qBCS - the BCS theory of q-deformed nucleon pairs

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We construct a coherent state of q-deformed zero coupled nucleon pairs distributed in several single-particle orbits. Using a variational approach, the set of equations of qBCS theory, to be solved self consistently for occupation probabilities, gap parameter Δ, and the chemical potential λ, is obtained. Results for valence nucleons in nuclear degenerate sdg major shell show that the strongly coupled zero angular momentum nucleon pairs can be substituted by weakly coupled q-deformed zero angular momentum nucleon pairs. A study of Sn isotopes reveals a well defined universe of (G, q) values, for which qBCS converges. While the qBCS and BCS show similar results for Gap parameter Δ in Sn isotopes, the ground state energies are lower in qBCS. The pairing correlations in N nucleon system, increase with increasing q (for q real).

I. ZERO COUPLED q-DEFORMED NUCLEON PAIRS

The creation and destruction operators for a zero coupled nucleon pair in a shell model orbit j are

\[ Z_0 = -\frac{1}{\sqrt{2}}(A^j \times A^j)^0 \quad \text{and} \quad \bar{Z}_0 = \frac{1}{\sqrt{2}}(B^j \times B^j)^0, \]  

\[ 21.60.Fw, 21.60.-n, 21.10.-Dr \]
where \( A_{jm} = a_{jm}^\dagger \); \( B_{jm} = (-1)^{j+m}a_{j,-m} \). From the anticommutation relations satisfied by the fermion creation and destruction operators \( a_{jm}^\dagger \) and \( a_{j,-m} \), we can verify that with number operator for fermions defined as \( n_{op}^j = \sum_m a_{jm}^\dagger a_{jm} \) and \( \Omega = (2j + 1)/2 \),

\[
[Z_0, Z_0] = \frac{n_{op} - \Omega}{\Omega}; [n_{op}, Z_0] = 2Z_0; [n_{op}, Z_0^\dagger] = -2Z_0.
\] (2)

These operators are easily related to well known quasi-spin operators by identifying

\[
S_+ = \sqrt{\Omega} Z_0; S_- = \sqrt{\Omega} Z_0^\dagger, \quad \text{and} \quad S_0 = \frac{(n_{op} - \Omega)}{2}.
\] (3)

The quasi-spin operators \( S_+ \), \( S_- \), and \( S_0 \) are the generators of Lie algebra of SU(2) and satisfy the commutation relations of angular momentum operators, that is

\[
[S_+, S_-] = 2S_0, \quad [S_0, S_\pm] = \pm S_\pm.
\] (4)

The generators of SU\(_q\)(2) on the other hand satisfy the \( q \)-commutation relations \[\[S_+(q), S_-(q)\] = \{2S_0(q)\}_q \quad \text{and} \quad \{S_0(q), S_\pm(q)\} = \pm S_\pm(q) ; \] (5)

where \( \{x\} = \frac{(x^r - x^{-r})}{(q^r - q^{-r})} \). Translated to \( q \)-deformed pair operators \( Z_0(q) \) and \( Z_0^\dagger(q) \) the new commutation relations give

\[
[Z_0(q), Z_0^\dagger(q)] = \frac{(n_{op} - \Omega)_q}{\Omega}; [n_{op}, Z_0(q)] = 2Z_0(q); [n_{op}, Z_0^\dagger(q)] = -2Z_0^\dagger(q) .
\] (6)

II. THE TRIAL WAVE FUNCTION

The proposed trial wave function for \( N \) nucleons distributed over \( m \) single particle orbits is, \( \Psi = \Phi_j \Phi_{j2} ... \Phi_{jm} \), where for the orbit \( j \),

\[
\Phi_j = u_j^{\Omega_j} \sum_{n=0}^{\Omega_j} \frac{v_j^n}{u_j^{\Omega_j-n}} \frac{\Omega_j!}{n!(\Omega_j-n)!} \frac{1}{2} [n]; \quad \Omega_j = \frac{2j+1}{2}
\] (7)

and

\[
|n] = \left[ \left\{ \frac{\Omega_j-n}{q}\right\}_q \left\{ \frac{\Omega_j}{q}\right\}_q \right]^{\frac{1}{2}} \left\{ \frac{\Omega_j-n}{q} \right\}_q \left\{ \frac{\Omega_j}{q}\right\}_q (S_+(q))^n |0] \]

is the normalized wave function for \( n \) zero coupled nucleon pairs with \( q \)-deformation occupying single particle orbit \( j \). The function \( \Psi \) is normalized in case, \( u_j^2 + v_j^2 = 1 \), for all single particle orbits. The single particle plus pairing Hamiltonian for \( q \)-deformed pairs is given by

\[
H = \sum_r \tilde{\epsilon}_r n_{op}^r - G \sum_{rs} S_{r+}(q) S_{s-}(q) \quad \text{where} \quad r, s \equiv j_1, j_2, .......j_m.
\] (8)

The matrix element \( \langle \Psi | -G S_{r+}(q) S_{s-}(q) | \Psi \rangle \) , obtained by using the \( q \)-commutation relations given in Eq. (5) and ignoring terms involving products of the type \( v_r^m u_r^m(m = 2, 4, ..., \Omega_r) \), is found to be

\[
\langle \Psi | -G S_{r+}(q) S_{s-}(q) | \Psi \rangle = -G v_r^2 \Omega_r \left\{ \Omega_r \right\}_q + G v_r^4 (\Omega_r - 1) \left\{ \Omega_r \right\}_q.
\]

We also calculate the gap parameter,

\[
\Delta(q) = G \left\{ \Psi | \sum_r S_{r+}(q) | \Psi \right\} = \sum_r \Delta_r(q) = \sum_r G \Omega_r \left\{ \Omega_r \right\}_q.
\]

Again the terms involving products of the type \( v_r^m u_r^m \) have been ignored. After these considerations, we can write the matrix element of the Hamiltonian \( H \) as

\[
\langle \Psi | H | \Psi \rangle = \sum_r \left( 2\tilde{\epsilon}_r \Omega_r v_r^2 - G v_r^2 \Omega_r \left\{ \Omega_r \right\}_q + G v_r^4 (\Omega_r - 1) \left\{ \Omega_r \right\}_q \right) \frac{\Delta_r^2(q)}{G} - \left( \Delta(q) \right)^2
\]
III. QBCS GAP EQUATION AND THE GROUND STATE ENERGY

In order to evaluate the ground state energy of $N$ nucleons, we minimize the expectation value of the Hamiltonian subject to the number constraint by varying $v_j$ and obtain $m$ equations to be solved self consistently, 

$$
4(\varepsilon'_j - \lambda)v_j \Omega_j - 2 \Delta(q) \{\Omega_j\}_q \left(1 - \frac{2v_j^2}{u_j}\right) - 4Gv_j^3 \{\Omega_j\}_q \left(\{\Omega_j\}_q - \Omega_j + 1\right) = 0,
$$

where $\varepsilon'_j = \varepsilon_j + \frac{G\{\Omega_j\}_q\{\Omega_j\}_q - \Omega_j}{2\Omega_j}$. Leaving out for the time being, the term containing $u_jv_j^3$, we solve these equations to obtain the occupancies,

$$
v_j^2 = 0.5 \left(1 - \frac{\varepsilon'_j - \lambda}{\sqrt{(\varepsilon'_j - \lambda)^2 + \left(\Delta(q) \{\Omega_j\}_q\right)^2}}\right),
$$

and consequently the gap equation

$$
\Delta(q) = \sum_j G \{\Omega_j\}_q 0.5 \left(1 - \frac{(\varepsilon'_j - \lambda)^2}{(\varepsilon'_j - \lambda)^2 + \left(\Delta(q) \{\Omega_j\}_q\right)^2}\right)^\frac{1}{2},
$$

To include the effect of terms containing $u_jv_j^3$ left out earlier, we now replace $\lambda$ by

$$
\lambda(q) = \lambda + \frac{Gv_j^2 \{\Omega_j\}_q}{\Omega_j} \left(\{\Omega_j\}_q - \Omega_j + 1\right).
$$

The ground state BCS energy, $\langle \Psi | H | \Psi \rangle$ is

$$
E_{bcs}(q) = \sum_{j=1}^m \left(2\varepsilon'_j \Omega_j v_j^2 - Gv_j^3 \{\Omega_j\}_q \left(\{\Omega_j\}_q - \Omega_j + 1\right)\right) - \frac{(\Delta(q))^2}{G}.
$$

IV. SINGLE ORBIT WITH $2\Omega$ DEGENERATE STATES

A very special situation arises, when the $N$ nucleons occupy a single orbit with an occupancy of $2\Omega$. Using the results of the previous section, the ground state wave function is now $\Psi = \Phi_j$ and the ground state energy $E_{bcs}(q)$ is

$$
E_{bcs}(q) = \varepsilon_j N - G \{\Omega_j\}_q \frac{N}{2\Omega} \left(2\{\Omega_j\}_q - N + \frac{N}{\Omega}\right),
$$

to be compared with the exact energy of the $N$ nucleon zero seniority state $E_{exact}$,

$$
E_{exact} = \varepsilon_j N - G' \frac{N}{4} (2\Omega_j - N + 2).
$$

We notice that we can have $E_{bcs}(q) = E_{exact}$ by choosing $q$ value and pairing strength $G$ such that
for the choice $\varepsilon_j = 0.0$. For the special case of nuclear sdg major shell with $\Omega = 16$, and 4, 14, 20, 30 valence nucleons occupying degenerate $1d_{\frac{3}{2}}, 0g_{\frac{7}{2}}, 2s_{\frac{1}{2}}, 1d_{\frac{1}{2}}$, and $0h_{\frac{1}{2}}$ orbits, we plot $G$ versus $q$ in Fig. 1 such that $E_{\text{bcs}}(q) = E_{\text{exact}}(G' = 0.187 \text{ MeV}, \varepsilon_j = 0.0 \text{ for all levels})$. The intensity of pairing strength required to reproduce $E_{\text{exact}}$ is seen to fall with increasing $q$ and ultimately $G \to 0$ for all cases. From the plot at hand we can say that strongly coupled zero coupled pairs of BCS theory may well be replaced by weakly coupled $q$-deformed zero coupled pairs of $q$BCS theory. The natural question is, is it possible to replace the pairing interaction by a suitable commutation relation between the pairs determined by a characteristic $q$ value for the system at hand? To get some clues to the answer, we next consider real nuclei for which we can get the pairing gap from the experiments.

V. SN ISOTOPES

We examine the heavy Sn isotopes with $N = 14, 16, 18, 20, 22$, and 24 neutrons outside $^{150}_{50}\text{Sn}_{50}$ core. The model space includes $1d_{\frac{3}{2}}, 0g_{\frac{7}{2}}, 2s_{\frac{1}{2}}, 1d_{\frac{1}{2}}$, and $0h_{\frac{1}{2}}$, single particle orbits, with excitation energies $0.0, 0.22, 1.90, 2.20$, and $2.80$ MeV respectively. Fig. 2 is a plot of pairing correlations function $D = \Delta(q)/\sqrt{G}$ versus $G$ for $N = 20$ in the cases where deformation parameter takes some typical successively increasing values varying from 1.0 to 1.7. We notice that in $^{120}_{50}\text{Sn}_{70}$, pairing correlations increase as $q$ increases if the pairing strength $G$ is kept fixed. For $q = 1.0$ that is conventional BCS theory the pairing correlation vanishes for $G < G_c(\sim 0.065 \text{ MeV})$ as expected. As the deformation $q$ of zero coupled pairs increases we find $D$ going to zero for successively lower values of coupling strength, for example $G_c \sim 0.04 \text{ MeV for } q = 1.3$. We may infer that the $q$BCS takes us beyond BCS theory.

The sets of $G, q$ values that reproduce the empirical $\Delta$ for $^{120}_{50}\text{Sn}_{70}$, are used to calculate the gap parameter $\Delta$ and the ground state BCS energy $E_N$, for even isotopes $^{114-124}\text{Sn}$ displayed in Fig. 3. The experimental values of $\Delta$ (filled triangles up) are also shown. As far as the gap parameter $\Delta$ is concerned all the sets of $G, q$ values fair equally in comparison with the experiment. The ground state energies from $q$BCS are however in general lower than those calculated by using BCS. The underlying $q$-deformed nucleon pairs show increasingly strong binding as the value of $q$ is increased. It opens the possibility of obtaining the exact correlation energies by choosing appropriately the combination of $G, q$ values.

VI. CONCLUSIONS

By looking at the results for 4, 14, 20, 30 valence nucleons in nuclear degenerate sdg major shell, we find that the strongly coupled zero angular momentum nucleon pairs may be replaced by weakly coupled $q$-deformed zero angular momentum nucleon pairs. The study of a realistic case i.e. Sn isotopes also indicates that their is a well defined universe of sets of values for pairing strength $G$ and deformation parameter $q$, for which $q$BCS converges and has a non-trivial solution. For $^{120}_{50}\text{Sn}_{70}$ we observe that by choosing the pairing strength $G \leq 0.217 \text{ MeV}$ a matching value of deformation parameter $q$ can be found such that the experimental pairing gap is reproduced. For the choice $G = 0.07 \text{ MeV for example a large deformation of } q = 1.7$ is needed to reproduce the empirical $\Delta$ for $^{120}_{50}\text{Sn}_{70}$. The results of $q$BCS for Sn isotopes are not much different from BCS as far as the Gap parameter $\Delta$ is concerned. The ground state binding energies are however lowered by the deformation. The pairing correlations, measured by $D = \Delta(q)/\sqrt{G}$, are seen to increase as $q$ increases (for $q$ real) while the pairing strength $G$ is kept fixed, in Sn isotopes. It is immediately seen that $q$ parameter is a very good measure of the pairing correlations left out in the conventional BCS theory.

The results of our present study are consistent with our earlier conclusions [2] that the $q$-deformed pairs with $q > 1 \text{ (q real)}$ are more strongly bound than the pairs with zero deformation and the binding energy increases with increase in the value of parameter $q$. In contrast by using complex $q$ values one can construct zero coupled deformed pairs with lower binding energy in comparison with the no deformation zero coupled nucleon pairs [3]. In general the pairing correlations in $N$ nucleon system, measured by $D = \Delta(q)/\sqrt{G}$, increase with increasing $q$ (for $q$ real) and $q$BCS takes us beyond the BCS theory. The formalism can be tested for several other systems, for example metal grains, where cooper pairing plays an important role.

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FIG. 1. $G$ versus $q$ for 4, 14, 20, 30 valence nucleons in sdg major shell with $\Omega = 16$ such that $E_{\text{bcs}}(q) = E_{\text{exact}}$, $G' = 0.187$ MeV, ($\varepsilon_j = 0.0$ for all single-particle orbits).
FIG. 2. The calculated pairing correlations function $D$ versus $G$ for $N = 20$ and deformation parameter values $q = 1.0, 1.2, 1.3, 1.4, 1.5, 1.6$ and $1.7$. Stars on the curves mark the $G$ value that reproduces empirical $\Delta$ for $^{120}$Sn.
FIG. 3. Calculated (a) $\Delta$ versus $N$ and (b) BCS Energy versus $N$, for $q = 1.0, 1.1, 1.2, 1.3, 1.4, 1.5$ and corresponding $G$ value chosen to reproduce the empirical neutron gap for $^{120}$Sn in each case.