Superconducting Coherent States for an Extended Hubbard Model

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Abstract

An extended Hubbard model with phonons is considered. q-coherent states relative to
the superconducting quantum symmetry of the model are constructed and their properties
studied. It is shown that they can have energy expectation lower than eigenstates constructed
via conventional processes and that they exhibit ODLRO.

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The Hubbard model [1], despite its simplicity, is certainly one of the important tools in
condensed matter physics. It is one of the simplest models to describe itinerant interacting
electrons on a lattice (for review see e.g. [2]). It is also believed that it may be used for the
description of high Tc-superconductivity.

In [3], the so-called η-pairing mechanism of superconductivity was introduced. This allows
the construction of states exhibiting off-diagonal long range order (ODLRO) which is regarded
as a definition for superconductivity [4]. The η operators involved in this construction generate
an su(2) algebra. More precisely, it has been shown [5] that the standard Hubbard model
have a SO(4) = SU(2) × SU(2)/Z₂ symmetry. The first SU(2) symmetry (spin symmetry)
is useful for the description of the antiferromagnetic properties of the electron systems. The
second SU(2) symmetry (pseudo spin), when broken, is responsible of the superconductivity
of the model.

In [6], an extended Hubbard model with phonons was shown to violate the superconduct-
ing SU(2) symmetry and that it can be only restored as a quantum (deformed) Uq(su(2))
symmetry.

In this letter, motivated by an idea [7] that coherent states [8, 9, 10] may be very relevant
for the study of the standard Hubbard model, we introduce q-coherent states related to the
extended Hubbard model of [6]. These states are nothing but the coherent states related to
the quantum algebra Uq(su(2)) (see e.g. [11]) and are shown to have, under some conditions,
energy expectation lower than states constructed through the η-pairing mechanism and even
from the Hamiltonian eigenstates constructed in [6]. We also show that this q-coherent states
exhibit ODLRO and are thus superconducting.

First, we begin by some preliminaries about the Hubbard model and recall the extended
one.

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Consider a D-dimensional lattice, $\Lambda$, with $L$ sites. The standard Hubbard Hamiltonian describing a system of itinerant interacting electrons in $\Lambda$, written in a grand-canonical formalism, is

$$H' = H'_{el}^{(loc)} + H_{el}^{(non-loc)}$$

where

$$H_{el}^{(loc)} = \sum_{i \in \Lambda} \left(-\mu(n_{i,\uparrow} + n_{i,\downarrow}) + u n_{i,\uparrow} n_{i,\downarrow}\right),$$

$$H_{el}^{(non-loc)} = \frac{1}{2} \sum_{<i,j>} \sum_{\sigma=\uparrow,\downarrow} (a_{i,\sigma}^+ a_{j,\sigma} + a_{j,\sigma}^+ a_{i,\sigma}).$$

We have used the conventional notations, namely,

- $a_{i,\sigma}$ and $a_{i,\sigma}^+$ are the canonical Fermi operators describing electrons on the lattice $\Lambda$ and obey the usual anticommutation relations.
- $i$ and $j$ are (real space) sites in $\Lambda$ and $<i,j>$ means that the summation is carried over nearest neighbor sites.
- $\sigma = \downarrow, \uparrow$ denoting spin down and spin up respectively.
- $n_{i,\sigma} = a_{i,\sigma}^+ a_{i,\sigma}$ denotes the number operator of electrons with spin $\sigma$ at site $i$.
- $\mu$ is the chemical potential, $u$ the on site repulsion energy and $t$ the hopping amplitude.

The model described by (1) has a natural $SU(2) \times SU(2)/\mathbb{Z}_2$ symmetry at half filling. The first $SU(2)$ symmetry, usually called spin or magnetic symmetry, is generated by the following spin operators

$$S^+ = \sum_{i \in \Lambda} a_{i,\uparrow}^+ a_{i,\downarrow}, \quad S^- = (S^+)^\dagger, \quad S^z = \frac{1}{2} \sum_{i \in \Lambda} (n_{i,\uparrow} - n_{i,\downarrow})$$

and is reminiscent of the antiferromagnetic properties of the system, see e.g. [2].

The second $SU(2)$ symmetry is generated by the $\eta$-pairing operators

$$\eta^+ = \sum_{i \in \Lambda} a_{i,\uparrow}^+ a_{i,\downarrow}^+, \quad \eta = (\eta^+)^\dagger, \quad \eta^z = \frac{1}{2} (N - L),$$

where $N = \sum_{i \in \Lambda} n_i := \sum_{i \in \Lambda} \sum_{\sigma=\uparrow,\downarrow} n_{i,\sigma} = \sum_{i \in \Lambda} n_{i,\uparrow} + n_{i,\downarrow}$ denotes the total number operator.

It is this latter symmetry that, when broken, leads to superconducting $\eta$-paired eigenstates of the Hamiltonian (for this reason it is called a superconducting symmetry).

Both symmetries can still be conserved when some additional terms and interactions are added to the Hamiltonian (1), see e.g. [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. However this is not the case in [1].

Montorsi and Rasetti considered the extension of the Hubbard model, described by (1), by including phonons in it to describe the ion vibrations. The relevant Hubbard Hamiltonian then is

$$H = H_{el}^{(loc)} + H_{ph}^{(loc)} + H_{el-ph}^{(loc)} + H_{non-loc}^{(non-loc)}.$$ ($6$)

$H_{el}^{(loc)}$ is given in (2), the other terms are

$$H_{ph}^{(loc)} = \sum_{i \in \Lambda} \frac{p_i^2}{2M} + \frac{1}{2} M \omega^2 x_i^2,$$

$$H_{el-ph}^{(loc)} = -\lambda \sum_{i \in \Lambda} (n_{i,\uparrow} + n_{i,\downarrow}) x_i,$$

$$H_{non-loc}^{(non-loc)} = \sum_{<i,j>} \sum_{\sigma=\uparrow,\downarrow} (t_{ij} a_{j,\sigma}^+ a_{i,\sigma} + h.c.).$$
where the hopping amplitude depends now on the ion displacement and is given by

\[ t_{ij} = t \exp \left\{ \zeta (x_i - x_j) \right\} \exp \left\{ ik(p_i - p_j) \right\}. \]  

(10)

For latter use we also define the q-factorial function as 

\[ [n]_q = \frac{q^n - 1}{q - 1} = \frac{\sinh(\alpha X)}{\sinh(\alpha)}. \]  

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(14)

The first constraint being the analogue of the half-filling requirement in the standard Hubbard model (i.e. \( \lambda = 0 \)). The second one constraining the choice of the parameter \( \phi \).

The extension of this local symmetry to a global one over \( \Lambda \) is achieved by means of the corresponding coproduct \( \Delta \). Note that, to be able to do this, is necessary to adopt some ordering of lattice sites.

The resultant (global) \( U_q (\mathfrak{su}(2)) \) algebra is generated by

\[ K^{(+)} = \sum_{j \in \Lambda} e^{iGJ} \prod_{k<j} e^{\alpha K_{ij}^{(z)}} K_{ij}^{(+)} \prod_{k>j} e^{-\alpha K_{ij}^{(z)}} \]  

(15)

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

(16)

The phase factor \( e^{GJ} \), with \( G = (\pi, ..., \pi) \), will be useful in what follows.

The above quantum algebra \( U_q (\mathfrak{su}(2)) \) describes a global symmetry of the model (i.e. the generators \( \{15, 19\} \)) if and only if

\[ \text{Re}(\alpha) = \frac{2\phi}{\hbar} \quad \text{and} \quad k = 2\phi, \]  

(17)

in addition to these two constraints, in \( \{12\} \) it has been shown that there are also additional constraints on the ordering of the lattice sites for the symmetry to hold. The authors of \( \{17\} \) thus concluded that this symmetry holds only on one-dimensional lattices.
The first relation in (18) gives a constraint on the real part of $\alpha$, so that its complex part can be chosen arbitrarily, without loss of generality we will take it null. The second relation, mainly, means that we can interpret $\phi_2$ as the parameter of a Lang-Firsov transformation [17].

In their paper [6] Montorsi and Rasetti also constructed eigenstates for the Hamiltonian (6) with energy expectation lower (or at least equal) to that of states constructed via the conventional $\eta$-pairing mechanism. These states are constructed from the vacuum state by successive action of the operator $K^{(+)}$:

$$|\phi_n> = \beta(n, L) \left(K^{(+)}\right)^n |vac>,$$

where the normalization constant is given by

$$\beta(n, L) = \left(\frac{[L-n]!}{[L]! [n]!}\right)^{1/2}.$$  

This is the case when the $U_q(su(2))$ symmetry holds.

When the model parameters have values such that this symmetry does not hold any more, one can still prove the following relation

$$[H, K^{(\pm)}] = \pm E K^{(\pm)},$$

where

$$E = u - 2\mu - \frac{4\lambda^2}{M\omega^2}.$$  

Now that we have reminded all the necessary materials, we can start developing our idea. This is an adaptation of an idea anticipated by Solomon and Penson in [7] for a standard Hubbard model ($SU(2)$ symmetry). In fact, they have used coherent (pairing) states in studying the Hubbard model and proved that this states can be useful for the description of the model. In the following, we shall follow a similar reasoning and use $q$-coherent states for the description of Montorsi and Rasetti’s Hubbard model.

Since this model have $U_q(su(2))$ symmetry it is natural to use $q$-coherent states, for instance see [11] and references therein.

The definition we adopt for this states is the following

$$|\nu> = N^{-\frac{1}{2}}(|\nu|^2) \exp_q(\nu K^{(-)}) |\phi_L>.$$  

Note that we have used the maximal state

$$|\phi_L> = \frac{1}{[L]!} \left(K^{(+)}\right)^L |vac>,$$

and the deformed exponential function

$$\exp_q = \sum_{n=0}^{\infty} \frac{x^n}{[n]_q!}.$$  

The normalization constant in (23) can easily be computed using some standard q-series technics [20] and is given by

$$\mathcal{N}(|\nu|^2) = (1 + |\nu|^2)^L_q$$

$$:= \prod_{k=1}^{L} \left(1 + q^{L-2k+1} |\nu|^2\right)$$

$$= \sum_{n=0}^{L} |\nu|^{2n} \left[ L \atop n \right] q.$$  

where the q-binomial is defined by
\[
\binom{L}{n}_q = \frac{[m]_q!}{[n]_q![m-n]_q!}.
\] (27)

The states |ν⟩ are clearly not eigenstates of the Hamiltonian (6) since the y involve eigenstates (|φn⟩) with different n’s. They possess, however, many interesting properties that we shall derive in the following.

First of all, let us notice that in the limit \( L \rightarrow \infty \), |ν⟩ is an eigenstate of \( K^{(\pm)} \sqrt{[L]_q} \). Thus, it (|ν⟩) can be seen as a q-harmonic oscillator coherent state, see e.g. [21]. This is not surprising since in the standard Hubbard model the coherent states constructed in [7] behave similarly, i.e. in that limit their coherent state is seen as a (standard) harmonic oscillator coherent state.

Let us evaluate the energy expectation in a q-coherent state (23). For this purpose we will use the following formulae, derived from (21 - 22),
\[
[H, (K^{(\pm)})^n] = \pm n E (K^{(\pm)})^n, \quad [H, \exp_q(\nu K^{(-)})] = -\nu E K^{(-)} \exp_q(\nu K^{(-)}).\] (28)

We obtain the following formula for the desired expectation value
\[
\langle \nu | H | \nu \rangle = N^{-1} \langle |\nu|^2 \rangle E \sum_{n=0}^{L} |\nu|^2 n \binom{L}{n}_q \langle \nu | (L-n) \rangle \] (29)
or, equivalently,
\[
\langle \nu | H | \nu \rangle = LE - N^{-1} \langle |\nu|^2 \rangle E \sum_{n=0}^{L} |\nu|^2 n \binom{L}{n}_q \] (30)

In contrast with the results of [7], this formula for the energy expectation can not be further simplified. However, it is easy to see its behavior as the different parameters involved change. For instance, in the limit \( q \rightarrow 1 \), as expected, one recovers a similar formulae to that obtained in [7].

Also, using the fact that \( [n]_q \geq n \) is always true, it is easy to see that as \( q \) tends to 1 the energy expectation (29) tends to \( E \) and after a critical value of \( q \) it gets even smaller than it.

All this is confirmed by the plots (see plot a, plot b and plot c).

Another important feature of the q-coherent states [24] is that they exhibit off-diagonal long range order (ODLRO) [4] and thus are superconducting states. In fact, the relevant off-diagonal matrix element of the reduced density matrix \( \rho_2 \), by considering the states |φn⟩, is equal to \( \langle \phi_n | a_{s,\uparrow} a_{r,\downarrow} a_{r,\uparrow} a_{s,\downarrow} | \phi_n \rangle \). And it was found [6] to be equal to
\[
e^{iG(r-s)} e^{\alpha (N+1-|r-s|)} \binom{L}{n-1}_q \binom{L}{n}_q \neq 0.\] (31)

Using this result and [24], one can show that the relevant expectation value to be evaluated, \( \langle \nu | a_{s,\uparrow} a_{s,\downarrow} a_{r,\downarrow} a_{r,\uparrow} | \nu \rangle \), equals
\[
e^{iG(r-s)} e^{\alpha (N+1-|r-s|)} \left\{ \frac{1 + |\nu|^2}{|\nu|^2} - \frac{N^{-1} \langle |\nu|^2 \rangle}{|\nu|^2} \right\} \] (32)
which is also different from zero (for large values of $|r - s|$). Thus the $q$-coherent states $|\nu\rangle$ are superconducting.

As a matter of fact, this is not surprising. It has been argued in [13, 15] that superconductivity based on $\eta$-pairing is a generic rather than an exotic phenomenon. On the other hand the states $|\phi_n\rangle$ were shown to have pairing [6]. Moreover, the coherent states of [7], which were constructed using an $\eta$-paired state, posses ODLRO. All these, permit us to conclude that superconductivity of coherent states, constructed from states which possess pairing, is not an exotic phenomenon.

In summary, we have constructed $q$-coherent states for the superconducting $U_q(su(2))$ symmetry of an extended Hubbard model with phonons. We have shown that they have energy expectation lower than that of the eigenstates $|\phi_n\rangle$ constructed in [6]. It was also shown that these states exhibit ODLRO, thus are superconducting. We concluded that these property (ODLRO) should be expected for any coherent states constructed using pairing states.

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Energy expectation $\langle \nu | H | \nu \rangle$, eq(29), versus:
- $|\nu|$ for $q = 0, 9, L = 10$ and normalized $E$; Plot a.
- $q$ for $|\nu| = 3, L = 10$ and normalized $E$; Plot b.
- $|\nu|$ and $q$ for $L = 10$ and normalized $E$; Plot c.