}_i - \boldsymbol{x}_j)]] = 2 \sinh(\tfrac{1}{2} \zeta \hbar \boldsymbol{R}_{ij} \cdot \boldsymbol{\Phi})(\delta_{l,j} - \delta_{l,i})$$
$$\times \exp[-\mathrm{i}\boldsymbol{\Phi} \cdot \boldsymbol{p}_l + \zeta \boldsymbol{R}_{ij} \cdot (\boldsymbol{x}_i - \boldsymbol{x}_j)] \tag{4.19}$$

$$[a_{l\uparrow}^\dagger a_{l\downarrow}^\dagger, a_{j\uparrow}^\dagger a_{i\uparrow} + a_{j\downarrow}^\dagger a_{i\downarrow}] = -\delta_{l,i}(a_{j\uparrow}^\dagger a_{i\downarrow}^\dagger + a_{i\uparrow}^\dagger a_{j\downarrow}^\dagger) \tag{4.20}$$

$$\exp(\alpha K_i^{(z)}) = 1 + 2K_i^{(z)}(1 - \exp(-\alpha/2)) + 2n_{i\uparrow} n_{i\downarrow}(\cosh(\alpha/2) - 1) \tag{4.21}$$

and, using equation (4.21),

$$[\exp(\alpha K_l^{(z)}), a_{j\uparrow}^\dagger a_{i\uparrow} + a_{j\downarrow}^\dagger a_{i\downarrow}] = (a_{j\uparrow}^\dagger a_{i\uparrow} + a_{j\downarrow}^\dagger a_{i\downarrow})(\delta_{l,j} - \delta_{l,i})(1 - \mathrm{e}^{-\alpha/2})$$
$$+(\delta_{l,j}(a_{j\uparrow}^\dagger a_{i\uparrow} n_{j\downarrow} + n_{j\uparrow} a_{j\downarrow}^\dagger a_{i\downarrow})$$
$$-\delta_{l,i}(a_{j\uparrow}^\dagger a_{i\uparrow} n_{i\downarrow} + n_{i\uparrow} a_{j\downarrow}^\dagger a_{i\downarrow}))(\mathrm{e}^{\alpha/2} + \mathrm{e}^{-\alpha/2} - 2). \tag{4.22}$$

We introduce the abbreviation

$$Z_{ij} = \sigma(\mathrm{i}) \exp[-\mathrm{i}(\boldsymbol{\Phi} - \boldsymbol{\kappa}) \cdot \boldsymbol{p}_i - \mathrm{i}\boldsymbol{\kappa} \cdot \boldsymbol{p}_j + \zeta \boldsymbol{R}_{ij} \cdot (\boldsymbol{x}_i - \boldsymbol{x}_j)]$$
$$\times \prod_{r<i, r\neq j} \exp(\alpha K_r^{(z)}) \prod_{r>i, r\neq j} \exp(-\alpha^* K_r^{(z)}). \tag{4.23}$$

Splitting the commutators, evaluating the expressions that are obtained by the use of (4.19)–(4.22), and using the delta functions which appear in (4.19), (4.20) and (4.22) to perform some of the sums, it can be seen that (4.18) becomes

$$\begin{aligned}
[K^{(+)}, H^{(\text{non-loc})}] = t \sum_{\langle i<j\rangle} \exp(-\hbar\zeta \boldsymbol{R}_{ij}\cdot\boldsymbol{\kappa})\{&(a^\dagger_{i\downarrow}a^\dagger_{i\uparrow}a^\dagger_{j\downarrow}a^\dagger_{j\uparrow}a_{i\uparrow}a_{j\downarrow} - a^\dagger_{i\downarrow}a^\dagger_{i\uparrow}a^\dagger_{j\downarrow}a^\dagger_{j\uparrow}a_{i\downarrow}a_{j\uparrow})\\
&\times[Z_{ij}(2\cosh(\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar) - 2\cosh(\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar + \tfrac{1}{2}\alpha^*))\\
&+Z_{ji}(2\cosh(\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar) - 2\cosh(\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar + \tfrac{1}{2}\alpha))]\\
&+(a^\dagger_{i\uparrow}a^\dagger_{j\downarrow}a^\dagger_{j\uparrow}a_{j\uparrow} + a^\dagger_{i\downarrow}a^\dagger_{j\downarrow}a^\dagger_{j\uparrow}a_{j\downarrow})\exp(\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\\
&\times[Z_{ij}(\exp(\tfrac{1}{2}\alpha^*) - 1) + Z_{ji}(\exp(-\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(-\tfrac{1}{2}\alpha) - 1)]\\
&+(a^\dagger_{i\downarrow}a^\dagger_{i\uparrow}a^\dagger_{j\downarrow}a_{i\downarrow} + a^\dagger_{i\downarrow}a^\dagger_{i\uparrow}a^\dagger_{j\uparrow}a_{i\uparrow})\exp(-\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\\
&\times[Z_{ij}(\exp(\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(\tfrac{1}{2}\alpha^*) - 1) + Z_{ji}(\exp(-\tfrac{1}{2}\alpha) - 1)]\\
&+(a^\dagger_{i\downarrow}a^\dagger_{j\uparrow} - a^\dagger_{i\uparrow}a^\dagger_{j\downarrow})[Z_{ij}\exp(\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(\tfrac{1}{2}\alpha^*)\\
&+Z_{ji}\exp(-\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(-\tfrac{1}{2}\alpha))]\}\\
&+\sum_l \sum_{\langle i,j\rangle, i<l<j} \sigma(l)\exp(-\hbar\zeta\boldsymbol{R}_{ij}\cdot\boldsymbol{\kappa})\exp(-\mathrm{i}\boldsymbol{\Phi}\cdot\boldsymbol{p}_l)a^\dagger_{l\uparrow}a^\dagger_{l\downarrow}\\
&\times\prod_{r<l, r\neq i}\exp(\alpha K^{(z)}_r)\prod_{r>l, r\neq j}\exp(-\alpha^* K^{(z)}_r)\\
&\times[\exp(\alpha K^{(z)}_i)\exp(-\alpha^* K^{(z)}_j), \exp[\mathrm{i}\boldsymbol{\kappa}\cdot(\boldsymbol{p}_i - \boldsymbol{p}_j)\\
&+\zeta\boldsymbol{R}_{ij}\cdot(\boldsymbol{x}_i - \boldsymbol{x}_j)]a^\dagger_{j\uparrow}a_{i\uparrow} + a^\dagger_{j\downarrow}a_{i\downarrow} + \text{HC}]. \qquad (4.24)
\end{aligned}$$

There are two sums containing six fermionic operators, four sums containing four fermionic operators, and two sums containing two fermionic operators. These sums must all be separately zero, because they depend on different numbers of such operators and hence are linearly independent. Let us study the term containing $a^\dagger_{i\downarrow}a^\dagger_{j\uparrow} - a^\dagger_{i\uparrow}a^\dagger_{j\downarrow}$:

$$\sum_{\langle i<j\rangle}(a^\dagger_{i\downarrow}a^\dagger_{j\uparrow} - a^\dagger_{i\uparrow}a^\dagger_{j\downarrow})[Z_{ij}\exp(\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(\tfrac{1}{2}\alpha^*) + Z_{ji}\exp(-\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(-\tfrac{1}{2}\alpha)]. \qquad (4.25)$$

The above sum can vanish only if each term with fixed i, j is separately zero, because there are no other terms which contain $a^\dagger_{i\downarrow}a^\dagger_{j\uparrow} - a^\dagger_{i\uparrow}a^\dagger_{j\downarrow}$. Therefore it is necessary that the expression between the square brackets is zero. For this reason we must require

$$Z_{ij}\exp(\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(\tfrac{1}{2}\alpha^*) + Z_{ji}\exp(-\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(-\tfrac{1}{2}\alpha) = 0. \qquad (4.26)$$

This is equivalent to the set of equations

$$Z_{ij} = -Z_{ji} \qquad (4.27)$$

$$\exp(\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(\tfrac{1}{2}\alpha^*) = \exp(-\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(-\tfrac{1}{2}\alpha) \qquad (4.28)$$

which in turn imply (i, j are nearest neighbours)

$$\sigma(i) = -\sigma(j) \qquad (4.29)$$

$$\begin{aligned}
&\exp[-\mathrm{i}(\boldsymbol{\Phi} - \boldsymbol{\kappa})\cdot\boldsymbol{p}_i - \mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{p}_j + \zeta\boldsymbol{R}_{ij}\cdot(\boldsymbol{x}_i - \boldsymbol{x}_j)]\\
&\qquad = \exp[-\mathrm{i}(\boldsymbol{\Phi} - \boldsymbol{\kappa})\cdot\boldsymbol{p}_j - \mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{p}_i + \zeta\boldsymbol{R}_{ij}\cdot(\boldsymbol{x}_i - \boldsymbol{x}_j)] \qquad (4.30)
\end{aligned}$$

$$\prod_{r<i}\exp(\alpha K^{(z)}_r)\prod_{r>i, r\neq j}\exp(-\alpha^* K^{(z)}_r) = \prod_{r<j, r\neq i}\exp(\alpha K^{(z)}_r)\prod_{r>j}\mathrm{e}(-\alpha^* K^{(z)}_r) \qquad (4.31)$$

$$\exp(-\tfrac{1}{2}\mathrm{i}\,\mathrm{Im}\,\alpha)(\exp(\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(\tfrac{1}{2}\,\mathrm{Re}\,\alpha) - \exp(-\tfrac{1}{2}\boldsymbol{R}_{ij}\cdot\boldsymbol{\Phi}\zeta\hbar)\exp(-\tfrac{1}{2}\,\mathrm{Re}\,\alpha)) = 0. \qquad (4.32)$$

Equation (4.29) means that nearest neighbours must have opposite signs. As we have already anticipated, this means that in order for the global commutation relations to hold, it should be possible to see the lattice Λ on which the model is defined, as the sum of two lattices Λ_1, Λ_2, such that nearest neighbours are always on different lattices. This gives a restriction on the possible lattices, e.g. a triangular lattice could not be chosen.

Equation (4.30) implies $\boldsymbol{\kappa} - \boldsymbol{\Phi} = -\boldsymbol{\kappa}$ and hence

$$2\boldsymbol{\kappa} = \boldsymbol{\Phi}. \tag{4.33}$$

This is one condition that must be satisfied for expression (4.25) to vanish. In particular it fixes the parameter of the transformation (3.17). It turns out, that the parameter has to be the same as the one used to transform the fermionic operators in the Hamiltonian.

Equation (4.32) implies

$$\operatorname{Re}\alpha = -\boldsymbol{R}_{ij} \cdot \boldsymbol{\Phi}\zeta\overline{h}. \tag{4.34}$$

This is the second condition which must be satisfied for expression (4.25) to vanish. It is important to notice that it is possible to fulfil this relation only if the ordering of the lattice sites is chosen to be the lexicographic one. So this imposes a first restriction on the ordering of the sites.

The strongest relation is (4.31)—it depends crucially on the ordering chosen for the lattice sites. In order for (4.31) to hold it is necessary that

$$\prod_{i<r<j} \exp(\alpha K_r^{(z)}) = \prod_{i<r<j} \exp(-\alpha^* K_r^{(z)}). \tag{4.35}$$

Let us apply (4.21) to expand the exponentials. Then we obtain an expression of the type

$$1 + 2(1 - \mathrm{e}^{-\alpha/2}) \sum_{i<r<j} K_r^{(z)} + \cdots = 1 + 2(1 - \mathrm{e}^{\alpha^*/2}) \sum_{i<r<j} K_r^{(z)} + \cdots. \tag{4.36}$$

(Here the terms which are indicated with '$\cdots$' are at least quadratic in the $K_r^{(z)}$ and therefore are independent of the first-order terms which have been written.) Equation (4.36) shows that in order for relation (4.35) to hold, it is necessary that

$$\mathrm{e}^{-\alpha/2} = \mathrm{e}^{\alpha^*/2} \Rightarrow \operatorname{Re}(\alpha) = 0.$$

But this would mean that the coproduct should be symmetric, and this is against the hypothesis that there is a true quantum symmetry.

This shows that we must look for a condition on the ordering of the lattice sites, so that we do not need to require (4.35): there cannot be any site r which satisfies the condition $i < r < j$ for any couple of nearest neighbours i, j. In other words it is necessary that if i, j is a couple of nearest neighbours then

$$(i < r \Rightarrow j \leqslant r,\ i > r \Rightarrow j \geqslant r) \qquad \forall r. \tag{4.37}$$

However, condition (4.37) implies that the lattice Λ on which the Hubbard model is defined is one dimensional, and that the 'normal' ordering of the sites is chosen, in which the sites are numbered from left to right in increasing or decreasing order.

It can be verified immediately that condition (4.37) is *sufficient* to guarantee that the sum with '$\sum_l \sum_{\langle i,j\rangle, i<l<j}$' is not present, because there is no longer any l satisfying $i < l < j$. In fact it can be verified with arguments similar to the ones used to study the term (4.25) that (4.37) is also *necessary* for such a sum to vanish. Because of (4.31) and (4.30) it is possible to combine the terms which contain the same products of fermionic operators. Further, it can be seen immediately, that conditions (4.29), (4.33), (4.34) and (4.37) are also necessary and sufficient for the sums with four and with six fermionic operators to vanish. Thus in order for the Hamiltonian $H^{(\text{non-loc})}$ (3.23) to commute with the generators (4.12)–(4.14) of $U_q(su(2))$ the conditions (4.29), (4.37), (4.33), (4.34) are necessary and sufficient.

5. Discussion

The computation of the previous section has shown that the Hamiltonian H, given for a D-dimensional lattice in (3.21)–(3.23), commutes with the generators of (global) $U_q su(2)$, $q \equiv e^{\alpha}$, provided that local conditions (4.16), (4.17), global conditions (4.33), (4.34) and either $D = 1$ or $\alpha = 0$ hold. (We will only consider $\mathrm{Im}(\alpha) = 0$ here.) We are now in a position to comment on the symmetries† of various Hamiltonians derived from the Hubbard model:

H_{Hub} (3.14) coincides with (3.21)–(3.23) for the particular choice of parameter $\boldsymbol{\kappa} = 0$. The global conditions (4.33), (4.34) imply $\boldsymbol{\Phi} = 0$, $\alpha = 0$ and hence $q = 1$. The local conditions (4.16), (4.17) imply $\boldsymbol{\lambda} = 0$ and $\mu = u/2$. We conclude that the Hubbard model with phonons (3.14) has no true quantum symmetry—not even in the one-dimensional case; it has an ordinary $SU(2)$ symmetry provided that there is no local electron–phonon coupling ($\boldsymbol{\lambda} = 0$).

The Hamiltonian H (3.21) studied in the previous section and considered by [5] is formally obtained from the Hubbard model with phonons by a Lang–Firsov transformation on the fermionic operators only. (See remark at the end of section 3.) The essential difference between H_{Hub} and H is that H_{Hub} uses coordinates $\boldsymbol{y}_i$ that commute with $b^{\dagger}_{i\sigma}, b_{i\sigma}$ while H is written in terms of new coordinates that commute with $a^{\dagger}_{i\sigma}$ and $a_{i\sigma}$ (and not with $b^{\dagger}_{i\sigma}, b_{i\sigma}$). To be able to compare the two Hamiltonians we have to relate the sets of coordinates. This is simply done by a Lang–Firsov transformation‡ (see (3.15)–(3.17))

$$\boldsymbol{x}_i = U(\boldsymbol{\kappa})\boldsymbol{y}_i U^{-1}(\boldsymbol{\kappa}). \tag{5.1}$$

The new coordinates are found to be

$$\boldsymbol{x}_i = \boldsymbol{y}_i + \overline{h}\boldsymbol{\kappa}\sum_{\sigma} n_{i\sigma} \tag{5.2}$$

i.e. the position of the ion at lattice site i is shifted according to the number of electrons at that site. Expressing H in terms of $y_i, b^{\dagger}_{i\sigma}, b_{i\sigma}$ we find

$$\begin{aligned} H_{q-\mathrm{sym}} = {} & u'\sum_i n_{i\uparrow}n_{i\downarrow} - \mu'\sum_{i,\sigma} n_{i\sigma} + \sum_i \left(\frac{\boldsymbol{p}_i^2}{2M} + \frac{1}{2}M\omega^2\boldsymbol{y}_i^2\right) - \boldsymbol{\lambda}'\cdot\sum_i (n_{i\uparrow}+n_{i\downarrow})\boldsymbol{y}_i \\ & + \Bigg(t\sum_{\langle i<j\rangle}\sum_{\sigma} \exp\{\zeta \boldsymbol{R}_{ij}\cdot(\boldsymbol{y}_i - \boldsymbol{y}_j)\}\exp(-\zeta\overline{h}\boldsymbol{R}_{ij}\cdot\boldsymbol{\kappa}) b^{\dagger}_{j\sigma}b_{i\sigma} \\ & \times(1 + (\exp(\zeta\overline{h}\boldsymbol{R}_{ij}\cdot\boldsymbol{\kappa}) - 1)n_{i,-\sigma})(1 + (\exp(-\zeta\overline{h}\boldsymbol{R}_{ij}\cdot\boldsymbol{\kappa}) - 1)n_{j,-\sigma}) + \mathrm{HC}) \end{aligned} \tag{5.3}$$

with a set of new parameters

$$\boldsymbol{\lambda}' = \boldsymbol{\lambda} - M\omega^2\overline{h}\boldsymbol{\kappa} \tag{5.4}$$

$$u' = u - 2\overline{h}\boldsymbol{\lambda}\cdot\boldsymbol{\kappa} + M\omega^2\overline{h}^2\kappa^2 \tag{5.5}$$

$$\mu' = \mu + \overline{h}\boldsymbol{\lambda}\cdot\boldsymbol{\kappa} - 1/2M\omega^2\overline{h}^2\kappa^2. \tag{5.6}$$

The model given by $H_{q-\mathrm{sym}}$ (5.3) has a true quantum symmetry (in the one-dimensional case). The local conditions (4.16), (4.17) for quantum symmetry expressed in terms of the *new* parameters are

$$\boldsymbol{\lambda}' = 0 \qquad \mu' = u'/2. \tag{5.7}$$

There is apparently no local coupling to the phonons and the condition for symmetry is 'half filling' as in the standard Hubbard model.

† The Hamiltonian will commute with *all* elements of $U_q SU(2)$ provided that its generators do so; this is equivalent to a full quantum symmetry (under quantum adjoint action), see section 2.

‡ This observation is also supported by the choice of $K_l^{(\pm)}, K_l^{(z)}$.

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