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APPROXIMATION

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On a q -covariant form of the BCS approximation

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Abstract

A quantum group formulation of the many-body BCS approximation for a pure pairing force in terms of $SU_q(N)$ -covariant fermion operators is presented. A set of quantum BCS equations is derived, as well as a q -analog to the gap equation. The quantum occupation probabilities and gap are shown to depend explicitly on the quantum parameter.

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In the last few years, q -deformed algebraic methods have been of much interest in many-body physics [1–9]. In the framework of the q -deformed quasi-spin algebra, the phenomenology of nuclear rotational states [1–4], the pairing problem for a single j -shell [5] and the Lipkin-Meshkov-Glick model [8,9], to quote some, were studied (for a brief review on these topics, see [10]); a recent application of this formalism to boson expansion methods can be found in ref. [11]. Nonetheless, the q -fermionic theory used in previous works, following [12–15], is a generalization - or *deformation* - of the usual one, compatible with the standard Drinfel'd-Jimbo quantization of $\mathcal{U}(su(2))$ rather than strictly covariant under some linear quantum group transformations [16–18]. This fact originated some confusion, mainly with respect to the language adopted in the literature, but we hope that concepts here will be clearly defined.

Recently, Ubrico [19] has studied thermodynamical properties of a free quantum group fermionic system with two “flavors”. In particular, it was given there a $SU_q(N)$ -covariant representation of the fermionic algebra for arbitrary N in terms of ordinary creation and annihilation operators. This enables one to attempt the construction of a quantum group invariant second quantized Hamiltonian for an arbitrary fermionic system. In this paper we propose a construction of the Bardeen-Cooper-Schrieffer (BCS) many-body formalism [20,21] for a pure pairing force in which the usual fermions are replaced by quantum group covariant ones satisfying appropriate anticommutation relations for a $SU_q(N)$ -fermionic algebra. Our main purposes are: 1) to study, in a simple case, the effects of introducing q -covariance in a many fermion system, 2) to introduce a many-body model based on quantum group covariance rather than in q -deformed fermionic symmetry and 3) to obtain the first results concerning with the application of the BCS framework in the $q \neq 1$ realm. In what follows, we write the quantum invariant pairing Hamiltonian and BCS vacuum wave function and apply the standard variational process to the this wave function obtaining the q -analog to the BCS and gap equations.

We will work in the usual spherical basis $\{j, -j \leq m \leq j\}$ and use the BCS phases for convenience (we are allowed to use BCS phases irrespectively of quantum group angular

momentum coupling coefficients because the coupling between $|j_1 j_2 m_1 m_2\rangle$ and $|j_1 j_2 IM\rangle$ states is unique and independent of q , see ref. [22]). In this basis, the usual BCS vacuum wave function is written in terms of particle operators as [21]:

$$|BCS\rangle = \prod_{jm>0} [u_j + v_j c_{jm}^\dagger c_{j-m}^\dagger] |0\rangle, \quad (1)$$

where the u_j and v_j are variational coefficients, c_{jm} and c_{jm}^\dagger are the usual particle fermion operators satisfying $\{c_{jm}, c_{j'm'}^\dagger\} = \delta_{jj'} \delta_{mm'}$ with all other anticommutators vanishing and $|0\rangle$ is the bare vacuum state. We assume that we can rewrite the wave function (1) as a quantum group invariant one in the following fashion:

$$|BCS\rangle_q \doteq \prod_{jm>0} [u_j^q + v_j^q C_{jm}^\dagger C_{j-m}^\dagger] |0\rangle_q, \quad (2)$$

where the operators C_{jm} and C_{jm}^\dagger play the role of creation and annihilation operators for $SU_q(2j+1)$ -fermions within the j -shell with angular momentum projection m . The q -bare vacuum ket is a vector in the product Fock space defined through $C_{jm} |0\rangle_q = 0$. The superscripts on the occupation probabilities mean that these quantities may now depend upon the quantum parameter q . Now, the q -fermion operators C_{jm} and C_{jm}^\dagger are required to satisfy an algebra covariant under quantum group transformations; we clearly want this algebra to act on *physical* vectors, that is, we want it to have a representation in the direct product Fock space generated by the eigenstates $|n_{j=1/2}, n_{j=3/2}, \dots\rangle = \prod_{jm} \otimes |n_j\rangle$ of the operator $N = \sum_{jm} c_{jm}^\dagger c_{jm}$ (we use n_j as a shorthand for n_{jm} , $n_j = \{n_{jm}\}$). If we put the quantum group operators in one-to-one correspondence with differentials in the quantum plane, then a q -fermionic algebra explicitly invariant under linear $SU_q(2j+1)$ transformations can be cast in the form (we assume real q and consider $q > 0$) [18,23]:

$$C_{jk} C_{jl} + q \mathcal{R}_{lkmn} C_{jm} C_{jn} = 0; \quad (3)$$

$$C_{jk} C_{jl}^\dagger + q^{-1} \mathcal{R}_{kmnl} C_{jm}^\dagger C_{jn} = \delta_{kl} \quad (4)$$

(sum over repeated indices), where $-j \leq \mu \leq j$, $\mu = k, l, m, n$ with the matrix $\mathcal{R}_{klmn} = \delta_{lm} \delta_{kn} [1 + (q-1)\delta_{kl}] + \delta_{km} \delta_{ln} \theta(m-k)(q-q^{-1})$, with the usual theta function $\theta(x-y)$

($\mathcal{R} = PR$, where P is the permutation matrix and R is the R -matrix of $GL_q(2j+1)$). It is easy to check that in the classical limit $q = 1$ these expressions become the usual $SU(2j+1)$ -invariant anticommutation relations for fermions. For a given j , a representation of this algebra can be given by [19]:

$$C_{jm} = c_{jm} \prod_{i=m+1}^j (1 + (q^{-1} - 1)c_{ji}^\dagger c_{ji}); \quad (5)$$

$$C_{jm}^\dagger = c_{jm}^\dagger \prod_{i=m+1}^j (1 + (q^{-1} - 1)c_{ji}^\dagger c_{ji}). \quad (6)$$

The q -fermions for various j orbits are given by $\mathcal{C} = \prod_j \otimes \mathcal{A}_j$, where \mathcal{A}_j is the algebra (3, 4).

The products in (5) and (6) can be written as:

$$\begin{aligned} M_{jm} &\doteq \prod_{i=m+1}^j (1 + (q^{-1} - 1)c_{ji}^\dagger c_{ji}) = 1 + \sum_{i_1=m+1}^j (q^{-1} - 1)c_{ji_1}^\dagger c_{ji_1} + \\ &+ \sum_{i_2 > i_1 = m+1}^j (q^{-1} - 1)^2 c_{ji_1}^\dagger c_{ji_1} c_{ji_2}^\dagger c_{ji_2} + \dots + (q^{-1} - 1)^{j-m} c_{jm+1}^\dagger c_{jm+1} \dots c_{jj}^\dagger c_{jj}. \end{aligned} \quad (7)$$

It is easy to see that the c_{jm} and c_{jm}^\dagger commute with M_{jm} . We may interpret the action of this operator on a given state as taking into account, in some effective way, not only the mean-field strength but also two-body and higher order contributions (a similar interpretation has already appeared in the literature when the consequences of q -deformation were concerned). Let us now assume that we can expand in a convergent manner the q -bare vacuum as:

$$|0\rangle_q \equiv \sum \dots \sum_{n_j=0}^{2j+1} \dots \sum \dots \xi(q, n_{j=1/2}, n_{j=3/2}, \dots) |n_{j=1/2}, n_{j=3/2}, \dots\rangle, \quad (8)$$

where the coefficients should satisfy $\xi(q = 1, 0, 0, \dots) = 1$ and $\xi(q = 1, \dots, 0, 0, n_j \neq 0, 0, 0, \dots) = 0$. Acting on the vacuum state with the operator C_{jm} , we obtain:

$$\begin{aligned} C_{jm} |0\rangle_q &= \sum \dots \sum_{n_{j'}=0}^{2j'+1} \dots \sum \dots \xi(q, n_{j'=1/2}, n_{j'=3/2}, \dots) \times \\ &\times m_{jm}(n_{j'=1/2}, n_{j'=3/2}, \dots) c_{jm} |n_{j'=1/2}, n_{j'=3/2}, \dots\rangle = 0, \end{aligned} \quad (9)$$

with $m_{jm} \geq 1$ the eigenvalue of M_{jm} (which can be immediately inferred from (7)). We should note that all states with occupation number n_{jm} originally equal to zero are automatically excluded from the sum; therefore, since all the state kets are orthogonal, all the coefficients corresponding to states with n_{jm} originally equal to one must vanish. But j and m are arbitrary, which implies that:

$$|0\rangle_q = \alpha e^{i\theta} |0\rangle. \quad (10)$$

Here the factor $\alpha e^{i\theta}$ is undefined, and we choose $\alpha^2 = 1$ independently of q . (Note that, due to $M_{jm} |0\rangle = |0\rangle$, $C_{jm} |0\rangle = 0$; with this it is shown the uniqueness of a ray in the product Fock space which is annihilated by the operator C_{jm} .) Thence, the BCS q -covariant vacuum ket reads:

$$\begin{aligned} |BCS\rangle_q &= \prod_{jm} [u_j^q + v_j^q C_{jm}^\dagger C_{j-m}^\dagger] |0\rangle = \prod_{jm} [u_j^q + v_j^q c_{jm}^\dagger c_{j-m}^\dagger M_{jm} M_{j-m}] |0\rangle = \\ &= \prod_{jm} [u_j^q + v_j^q c_{jm}^\dagger c_{j-m}^\dagger] |0\rangle. \end{aligned} \quad (11)$$

(The superscripts will hereafter be omitted in v_j^q and u_j^q). We now turn to the expression of the q -Hamiltonian. We are interested in a pure pairing Hamiltonian, whose $q = 1$ version we write as [21]:

$$H = \sum_{jm} \epsilon_j c_{jm}^\dagger c_{jm} - G \sum_{jj'm_1m_2} c_{jm_1}^\dagger c_{j-m_1}^\dagger c_{j'-m_2} c_{j'm_2}, \quad (12)$$

where G is the pairing strength and the ϵ_j are the single-particle energies; here we understand that the indices m_1 and m_2 are greater than zero. We write a q -Hamiltonian following expression (12) in the form:

$$H_q \doteq \sum_{jm} \epsilon_j c_{jm}^\dagger c_{jm} (M_{jm})^2 - G \sum_{jj'm_1m_2} c_{jm_1}^\dagger c_{j-m_1}^\dagger M_{jm_1} M_{j-m_1} c_{j'-m_2} M_{j'-m_2} c_{j'm_2} M_{j'm_2}. \quad (13)$$

One can observe that the "mean-field" term in (13) already contains explicit interaction among different levels (see also eq. (16) of ref. [19]). Using expression (7), and anticommutation properties of ordinary fermion operators, one can perform straightforwardly the calculation of the mean-value of (13) between $|BCS\rangle_q$ states. The result is:

$$\begin{aligned}
{}_q\langle BCS|H_q|BCS\rangle_q &= \sum_j \epsilon_j v_j^2 \times \frac{\left(\frac{1}{q}\right)^{4\Omega_j} - 1}{\left(\frac{1}{q}\right)^2 - 1} - G \sum_{j \neq j'} v_j v_{j'} u_j u_{j'} \times \left(\frac{1}{q}\right)^{2j+2j'} \times \Omega_j \Omega_{j'} - \\
&\quad - \frac{G}{2} \sum_{jm>0} v_j^2 u_j^2 \left[\left(\frac{1}{q}\right)^{3j-m} \zeta_{2j-m} + \left(\frac{1}{q}\right)^{2j} \zeta_{1jm} \zeta_{1j-m} \right] \times \Omega_j, \tag{14}
\end{aligned}$$

where

$$\begin{aligned}
\zeta_{njm} &\doteq 1 + (q^{-1} - 1)(j - m - n) + (q^{-1} - 1)^2 \times \\
&\quad \times \left[\frac{(j - m)(j - m - 1)}{2!} - nj - nm - n \right] + \dots + (q^{-1} - 1)^{j-m-1} \times \\
&\quad \times [(j - m) - n(m + 3)(m + 2) \dots (j - m - 3) - n(-m - 1) \times (m + 2)(m + 1) \dots (j - m - 2) - \dots] \tag{15}
\end{aligned}$$

and Ω_j is the pair degeneracy of the j -shell. The coefficients of each power of $(q^{-1} - 1)$ in ζ obviously have to be either positive or zero. The variational q -Hamiltonian is $\tilde{H}' = \tilde{H} - \lambda_q \sum_j 2v_j^2$. Performing a naive variation with respect to the Lagrange multiplier λ_q one obtains:

$$\lambda_q = \frac{d {}_q\langle BCS|H_q|BCS\rangle_q}{d \sum_j 2v_j^2}, \tag{16}$$

which means that λ_q works as the chemical potential in the frame of the q -energy $E_q = {}_q\langle BCS|H_q|BCS\rangle_q$. One may now calculate the variation with respect to the occupation probabilities:

$$\delta {}_q\langle BCS|H_q - \lambda_q \sum_j 2v_j^2|BCS\rangle_q = \left(\frac{\partial}{\partial v_j} + \frac{u_j}{v_j} \frac{\partial}{\partial u_j} \right) {}_q\langle BCS|H_q - \lambda_q \sum_j 2v_j^2|BCS\rangle_q, \tag{17}$$

which one then imposes to vanish for some fixed q . The resulting q -BCS equations are:

$$u_j v_j (\epsilon_j \times \left(\frac{\left(\frac{1}{q}\right)^{4\Omega_j} - 1}{\left[\left(\frac{1}{q}\right)^2 - 1\right] \Omega_j} \right) - 2\lambda_q) + (u_j^2 - v_j^2) \Delta_j^q = 0, \tag{18}$$

where

$$\Delta_j^q \doteq G \left[\sum_{j' \neq j} u_{j'} v_{j'} \left(\frac{1}{q}\right)^{2j+2j'} \Omega_{j'} + \frac{u_j v_j}{2} \sum_{m>0} \left(\frac{1}{q}\right)^{3j-m} \zeta_{2j-m} + \left(\frac{1}{q}\right)^{2j} \zeta_{1jm} \zeta_{1j-m} \right] \quad (19)$$

is the quantum gap parameter (which, in opposition to the standard pure pairing case, depends upon the shell label j). It is easy to verify that when $q = 1$, the quantum equations (18) are the BCS equations:

$$2u_j v_j (\epsilon_j - \lambda) + (u_j^2 - v_j^2) \Delta = 0 \quad (20)$$

for the nuclear pairing problem, with the non-quantum gap parameter $\Delta = G \sum_j u_j v_j \Omega_j$.

The solution of equations (18) for the variational parameters u_j and v_j is:

$$\left. \begin{array}{l} u_j^2 \\ v_j^2 \end{array} \right\} = \frac{1}{2} \left[1 \pm \frac{\left(\epsilon_j \times \left(\frac{(\frac{1}{q})^{4\Omega_j} - 1}{2[(\frac{1}{q})^2 - 1]\Omega_j} \right) - \lambda_q \right)}{\sqrt{\left(\epsilon_j \times \left(\frac{(\frac{1}{q})^{4\Omega_j} - 1}{2[(\frac{1}{q})^2 - 1]\Omega_j} \right) - \lambda_q \right)^2 + (\Delta_j^q)^2}} \right] \quad (21)$$

The quantum gap equation is obtained in an analog way as for the standard case by substitution of (21) into (19):

$$\Delta_j^q = \frac{G}{2} \left[\sum_{j' \neq j} \left(\frac{1}{q}\right)^{2j+2j'} \Omega_{j'} \frac{\Delta_{j'}^q}{\sqrt{\left(\epsilon_{j'} \times \left(\frac{(\frac{1}{q})^{4\Omega_{j'}} - 1}{2[(\frac{1}{q})^2 - 1]\Omega_{j'}} \right) - \lambda_q \right)^2 + (\Delta_{j'}^q)^2}} + \frac{\Delta_j^q}{\sqrt{\left(\epsilon_j \times \left(\frac{(\frac{1}{q})^{4\Omega_j} - 1}{2[(\frac{1}{q})^2 - 1]\Omega_j} \right) - \lambda_q \right)^2 + (\Delta_j^q)^2}} \sum_{m>0} \left(\frac{1}{q}\right)^{3j-m} \zeta_{2j-m} + \left(\frac{1}{q}\right)^{2j} \zeta_{1jm} \zeta_{1j-m} \right] \quad (22)$$

For the case of a single j -shell, the quantum gap parameter assumes the form:

$$\Delta_j^q = \left[\frac{G^2}{4} \left(\sum_{m>0} \left(\frac{1}{q}\right)^{3j-m} \zeta_{2j-m} + \left(\frac{1}{q}\right)^{2j} \zeta_{1jm} \zeta_{1j-m} \right)^2 - \left(\epsilon_j \times \left(\frac{(\frac{1}{q})^{4\Omega_j} - 1}{2[(\frac{1}{q})^2 - 1]\Omega_j} \right) - \lambda_q \right)^2 \right]^{1/2} \quad (23)$$

The qualitative behavior of Δ_j^q is, as one can see, independent of the shell label. A 3D plot shows the dependence of the curve $v_j^2 \times \epsilon_j$ upon the parameter q , for a $j = \frac{3}{2}$ shell (Fig. 1a). Figure 1b shows the behavior of $v_j^2 \times \epsilon_j$ for three different values of q .

In summary, we presented a quantum group form of the BCS method for the case of a pure pairing force, following the $SU_q(N)$ -covariant representation of the fermionic algebra given by Ubrico in ref. [19]. The quantum bare vacuum was shown to be identical (apart from a multiplicative constant) to the product Fock space vacuum. The q -analogues to the BCS equations (18) were derived along with the quantum gap equation (22). The quantum gap (19) was shown to depend explicitly on the deformation parameter; we found that the quantum gap is reduced as the deformation increases, as if the system collapsed into its ground-state and, conversely, that it goes to infinity as q tends to zero making the system unexcitable. A 3D plot was made to illustrate the dependence of the occupation probabilities v_j^2 versus the single-particle energies on the quantum parameter. One can check this dependence is qualitatively in agreement with the remark in the first paragraph below eq. (19) in ref. [19]. The study of introduction of q -covariance may be interesting in other many-body systems, in special in toy models such as the Moszkowski and the Lipkin-Meshkov-Glick ones, studied previously (in the deformed algebraic approach) in [6,7] and [8,9]. A q -analog of two-level pairing is under study and we hope to address it in a future publication.

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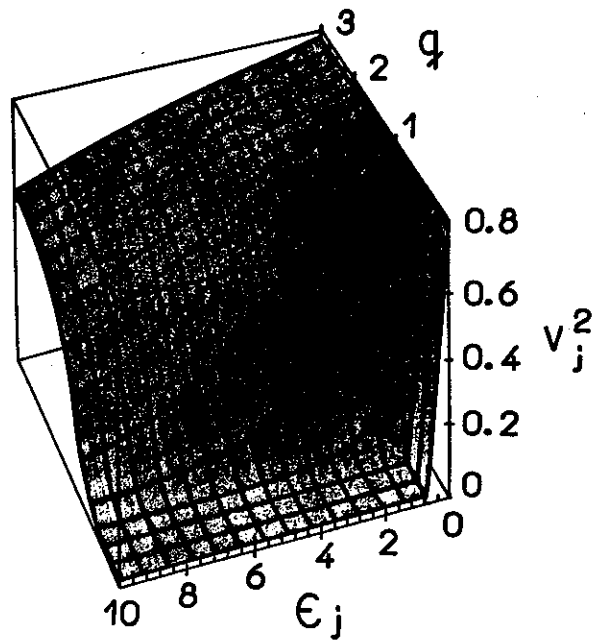
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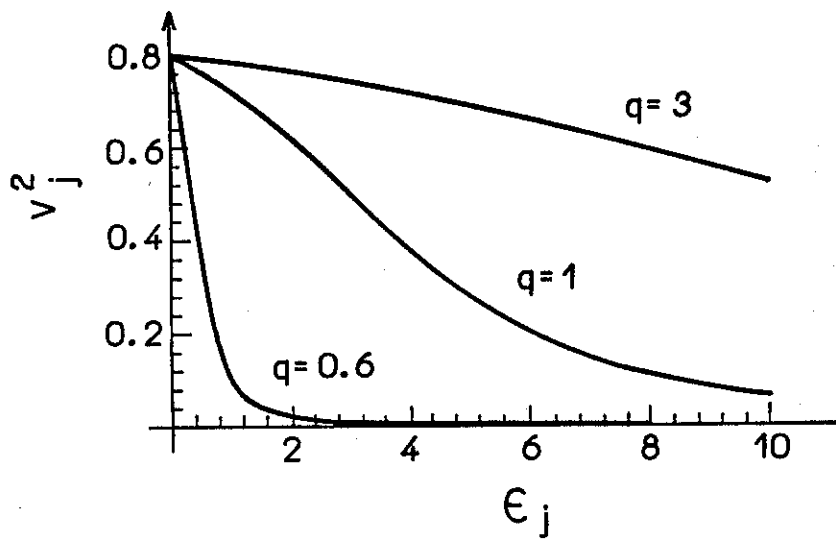
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Figure Captions

Figure 1. Quantum occupation probabilities v_j^2 as a function of the single particle energy ϵ_j and the quantum parameter q for $j = 3/2$. Figure 1a is a 3D view whereas Figure 1b presents the behavior for three different values of q .



(a)



(b)