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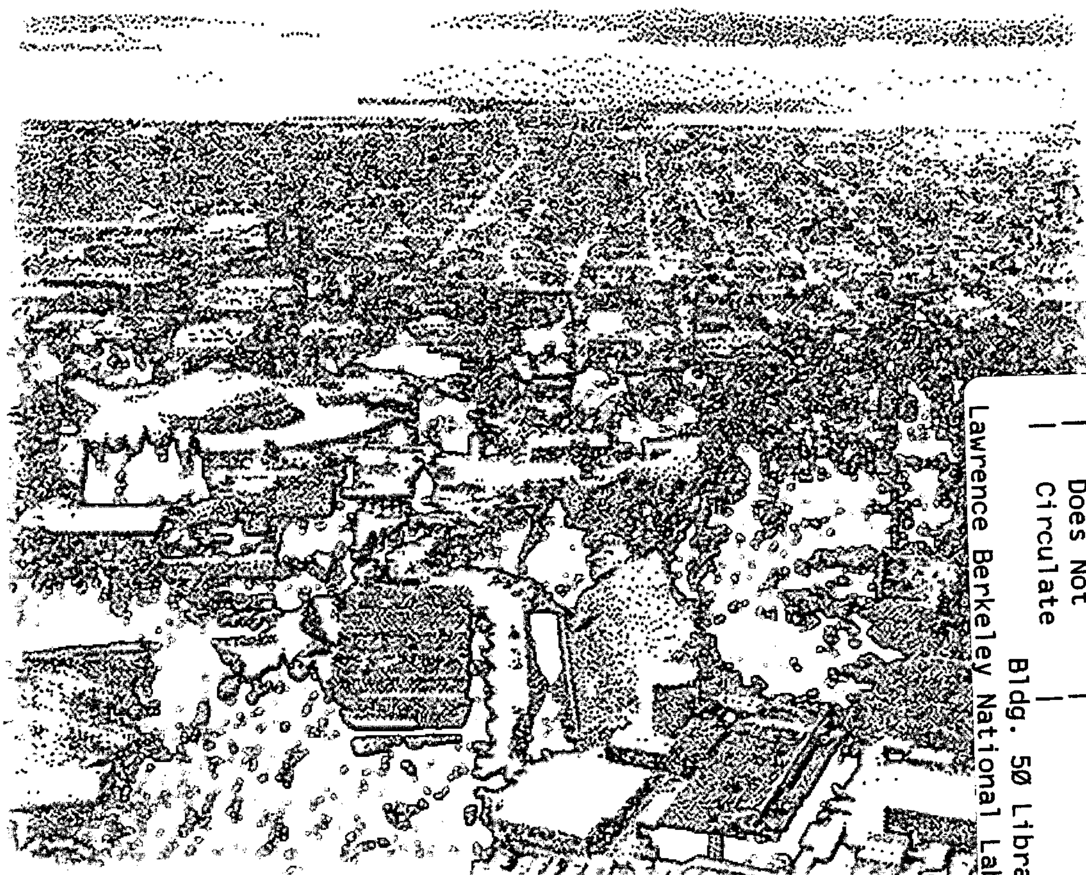

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Quantum Symmetry of Hubbard Model Unraveled*

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Superconducting quantum symmetries in extended one-band one-dimensional Hubbard models are shown to originate from the classical (pseudo-)spin symmetry of a new class of models; the standard Hubbard model is a special case. The quantum symmetric models provide extra parameters but are restricted to one dimension. All models discussed are related by generalized Lang-Firsov transformations, some have symmetries away from half filling.

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The exploration of high temperature superconductivity in cuprates has greatly revived interest in the Hubbard model [1] as a model of strongly correlated electron systems [2–4]. Despite its formal simplicity this model continues to resist complete analytical or numerical understanding. Symmetries of the Hubbard Hamiltonian play a major role in the reduction of the problem. They have for instance been used to construct eigenstates of the Hamiltonian with off-diagonal long range order [5], to simplify numerical diagonalization [6] and to show completeness of the solution [7] to the one-dimensional model [8].

The well-known (pseudo-)spin symmetries [9,5,10] of the standard Hubbard model are restricted to the case of an average of one electron per site (half-filling), so recent speculations [11] about extended Hubbard models with generalized (quantum group) symmetries away from half-filling attracted some attention. A careful analysis of the new models reveals that this quantum symmetry exists only on one-dimensional lattices and in an appropriate approximation seems still to be restricted to half-filling. Despite these shortcomings the existence of novel symmetries in Hubbard models is very interesting and worth investigating. Quantum symmetries of the Hubbard model were first investigated in the form of Yangians [12]; quantum supersymmetries of Hubbard models have also been considered [13].

In this letter we shall investigate the origin of quantum symmetries in extended Hubbard models. We will find a one-to-one correspondence between Hamiltonians with quantum and classical symmetries. Guided by our results we will then be able to identify models whose symmetries are neither restricted to one-dimensional lattices nor to half filling.

Originally introduced as a simplistic description of narrow d-bands in transition metals, the Hubbard model combines band-like and atomic behavior. In the standard Hubbard Hamiltonian

$$H_{\text{Hub}} = u\sum_i n_{i\uparrow}n_{i\downarrow} - \mu\sum_{i,\sigma} n_{i\sigma} + t\sum_{\langle i,j\rangle\sigma} a^\dagger_{j\sigma}a_{i\sigma}, \quad (1)$$

this is achieved by a local Coulomb term and a competing non-local hopping term. Here $a^\dagger_{i\sigma}$, $a_{i\sigma}$ are creation and annihilation operators[1] for electrons of spin $\sigma \in \{\uparrow, \downarrow\}$ at site i of a D-dimensional lattice, $\langle i,j\rangle$ denotes nearest neighbor sites and $n_{i\sigma} \equiv a^\dagger_{i\sigma}a_{i\sigma}$. The average number of electrons $\langle\sum_{i,\sigma} n_{i\sigma}\rangle$ is fixed by the chemical potential μ.

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[1] We will use the convention that operators at different sites *commute*. On a bipartite lattice one can easily switch to anticommutators without changing any of our results.

The *standard Hubbard model* has a $\mathrm{SU}(2) \times \mathrm{SU}(2)/\mathbf{Z}_2$ symmetry at $\mu = u/2$, the value of μ corresponding to half filling in the band-like limit. This symmetry is the product of a *magnetic* $\mathrm{SU}(2)_m$ (spin) with local generators

$$X_m^+ = a_\uparrow^\dagger a_\downarrow, \quad X_m^- = a_\downarrow^\dagger a_\uparrow, \quad H_m = n_\uparrow - n_\downarrow, \tag{2}$$

and a *superconducting* $\mathrm{SU}(2)_s$ (pseudo-spin) with local generators

$$X_s^+ = a_\uparrow^\dagger a_\downarrow^\dagger, \quad X_s^- = a_\downarrow a_\uparrow, \quad H_s = n_\uparrow + n_\downarrow - 1, \tag{3}$$

modulo a $\mathbf{Z}_2$, generated by the unitary transformation $(a_\downarrow \leftrightarrow a_\downarrow^\dagger)$ that interchanges the two sets of local generators. The mutually orthogonal algebras generated by (2) and (3) are isomorphic to the algebra generated by the Pauli matrices and have unit elements $1_s = H_s^2$, $1_m = H_m^2$ with $1_s + 1_m = 1$. The superconducting generators commute with each term of the local part $H^{(\mathrm{loc})}$ (first two terms) of the Hubbard Hamiltonian (1) provided that $\mu = u/2$. This can either be seen by direct computation or by studying the action of the generators on the four possible electron states at each site. It is also easily seen that the magnetic generators commute with each term of $H^{(\mathrm{loc})}$; in the following we will however focus predominantly on the superconducting symmetry.

To check the symmetry of the non-local hopping term we have to consider global generators $\mathcal{O}$: These generators are here simply given by the sum $\sum \mathcal{O}_i$ of the local generators for all sites i. The rule that governs the combination of representations for more than one lattice site is abstractly given by the diagonal map or coproduct Δ of $U(su(2))$. Generators for two sites are directly obtained from the coproduct

$$\Delta(X^\pm) = X^\pm \otimes 1 + 1 \otimes X^\pm, \quad \Delta(H) = H \otimes 1 + 1 \otimes H,$$

while generators for N sites require $(N-1)$-fold iterative application of Δ. Coassociativity of Δ ensures that it does not matter which tensor factor is split up at each step. Another distinguishing property of this *classical* coproduct is its symmetry (cocommutativity). This property and coassociativity ensure that we can arrange that the two factors of the last coproduct coincide with any given pair $\langle i,j \rangle$ of next-neighbor sites; see Fig. 1. It is hence enough to study symmetry of a single next-neighbor term of the Hamiltonian to prove global symmetry.

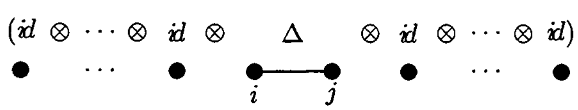

FIG. 1. Coassociativity of Δ reduces global symmetry to symmetry of next-neighbor terms $\langle i,j \rangle$ if $D = 1$.

The search for quantum group symmetries in the Hubbard model is motivated by the observation that the local generators X_s^+, X_s^- and H_s in the superconducting representation of SU(2) also satisfy the $\mathrm{SU}_q(2)$ algebra as given in the Jimbo-Drinfel'd basis [14]

$$[X^+, X^-] = \frac{q^H - q^{-H}}{q - q^{-1}}, \qquad [H, X^\pm] = \pm 2 X^\pm. \tag{4}$$

(The proof uses $H_s^3 = H_s$.) It immediately follows that $H^{(\mathrm{loc})}$ has a local quantum symmetry. As is, this is a trivial statement because we did not yet consider global quantum symmetries. Global generators are now defined via the deformed coproduct of $\mathrm{SU}_q(2)$, $q \in \mathbf{R}\backslash\{0\}$

$$\begin{aligned} \Delta_q(X^\pm) &= X^\pm \otimes q^{-H/2} + q^{H/2} \otimes X^\pm, \\ \Delta_q(H) &= H \otimes 1 + 1 \otimes H. \end{aligned} \tag{5}$$

The local symmetry can be extended to a non-trivial global quantum symmetry by a modification of the Hubbard Hamiltonian. The idea of [11] was to achieve this by including phonons. Before we proceed to study the resulting extended Hubbard Hamiltonian H_{ext}, we would like to make two remarks: (i) We call a Hamiltonian quantum symmetric if it commutes with all global generators. This implies invariance under the quantum adjoint action and vice versa. (ii) Coproducts of quantum groups are coassociative but not cocommutative. This means that the reduction of global symmetry to that of next-neighbor terms holds only for one-dimensional lattices. The practical implication is an absence of quantum symmetries for higher-dimensional lattices. (For a triangular lattice this is illustrated in Fig. 2.)

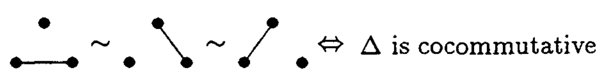

FIG. 2. In $D \neq 1$ symmetry of next-neighbor terms implies global symmetry only if Δ is classical.

The *extended Hubbard model* of [11] (with some modifications [15]) introduces Einstein oscillators (parameters: M, ω) and electron-phonon couplings (local: $\vec{\lambda}$-term, non-local: via $T_{ij\sigma}$):

$$\begin{aligned} H_{\mathrm{ext}} = u \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} - \vec{\lambda} \cdot \sum_{i\sigma} n_{i\sigma} \vec{x}_i \\ + \sum_i \left(\frac{\vec{p}_i^{\,2}}{2M} + \frac{1}{2} M \omega^2 \vec{x}_i^2 \right) + \sum_{\langle i,j \rangle \sigma} a_{j\sigma}^\dagger a_{i\sigma} T_{ij\sigma}, \end{aligned} \tag{6}$$

with hopping amplitude

$$T_{ij\sigma} = T_{ji\sigma}^\dagger = t \exp(\zeta \hat{e}_{ij} \cdot (\vec{x}_i - \vec{x}_j) + i\kappa \cdot (\vec{p}_i - \vec{p}_j)). \tag{7}$$

The displacements $\vec{x}_i$ of the ions from their rest positions and the corresponding momenta $\vec{p}_i$ satisfy canonical commutation relations. The $\hat{e}_{ij}$ are unit vectors from site i to site j. For $\vec{\kappa}=0$ the model reduces to the Hubbard model with phonons and atomic orbitals $\psi(r) \sim \exp(-\zeta r)$ in s-wave approximation [15].

The local part of H_{ext} commutes with the generators of $\mathrm{SU}_q(2)_s$ iff

$$\mu = \frac{u}{2} - \frac{\vec{\lambda}^2}{M\omega^2}. \tag{8}$$

(For technical reasons one needs to use modified generators $\tilde{X}^{\pm}_s \equiv e^{\mp 2i\vec{\kappa}\cdot\vec{p}} X^{\pm}_s$ here that however still satisfy the $\mathrm{SU}_q(2)$ algebra.)
The nonlocal part of H_{ext} and thereby the whole extended Hubbard Hamiltonian commutes with the global generators iff

$$\vec{\lambda} = \hbar M\omega^2\vec{\kappa}, \qquad q = \exp(2\kappa\zeta\hbar), \tag{9}$$

where $\kappa \equiv -\hat{e}_{ij}\cdot\vec{\kappa}$ for i,j ordered next neighbour sites. *For $q \neq 1$ the symmetry is restricted to models given on a 1-dimensional lattice with naturally ordered sites.*

From what we have seen so far we could be let to the premature conclusion that the quantum symmetry is due to phonons and that we have found symmetry away from half filling because $\mu \neq u/2$. However: the pure Hubbard model with phonons has $\vec{\kappa}=0$ and hence a classical symmetry ($q=1$). Furthermore $\vec{\lambda} \neq 0$ implies non-vanishing local electron-phonon coupling so that a mean field approximation cannot be performed and we simply do not know how to compute the actual filling. Luckily there is an equivalent model that is not plagued with this problem: A *Lang-Firsov transformation* with unitary operator $U = \exp(i\vec{\kappa}\cdot\sum_j \vec{p}_j n_{j\sigma})$. leads to the Hamiltonian

$$H_{q\text{-sym}} = UH_{\text{ext}}U^{-1} = H_{\text{ext}}(\vec{\lambda}', u', \mu', T'_{ij\sigma}), \tag{10}$$

of what we shall call the *quantum symmetric Hubbard model*. It has the same form as H_{ext}, but with a new set of parameters

$$\vec{\lambda}' = \vec{\lambda} - M\omega^2\hbar\vec{\kappa} \tag{11}$$

$$u' = u - 2\hbar\vec{\lambda}\cdot\vec{\kappa} + M\omega^2\hbar^2\kappa^2 \tag{12}$$

$$\mu' = \mu + \hbar\vec{\lambda}\cdot\vec{\kappa} - \frac{1}{2}M\omega^2\hbar^2\kappa^2 \tag{13}$$

and a modified hopping amplitude

$$T'_{ij,-\sigma} = \tilde{t}_{ij}(1+(q^{\frac{\hat{e}_{ji}}{2}}-1)n_{i\sigma})(1+(q^{\frac{\hat{e}_{ij}}{2}}-1)n_{j\sigma}) \tag{14}$$

where $\tilde{t}_{ij} = t\exp(\zeta\hat{e}_{ij}\cdot(\vec{x}_i-\vec{x}_j))$. The condition for symmetry expressed in terms of the new parameters is

$$\vec{\lambda}' = 0, \qquad \mu' = \frac{u'}{2}, \tag{15}$$

i.e. requires vanishing local phonon coupling and corresponds to *half filling*! $\tilde{t}_{ij}$ may also be turned into a (temperature-dependent) constant via a mean field approximation. This approximation is admissible for the quantum symmetric Hubbard model because $\vec{\lambda}'=0$.

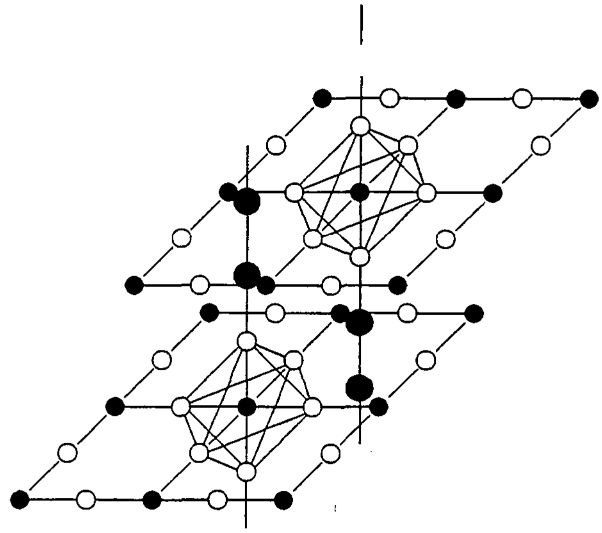

FIG. 3. Typical cuprate superconductor with CuO_2 conduction planes

We have so far identified several quantum group symmetric models (with and without phonons) and have achieved a better understanding of H_{ext}'s superconducting quantum symmetry. There are however still open questions: (i) Does a new model exist that is equivalent to $H_{q\text{-sym}}$ in 1-D but can also be formulated on higher dimensional lattices without breaking the symmetry? This would be important for realistic models, see Fig. 3. (ii) Are there models with symmetry away from half-filling? (iii) What is the precise relation between models with classical and quantum symmetry in this setting?

As we shall see the answer to the last question also leads to the resolution of the first two. Without loss of generality (see argument given above) we will focus on one pair of next-neighbor sites in the following. We shall present two approaches that supplement each other:

a. Generalized Lang-Firsov transformation We recall that the Hubbard model with phonons (with classical symmetry) can be transformed into the standard Hubbard Hamiltonian in two steps: A Lang-Firsov transformation changes the model to one with vanishing local phonon coupling and a mean field approximation removes the phonon operators from the model by averaging over Einstein oscillator eigenstates [17]. There exists a similar transformation that relates the extended Hubbard model (with quantum symmetry) to the standard Hubbard model:

$$H_{\text{ext}} \longleftrightarrow H_{q\text{-sym}} \longleftrightarrow H_{\text{Hub}}.$$

(We have already seen the first step of this transformation above in (10).) It is easy to see that the hopping terms of $H_{q\text{-sym}}$ and H_{Hub} have different spectrum so the transformation that we are looking for cannot be an equivalence transformation. There exists however an invertible operator M, with $MM^* = 1+(\alpha^2-1)\xi$, $\xi^2=\xi$ (*i.e.* similar to a partial isometry), that transforms the coproducts of the classical Chevalley generators into their Jimbo-Drinfel'd quantum counterparts

$$\begin{aligned} M\Delta_c(X^{\pm})_s M^* &= \Delta_q(X^{\pm})_s \\ M\Delta_c(H)_s M^* &= \Delta_q(H)_s, \end{aligned} \tag{16}$$

and the standard Hubbard Hamiltonian into $H_{q\text{-sym}}$

$$M H_{\text{Hub}} M^* = H_{q\text{-sym}}. \tag{17}$$

This operator M is

$$M = 1 \otimes 1 + (\alpha - 1)\xi + \beta f, \tag{18}$$

with $f = X_s^- \otimes X_s^+ - X_s^+ \otimes X_s^-$, $\xi = -f^2 = \frac{1}{2}(H_s^2 \otimes H_s^2 - H_s \otimes H_s)$ and $\alpha \pm \beta = q^{\pm\frac{1}{2}}$. With this knowledge the proof of the quantum symmetry of H_{ext} is greatly simplified.

b. Quantum vs. Classical Groups—Twists A systematic way to study the relation of quantum and classical symmetries was given by Drinfel'd [18]. He argues that the classical U(g) and q-deformed $U_q(g)$ universal enveloping algebras are isomorphic *as algebras*. The relation of the Hopf algebra structures is slightly more involved: the undeformed universal enveloping algebra U(g) of a Lie algebra, interpreted as a quasi-associative Hopf algebra whose coassociator is an invariant 3-tensor, is twist-equivalent to the Hopf algebra $U_q(g)$ (over [[ln q]]).

All we need to know here is that classical (Δ_c) and quantum (Δ_q) coproducts are related via conjugation ("twist") by the so-called universal $\mathcal{F} \in U_q(su_2)^{\hat{\otimes}2}$:

$$\Delta_q(x) = \mathcal{F}\Delta_c(x)\mathcal{F}^{-1}. \tag{19}$$

(For notational simplicity we did not explicitly write the map that describes the algebra isomorphism of U(su$_2$) and $U_q(su_2)$ but we should not be fooled by the apparent similarity between (16) and (19): The algebra isomorphism does not map Chevalley generators to Jimbo-Drinfel'd generators and M is not a representation of $\mathcal{F}$.)

The fundamental matrix representation of the universal $\mathcal{F}$ for SU(N) is an orthogonal matrix [19]

$$\begin{aligned} \rho^{\otimes 2}(\mathcal{F}) &= \sum_i e_{ii} \otimes e_{ii} + \cos\varphi \sum_{i \neq j} e_{ii} \otimes e_{jj} \\ &+ \sin\varphi \sum_{i<j} (e_{ij} \otimes e_{ji} - e_{ji} \otimes e_{ij}), \end{aligned} \tag{20}$$

where $\cos\varphi \pm \sin\varphi = \sqrt{2q^{\pm 1}/(q+q^{-1})}$, $i, j = 1 \ldots N$ and e_{ij} are N×N matrices with lone "1" at position (i,j). The universal $\mathcal{F}$ in the superconducting spin-$\frac{1}{2}$ representation, *i.e.* essentially the $N = 2$ case with the Pauli matrices replaced by (3), is

$$F_s = \exp(\varphi f)_s = \tilde{\xi} + \cos\varphi\, \xi + \sin\varphi\, f \tag{21}$$

and $\tilde{\xi} + \xi = 1_s \otimes 1_s$. We are interested in a representation of the universal $\mathcal{F}$ on the 16-dimensional Hilbert space of states of two sites:

$$\begin{aligned} F &= (\epsilon_m \oplus \rho_s)^{\otimes 2}(\mathcal{F}) = \exp(\varphi f) \\ &= 1 \otimes 1 - 1_s \otimes 1_s + F_s. \end{aligned} \tag{22}$$

Note that the trivial magnetic representation ϵ_m enters here even though we decided to study only deformations of the superconducting symmetry—F_s alone would have been identically zero on the hopping term and would hence have lead to a trivial model.

We now face a puzzle: By construction $F^{-1}H_{q\text{-sym}}F$ should commute with the (global) generators of $SU_q(2)_s$ just like H_{Hub}. But $F^{-1}H_{q\text{-sym}}F$ obviously has the same spectrum as $H_{q\text{-sym}}$ so it cannot be equal to H_{Hub}. There must be other models with the same symmetries. In fact we find a six-parameter family of classically symmetric models in any dimension. In the one-dimensional case twist-equivalent quantum symmetric models can be constructed as deformations of each of these classical models. H_{Hub} and $H_{q\text{-sym}}$ are not a twist-equivalent pair but all models mentioned are related by generalized Lang-Firsov transformations.

To close we would like to present the most general Hamiltonian with SU(2) × SU(2)/$\mathbf{Z}_2$ symmetry and symmetric next-neighbor terms. (A group-theoretical derivation and detailed description of this model is however beyond the scope of this letter and will be given elsewhere.) The Hamiltonian is written with eight real parameters (μ, r, s, t, u, v, Re(z), Im(z)):

$$\begin{aligned} H_{\text{sym}} = u &\sum_i n_{i\uparrow}n_{i\downarrow} \quad - \mu \sum_{i,\sigma} n_{i\sigma} \quad + t \sum_{\langle i,j\rangle\sigma} a_{i\sigma}^\dagger a_{j\sigma} \\ &+ r \sum_{\langle i,j\rangle\sigma} n_{i\sigma}n_{j-\sigma} \quad + s \sum_{\langle i,j\rangle\sigma} n_{i\sigma}n_{j\sigma} \\ &+ \frac{2\mu - u}{e} \sum_{\langle i,j\rangle\sigma} a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger a_{j\uparrow} a_{j\downarrow} \\ &+ (s - r) \sum_{\langle i,j\rangle\sigma} a_{i\sigma}^\dagger a_{i-\sigma} a_{j-\sigma}^\dagger a_{j\sigma} \\ &+ v \sum_{\langle i,j\rangle\sigma} (n_{i\uparrow}n_{i\downarrow}n_{j\uparrow}n_{j\downarrow} - n_{i\uparrow}n_{i\downarrow}n_{j\sigma} - n_{i\sigma}n_{j\uparrow}n_{j\downarrow}) \\ &+ \sum_{\langle i,j\rangle\sigma} a_{i-\sigma}^\dagger a_{j-\sigma} \left(z(n_{i\sigma} - 1)n_{j\sigma} + z^* n_{i\sigma}(n_{j\sigma} - 1)\right) \\ &+ \text{H.C.} \end{aligned} \tag{23}$$

For symmetry $v = r + s + u - 2\mu$ must hold. One parameter can be absorbed into an overall multiplicative constant, so we have six free parameters. The first three terms comprise the standard Hubbard model but now without the restriction to half-filling. The filling factor is fixed by the coefficient of the pair hopping term (6^{th} term). The number e in the denominator of this coefficient is the number of edges per site. For a single pair of sites $e = 1$, for a one-dimensional chain $e = 2$, for a honeycomb lattice $e = 3$, for a square lattice $e = 4$, for a triangular lattice $e = 6$ and for a D-dimensional hypercube $e = 2D$. For a model on a general graph e will vary with the site. The 4^{th} and 5^{th} term describe density-density interaction for anti-parallel and parallel spins respectively. The balance of these two interactions is governed by the coefficient of the spin-wave term (7^{th} term). The last term is a modified hopping term that is reminiscent of the hopping term in the t-J model with hopping strength depending on the occupation of the sites; after deformation this term is the origin of the non-trivial quantum symmetries of H_{sym}.

The known and many new quantum symmetric Hubbard models can be derived from H_{sym} by twisting as described above. While the deformation provides up to two extra parameters for the quantum symmetric models the advantage of the corresponding classical models is that they are not restricted to one dimension. There are both classically and quantum symmetric models with symmetries away from half filling.

The way the filling and the spin-spin interactions appear as coefficients of the pair-hopping and spin-wave terms respectively looks quite promising for a physical interpretation. Due to its symmetries H_{sym} should share some of the nice analytical properties of the standard Hubbard Hamiltonian and could hence be of interest in its own right.

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