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Quantum Symmetries Induced by Phonons in the Hubbard Model

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We show how the addition of a phonon field to the Hubbard model deforms the *superconducting* $su(2)$ part of the global symmetry Lie algebra $su(2) \otimes su(2)/\mathbb{Z}_2$, holding at half filling for the customary model, into a *quantum* $[su(2)]_q$ symmetry, holding for a filling which depends on the electron-phonon interaction strength. Such symmetry originates in the feature that in the presence of phonons the hopping amplitude turns out to depend on the coupling strength. The states generated by resorting to this new q symmetry exhibit both off-diagonal long-range order and pairing.

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The interest in itinerant interacting electron systems has been greatly revived since the discovery of high- T_c materials, for which the interplay between itinerant magnetism and insulating behavior is believed to play a relevant role. The Hubbard model [1] provides the simplest description of such systems, by assuming that the itinerant electrons interact only via an on-site Coulomb repulsion term, and it has therefore been intensively studied. In particular, it is known that at half filling the model has a $su(\tilde{2}) \oplus su(2)$ symmetry algebra [2], where $su(\tilde{2})$ refers to the magnetic part (spin conserving) and $su(2)$ to the superconducting part (number conserving) of the global symmetry. Korepin and co-workers [3] utilized the corresponding $SO(4) = SU(\tilde{2}) \otimes SU(2)/\mathbb{Z}_2$ group to prove completeness of the solution for the one-dimensional model given by Lieb and Wu [4]. Also, in 1D, such symmetry extends to an ∞ -dimensional one, generated by deformations of the corresponding Kac-Moody algebra [5]. Yang [6] showed that, due to the algebraic structure underlying the symmetry, at any filling it is possible to construct in any dimension eigenstates of the Hubbard Hamiltonian characterized by off-diagonal long-range order (ODLRO), and these can be labeled in terms of two quantum numbers connected with the above symmetry, one of which is related to the existence of superconductivity. These eigenstates can be shown to be of high energy compared to the global ground state, but for $U < 0$ turn out to be metastable states. Because of the above results, even though there is still no exact solution in more than one dimension, it has by now become clear that, at least as far as s -wave pairing is concerned, the repulsive Hubbard model itself is not able to describe a superconducting phase. Many generalizations have then been proposed in order to make it capable of exhibiting the latter feature, some of which, having in mind the role which phonons play for conventional superconductivity, explicitly consider the electron-phonon coupling as a possible mechanism for the formation of electron pairs [7].

In this Letter, we show that the addition of a phonon field to the Hubbard model, although breaking the superconductive part of the symmetry, restores it as a deformed (*quantum group*) $[su(2)]_q$ symmetry, where q is

related to the strength of electron-phonon coupling. Also, the filling at which symmetry is restored turns out to depend on the same interaction strength. Moreover, at any filling we can still build eigenstates of the Hamiltonian with nonvanishing pairing, which have energy lower than the corresponding (η -paired) states of Yang, exhibit ODLRO, and could possibly be metastable for some $U > 0$.

The grand-canonical Hubbard Hamiltonian reads

$$H_{\text{Hub}} = H_{\text{el}}^{(\text{loc})} + H_{\text{el}}^{(\text{hop})}, \quad (1)$$

where

$$H_{\text{el}}^{(\text{loc})} = \sum_j [-\mu(n_{j,\uparrow} + n_{j,\downarrow}) + Un_{j,\uparrow}n_{j,\downarrow}], \quad (2)$$

$$H_{\text{el}}^{(\text{hop})} = -\frac{1}{2}t \sum_{\langle j,\mathbf{k} \rangle} \sum_{\sigma} (a_{j,\sigma}^{\dagger} a_{\mathbf{k},\sigma} + a_{\mathbf{k},\sigma}^{\dagger} a_{j,\sigma}), \quad (3)$$

the first representing the contributions to the electron local energy, the second the nonlocal kinetic part of the energy. In (2) and (3) $a_{j,\sigma}^{\dagger}, a_{j,\sigma}$ are fermionic creation and annihilation operators ($\{a_{j,\sigma}, a_{\mathbf{k},\sigma}\} = 0$, $\{a_{j,\sigma}^{\dagger}, a_{\mathbf{k},\sigma}^{\dagger}\} = \delta_{j,\mathbf{k}} \delta_{\sigma,\sigma} \mathbb{1}$, $n_{j,\sigma} \doteq a_{j,\sigma}^{\dagger} a_{j,\sigma}$) over a d -dimensional lattice Λ ($j, \mathbf{k} \in \Lambda$, $\sigma \in \{\uparrow, \downarrow\}$), and $\langle j, \mathbf{k} \rangle$ stands for nearest neighbors (nn) in Λ . μ is the chemical potential and $U > 0$ is the on-site Coulomb repulsion between electrons [1], whereas t denotes the hopping integral of the band electrons, given by the overlap integral [8]

$$t = \int d\mathbf{r} \phi^*(\mathbf{r} - R_j) \left[-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}, \{R_l\}) \right] \phi(\mathbf{r} - R_{\mathbf{k}}), \quad (4)$$

where $\phi(\mathbf{r} - R_j)$ denotes the atomic wave function for an electron of mass m on the atom centered at site R_j of Λ , and $V(\mathbf{r}, \{R_l\})$ the crystal ion potential seen by a single electron.

As for the phonons, since only the local modes are relevant [7], they are identified—for simplicity—with an ensemble of independent Einstein oscillators, all with the same frequency ω , and may be thought of as describing nothing but the ion oscillations around the lattice posi-

tions. When one switches on the phonon field, therefore, the Hamiltonian (1) is simply changed into

$$H = H_{\text{el}}^{(\text{loc})} + H_{\text{ph}} + H_{\text{el-ph}}^{(\text{hop})}, \quad (5)$$

where

$$H_{\text{ph}} = \sum_{\mathbf{j}} \left[\frac{p_{\mathbf{j}}^2}{2M} + \frac{1}{2} M \omega^2 x_{\mathbf{j}}^2 \right]. \quad (6)$$

Here M is the ion mass and $x_{\mathbf{j}}, p_{\mathbf{j}}$ the local ion displacement and momentum operators, respectively ($[x_{\mathbf{j}}, p_{\mathbf{k}}] = i\hbar \delta_{\mathbf{j}, \mathbf{k}}$), commuting with the Fermi operators, and

$$H_{\text{el-ph}}^{(\text{hop})} = \sum_{(\mathbf{j}, \mathbf{k})} \sum_{\sigma} (t_{\mathbf{j}, \mathbf{k}} a_{\mathbf{k}, \sigma}^{\dagger} a_{\mathbf{j}, \sigma} + \text{H.c.}), \quad (7)$$

with $t_{\mathbf{j}, \mathbf{k}}$ given by the obvious generalization [9] of (4) taking into account the fact that, due to the phonon field, the orbitals should be centered at the displaced ion sites:

$$t_{\mathbf{j}, \mathbf{k}} = \int d\mathbf{r} \phi^*(\mathbf{r} - R_{\mathbf{j}} - x_{\mathbf{j}}) \left[-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}, \{R_{\mathbf{l}} + x_{\mathbf{l}}\}) \right] \times \phi(\mathbf{r} - R_{\mathbf{k}} - x_{\mathbf{k}}). \quad (8)$$

The hopping amplitude $t_{\mathbf{j}, \mathbf{k}}$ should then be thought of as an operator, commuting with all fermionic operators, depending on the phonon bosonic dynamical variables. There follows that the hopping Hamiltonian (7) turns out to be the sum of two terms: $H_{\text{el-ph}}^{(\text{hop})} = H_{\text{el-ph}}^{(\text{loc})} + H_{\text{el-ph}}^{(\text{nonloc})}$. The former, due to the direct contribution of $V(\mathbf{r}, \{R_{\mathbf{l}}\})$ to (8), is readily seen, via the usual Holstein mechanism [10] of linear variation of $V(\mathbf{r}, \{R_{\mathbf{l}}\})$ in (8) to consist essentially in a purely local term,

$$H_{\text{el-ph}}^{(\text{loc})} \approx -\lambda \sum_{\mathbf{j}} (n_{\mathbf{j}, \uparrow} + n_{\mathbf{j}, \downarrow}) x_{\mathbf{j}}, \quad (9)$$

which describes coupling of the phonons with strength λ to the charge density of the band electrons. λ (independent on site \mathbf{l}) is given by

$$\lambda \approx - \int d\mathbf{r} \phi^*(\mathbf{r} - R_{\mathbf{j}}) [\nabla_{R_{\mathbf{l}}} V(\mathbf{r}, \{R_{\mathbf{l}}\})] \phi(\mathbf{r} - R_{\mathbf{l}}). \quad (10)$$

Clearly, $\lambda \neq 0$ dynamically breaks the $\text{su}(2)$, *not* the $\text{su}(\tilde{2})$ symmetry.

On the other hand, $H_{\text{el-ph}}^{(\text{nonloc})}$ contains the contribution of the ion displacement to the hopping amplitude $t_{\mathbf{j}, \mathbf{k}}$ induced in (8) by the Laplacian, depending on the electron orbital gradients overlap integral:

$$\tilde{t}_{\mathbf{j}, \mathbf{k}} = -\frac{\hbar^2}{2m} \int d\mathbf{r} \nabla \phi^*(\mathbf{r} - R_{\mathbf{j}} - x_{\mathbf{j}}) \cdot \nabla \phi(\mathbf{r} - R_{\mathbf{k}} - x_{\mathbf{k}}). \quad (11)$$

In view of the exponential character of $\phi(\mathbf{r} - R_{\mathbf{k}})$ far from the \mathbf{k} th ion, and of the fact that $|x_{\mathbf{k}}| \ll |R_{\mathbf{k}}|$, the corresponding variation of the overlap integral $\tilde{t}_{\mathbf{j}, \mathbf{k}}$ with respect to the original amplitude t can be seen to consist [11] in the factor $\exp[\zeta(x_{\mathbf{j}} - x_{\mathbf{k}})]$, accounting for the modulus and $\exp[i\kappa(p_{\mathbf{j}} - p_{\mathbf{k}})]$ for the phase. Here ζ and

κ are real constants, the former depending ultimately, once more, on the form of the potential $V(\mathbf{r}, \{R_{\mathbf{l}}\})$ that each single ion exerts on the electron, which determines the exponential decay of the wave function $\phi(\mathbf{r})$ far from the origin; the latter depends on the lattice structure, in particular on the interatomic distance $\delta = |R_{\mathbf{j}} - R_{\mathbf{k}}|$, in view of the Bloch theorem and the fact that one can think of $(p_{\mathbf{j}} - p_{\mathbf{k}})$ as the relative variation of the electron momentum eigenvalues induced by the ion displacements. We write therefore

$$H_{\text{el-ph}}^{(\text{nonloc})} = t \sum_{(\mathbf{j}, \mathbf{k})} \sum_{\sigma} (\exp[\zeta(x_{\mathbf{j}} - x_{\mathbf{k}})] \times \exp[i\kappa(p_{\mathbf{j}} - p_{\mathbf{k}})] a_{\mathbf{k}, \sigma}^{\dagger} a_{\mathbf{j}, \sigma} + \text{H.c.}). \quad (12)$$

In a recent paper [12] it was pointed out how—in the limit in which $H_{\text{el-ph}}^{(\text{loc})}$ is retained, but $H_{\text{el-ph}}^{(\text{nonloc})}$ is approximated by $H_{\text{el-ph}}^{(\text{hop})}$ —the Hamiltonian H can be rewritten as a purely Hubbard-like anyonic oscillator Hamiltonian (whose building operators are no longer fermionic electron operators, but satisfy a q -deformed Gel'fand-Fairlie algebra [13]) plus H_{ph} .

In the following we shall show how a global symmetry of the model described by the complete H in (5) might in fact be restored at the *quantum group* level [14]. In other words we look for a global symmetry algebra of the form $\text{su}(\tilde{2}) \oplus [\text{su}(2)]_q$. We shall do this following the same scheme used by Yang and Zhang in [2], constructing first a local $[\text{su}(2)]_{q, \mathbf{j}}, \mathbf{j} \in \Lambda$, and requiring that it commute with the \mathbf{j} th part of the local Hamiltonian, $H^{(\text{loc})} = H_{\text{ph}} + H_{\text{el}}^{(\text{loc})} + H_{\text{el-ph}}^{(\text{loc})}$, and extending it successively to a global $[\text{su}(2)]_q$ generating a symmetry of the whole Hamiltonian H .

Dealing first with the local symmetry, we set

$$K_{\mathbf{j}}^{(+)} = e^{-i\phi_{\mathbf{j}}} a_{\mathbf{j}, \uparrow}^{\dagger} a_{\mathbf{j}, \downarrow}^{\dagger}, \quad K_{\mathbf{j}}^{(-)} = K_{\mathbf{j}}^{(+)\dagger}, \quad (13)$$

$$K_{\mathbf{j}}^{(z)} = \frac{1}{2} (n_{\mathbf{j}, \uparrow} + n_{\mathbf{j}, \downarrow} - 1).$$

The three operators $K_{\mathbf{j}}^{(\gamma)}$, $\gamma = \pm, z$, close both under a quantum $[\text{su}(2)]_q$ algebra [15] with $q = e^{-\alpha}$, $\alpha \in \mathbb{C}$ arbitrary:

$$[K_{\mathbf{j}}^{(z)}, K_{\mathbf{j}}^{(\pm)}] = \pm K_{\mathbf{j}}^{(\pm)}, \quad [K_{\mathbf{j}}^{(+)}, K_{\mathbf{j}}^{(-)}] = [2K_{\mathbf{j}}^{(z)}]_q \quad (14)$$

(where the notation, standard in quantum group theory, $[x]_q = (q^x - q^{-x}) / (q - q^{-1}) = \sinh(\alpha x) / \sinh \alpha$ was used), as well as under a customary $\text{su}(2)$ Lie algebra $([K_{\mathbf{j}}^{(+)}, K_{\mathbf{j}}^{(-)}] = 2K_{\mathbf{j}}^{(z)})$, since $[2K_{\mathbf{j}}^{(z)}]^{2n+1} = 2K_{\mathbf{j}}^{(z)}$ ($n \geq 0$) in the representation adopted.

It is straightforward to check that $H^{(\text{loc})}$ commutes with all the above $K_{\mathbf{j}}^{(\gamma)}$'s, provided the conditions $\phi = 2\xi$ and $\mu = \frac{1}{2}(U - 4\lambda\xi)$ are satisfied, with $\xi = \lambda/M\omega^2$ [observe that for $\xi = 0$ the former leads to the customary fermionic realization of $\text{su}(2)$ and the latter reduces to the condition of half filling]. Even when the two above conditions do not hold, the local Hamiltonian commutes with

$K_j^{(z)}$, in which case the local symmetry reduces to $u(1)$.

We intend to show first that the global extension to the whole lattice Λ of the above local algebras gives rise to a physically nontrivial symmetry of the Hamiltonian (5) only in the quantum algebra case.

In view of the adoption of the quantum group scheme, the correct extension must naturally be performed resorting to the notion of coproduct. For $[\text{su}(2)]_q$ the Cartan element $K^{(z)}$ is primitive, and its coproduct $\Delta(K^{(z)}) = \mathbb{I} \otimes K^{(z)} + K^{(z)} \otimes \mathbb{I}$, whereas

$$\Delta(K^{(+)}) = e^{\alpha K^{(z)}} \otimes K^{(+)} + K^{(+)} \otimes e^{-\alpha K^{(z)}}, \tag{15}$$

$$\Delta(K^{(-)}) = [\Delta(K^{(+)})]^\dagger.$$

Notice that in the limiting case $\alpha=0$ such a coproduct turns into the usual tensor product. For the sake of simplicity, and without any loss of generality in the thermodynamic limit, we assume the lattice number of sites N of the form $N=2^v$; hence the extension to the whole Λ of the local $[\text{su}(2)]_q$ is given by $\hat{K}^{(\gamma)} = \Delta^{(v)}(K^{(\gamma)})$, $\gamma = \pm, z$, with the iterated coproduct defined through $\Delta^{(n+1)}(K^{(\gamma)}) = \Delta(\Delta^{(n)}(K^{(\gamma)}))$. Explicitly,

$$\hat{K}^{(z)} = \sum_j K_j^{(z)} \equiv \sum_j \mathbb{I} \otimes \dots \otimes \mathbb{I} \otimes K^{(z)} \otimes \mathbb{I} \dots \otimes \mathbb{I},$$

$$\hat{K}^{(+)} \equiv [\hat{K}^{(-)}]^\dagger = \sum_j e^{i\mathbf{G} \cdot \mathbf{j}} \prod_{\mathbf{k} < \mathbf{j}} e^{\alpha K_{\mathbf{k}}^{(z)}} K_j^{(+)} \prod_{\mathbf{k} > \mathbf{j}} e^{-\alpha K_{\mathbf{k}}^{(z)}} \equiv \sum_j e^{i\mathbf{G} \cdot \mathbf{j}} e^{\alpha K^{(z)}} \otimes \dots \otimes e^{\alpha K^{(z)}} \otimes K^{(+)} \otimes e^{-\alpha K^{(z)}} \dots \otimes e^{-\alpha K^{(z)}}. \tag{16}$$

Here the multiple tensor products consist of N factors, the single one of which not equal to the identity \mathbb{I} (or to the exponential of $K^{(z)}$) is at position \mathbf{j} . Also, following [2], we redefined the local generator $K_j^{(+)}$ (13) with a multiplicative phase factor $\exp(i\mathbf{G} \cdot \mathbf{j})$ (\mathbf{G} is a vector with all its components equal to π). This of course does not affect the structure of the algebra and will allow us to deal with the nn hopping term in the correct way. Moreover, we introduced the notation $\mathbf{k} > \mathbf{j}$ or $\mathbf{k} < \mathbf{j}$ with respect to the arbitrary order of the lattice sites adopted in the direct product.

The global $[\text{su}(2)]_q$ defined above manifestly commutes with $H^{(\text{loc})}$. The requirement that H has $\text{su}(2) \oplus [\text{su}(2)]_q$ as global symmetry thus reduces to checking that $[H_{\text{el-ph}}^{(\text{nonloc})}, [\text{su}(2)]_q] = 0$. On the other hand, as the hopping term in H conserves the total number of electrons, in view of its definition $\hat{K}^{(z)}$ always commutes with H . The symmetry condition implies therefore simply that $[H_{\text{el-ph}}^{(\text{nonloc})}, \hat{K}^{(\pm)}] = 0$. A lengthy but straightforward calculation shows that this happens if the parameter α , so far undefined, has real part $\text{Re}\alpha = 2\zeta\kappa/\hbar$, and κ is constrained by the condition $\kappa = \xi$. Naturally the former condition suggests that α can be chosen to be real. The above discussion shows that only $\zeta=0$ implies $\alpha=0$; thus the quantum symmetry can be ignored only if the effect of ion displacements due to the phonon field on the hopping amplitude is neglected. It should be remarked, on the other hand, that setting $\zeta=0$, but still keeping $\kappa = \xi$, generates a Hamiltonian which, by a unitary transformation R essentially equal to the inverse of that of Lang-Firsov [16,17] [$R = \exp(i\xi \sum_j p_j (n_{j,1} + n_{j,1}))$], can be reconducted to one describing a system of interacting electrons plus a field of phonons (uncorrelated with electrons). It should moreover be pointed out that the conditions that guarantee quantum symmetry impose two constraints, $\kappa = \xi$, $\mu = \frac{1}{2}(U - 4\lambda^2/M\omega^2)$, among the four physical parameters λ , U , ω , and the filling n_0 (through the chemical potential μ), in terms of the atomic parameters M , ξ , and ζ . As discussed above, among the latter, ζ has only the

role of fixing the quantum group deformation parameter q .

Following an argument quite similar to that of Yang [6], we now consider the family of states $|\psi_n\rangle$, characterized by nonvanishing pairing (referred to as η pairing), of the generic form

$$|\psi_n\rangle = \frac{1}{\sqrt{\mathcal{N}_\eta}} (\eta^\dagger)^n |\text{vac}\rangle, \tag{17}$$

where, however, the η -pairing operator is phonon dependent, defined, in terms of the set of parameters $w, \{\vartheta_j\}$, by

$$\eta^\dagger = \sum_j e^{i\vartheta_j} a_{j,1}^\dagger a_{j,1}^\dagger e^{i w p_j}, \quad w, \vartheta_j \in \mathbb{R}, \tag{18}$$

and $\mathcal{N}_\eta^{-1} = n!N!/(N-n)!$. A direct calculation shows that the state among the $|\psi_n\rangle$'s, which minimizes the energy expectation $\mathcal{E}_n = \langle \psi_n | H | \psi_n \rangle$ with respect to w has $w = 2\xi$ ($\equiv \phi$) and gives $\mathcal{E}_n = \frac{1}{2} \hbar \omega N$, which are the same values as for the q -symmetric eigenstates $|\phi_n\rangle = (1/\sqrt{\mathcal{N}}) \times (\hat{K}^{(+)})^n |\text{vac}\rangle$ of H . Here the normalization is

$$\mathcal{N}^{-1} = \prod_{l=0}^{n-1} \left(\sum_{p=0}^l \left[\frac{N}{2} - p \right]_q \right) = \frac{[n]_q! [N]_q!}{[N-n]_q!}.$$

Both Yang's η -paired state [6] and the BCS ground state turn out to have—for the filling corresponding to full symmetry—energy $\mathcal{E}_n + 2\lambda^2/M\omega^2 > \mathcal{E}_n$.

If the chemical potential does not fulfill the symmetry condition, it is still possible to work out eigenstates of H , due to the fact that $[H, \hat{K}^{(\pm)}] = \delta \mathcal{E} \hat{K}^{(\pm)}$, with $\delta \mathcal{E} = U - 2\mu - 4\lambda^2/M\omega^2$, and starting from any eigenstate $|\mathcal{E}\rangle$ of H one can construct a sequence of other eigenstates in the form $[\hat{K}^{(\pm)}]^n |\mathcal{E}\rangle$, $n \leq N$, with decreasing energy eigenvalues $\mathcal{E}'_n = \mathcal{E} + n\delta \mathcal{E}$, provided $\mu + 2\lambda^2/M\omega^2 > \frac{1}{2}U$. μ here is to be intended as a parameter, and a detailed analysis of its dependence on the filling would require the knowledge of the ground state of the system, or some ansatz about it, which is beyond the purposes of the present

paper. Moreover, as in the case analyzed by Yang, the state $|\phi_n\rangle$ exhibits ODLRO [18], in that for large $(\mathcal{O}(N))|r-s|$, the expectation value

$$\langle \phi_n | a_s^\dagger | a_s^\dagger | a_r | a_r | \phi_n \rangle$$

equals

$$e^{i\mathbf{G}\cdot(\mathbf{r}-\mathbf{s})} e^{a(N+1-|\mathbf{r}+\mathbf{s}|)} \frac{[N-1]_q}{[N]_q} \neq 0, \quad (19)$$

where

$$\begin{bmatrix} N \\ n \end{bmatrix}_q = \frac{[N]_q!}{[n]_q! [N-n]_q!}$$

is the *quantum* binomial coefficient. The states $|\phi_n\rangle$ manifestly have *pairing* as well. It is worth noticing that $|\phi_n\rangle$ cannot be the ground state because, provided that $w=2\xi$, $|\psi_n\rangle$ gives the same \mathcal{E}_n for whatever value of the phase θ_j in (17), whereas only for $\theta_j=\pi|\psi_n\rangle$ is an eigenstate of H . Nevertheless one could argue that, similarly to what happens in Yang's case, for $\delta\mathcal{E} < 0$, $|\phi_n\rangle$ turns into a metastable state.

In conclusion, one can thus observe that the superconducting eigenstates $|\phi_n\rangle$ of a Hamiltonian of the form (5) for systems whose ionic structure implies that the constraint $\kappa=\xi$ is satisfied by the parameters could be favorable also for some range of positive U values, immediately upon doping away from the filling at which the q symmetry holds. Moreover, switching off of the phonon field raises the paired states energy.

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