BCS theory of q-deformed nucleon pairs: qBCS

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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 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).

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The problem of nucleon pairing has been of great interest to those interested in solving the riddles about nuclear structure. BCS theory of superconductivity [1] turned out to be a great ally in efforts to take into account short range interactions between nucleons. In many nuclear structure calculations BCS is taken as the starting point as the BCS wave function offers a good approximation to the ground state of even-even nuclei. Another approach to the nucleon pairing problem is the seniority scheme. In order to include the pairing correlations left out in these approximate schemes, we studied the zero coupled nucleon pairs with q deformations [2] expressing these in terms of the generators of quantum group $SU_q(2)$. The quantum group $SU_q(2)$, a q-deformed version of Lie algebra $SU(2)$, has been studied extensively [3–5], and a q-deformed version of quantum harmonic oscillator developed [6,7]. The quantum group $SU_q(2)$ is more general than $SU(2)$ and contains the latter as a special case. The underlying idea in using the zero coupled nucleon pairs with q deformations is that the commutation relations of nucleon pair creation and destruction operators are modified by the correlations and as such are somewhat different in comparison with those used in deriving the usual theories. The seniority scheme for q-deformed nucleon pairs in a single j orbit and zero seniority states for nuclei with q-deformed nucleon pairs distributed over several orbits have also been constructed in Ref. [2]. On the same lines random phase approximation equations for the pairing vibrations of nuclei have been derived and applied to study pairing vibrations in Pb isotopes [8]. Further a q-deformed version of quasiboson approximation for 0^+ states in superconducting nuclei was developed. The q-deformed theories reduce to the corresponding usual theories in the limit $q\to 1$. The nucleon pairing in a single j shell has also been treated by Bonatsos and co-workers [9–11] by associating two Q oscillators, one describing the $J=0$ pairs and the other associated with $J\neq 0$ pairs. In their formalism, Q oscillators involved reduce to usual harmonic oscillators as $Q\to 1$ and the deformation is introduced in a way different from ours. Following the idea of building in correlations into the theory by using pair generators satisfying q-commutation relations, we now construct the q analog of BCS theory (qBCS) for nuclei. The single orbit limit of qBCS is applied to nuclear *sdg* major shell with $\Omega=16$. In addition, the gap parameter and ground state energies are calculated for $^{114-124}$Sn, to elucidate the role played by q deformation in these nuclei.

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

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

where $A_{jm}=a^\dagger_{jm}$; $B_{jm}=(-1)^{j+m}a_{j,-m}$. From the anticommutation relations satisfied by the fermion creation and destruction operators $a^\dagger_{jm}$ and $a_{j,-m}$, we can verify that with number operator for fermions defined as $n^j_{op}=\Sigma_m a^\dagger_{jm}a_{jm}$ and $\Omega=(2j+1)/2$,

$$[Z_0,\overline{Z}_0]=\frac{n_{op}-\Omega}{\Omega};\ [n_{op},Z_0]=2Z_0;\ [n_{op},\overline{Z}_0]=-2\overline{Z}_0. \tag{2}$$

These operators are easily related to well-known quasispin operators by identifying

$$S_+=\sqrt{\Omega}\,Z_0;\ S_-=\sqrt{\Omega}\,\overline{Z}_0, \quad \text{and} \quad S_0=\frac{(n_{op}-\Omega)}{2}. \tag{3}$$

The quasispin 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,

$$[S_+,S_-]=2S_0,\ [S_0,S_\pm]=\pm S_\pm . \tag{4}$$

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The generators of $SU_q(2)$ on the other hand satisfy the q-commutation relations [2]

$$[S_+(q),S_-(q)]=\{2S_0(q)\}_q\,,\ \ [S_0(q),S_\pm(q)]=\pm S_\pm(q), \tag{5}$$

where $\{x\}_q=(q^x-q^{-x})/(q-q^{-1})$. Translated to q-deformed pair operators $Z_0(q)$ and $\overline{Z_0(q)}$ The new commutation relations give

$$[Z_0(q),\overline{Z_0(q)}]=\frac{\{n_{op}-\Omega\}_q}{\Omega};$$

$$[n_{op},Z_0(q)]=2Z_0(q);\ \ [n_{op},\overline{Z_0(q)}]=-2\overline{Z_0(q)}. \tag{6}$$

II. THE TRIAL WAVE FUNCTION

The proposed trial wave function for N nucleons distributed over m single particle orbits is, $\Psi=\Phi_{j_1}\Phi_{j_2}\cdots\Phi_{j_m}$, where for the orbit j,

$$\Phi_j=u_j^{\Omega_j}\sum_{n=0}^{\Omega_j}\left(\frac{v_j}{u_j}\right)^n\left[\frac{\Omega_j!}{n!(\Omega_j-n)!}\right]^{1/2}|n\rangle;\ \ \Omega_j=\frac{2j+1}{2} \tag{7}$$

and

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

is the normalized wave function for n zero coupled nucleon pairs with q deformation occupying single particle orbit j. The function Ψ 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

$$H=\sum_r\ \varepsilon_r n_{op}^r-G\sum_{rs}\ S_{r+}(q)S_{s-}(q)\quad \text{where}$$

$$r,s\equiv j_1,j_2,\ldots,j_m. \tag{8}$$

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

$$\langle\Psi|-G\,S_{r+}(q)S_{r-}(q)|\Psi\rangle$$
$$=-G\,v_r^2\Omega_r\{\Omega_r\}_q+G\,v_r^4(\Omega_r-1)\{\Omega_r\}_q.$$

We also calculate the gap parameter

$$\Delta(q)=G\left\langle\Psi\left|\sum_r\ S_{r+}(q)\right|\Psi\right\rangle$$

$$=\sum_r\ \Delta_r(q)=\sum_r\ Gu_rv_r\{\Omega_r\}_q.$$

Again the terms involving products of the type $v_r^3u_r^m$ have been ignored. After these considerations, we can write the matrix element of the Hamiltonian H as

$$\langle\Psi|H|\Psi\rangle=\sum_r\ \Bigg(2\varepsilon_r\,\Omega_r\,v_r^2-G\,v_r^2\,\Omega_r\{\Omega_r\}_q+G\,v_r^4(\Omega_r-1)$$
$$\times\{\Omega_r\}_q+\frac{\Delta_r^2(q)}{G}\Bigg)-\frac{[\Delta(q)]^2}{G}.$$

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,

$$4(\varepsilon_j'-\lambda)v_j\Omega_j-2\,\Delta(q)\,\{\Omega_j\}_q\left(\frac{1-2v_j^2}{u_j}\right)$$
$$-4G\,v_j^3\{\Omega_j\}_q(\{\Omega_j\}_q-\Omega_j+1)=0, \tag{9}$$

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

$$v_j^2=0.5\left(1-\frac{\varepsilon_j'-\lambda}{\sqrt{(\varepsilon_j'-\lambda)^2+[\Delta(q)(\{\Omega_j\}_q/\Omega_j)]^2}}\right), \tag{10}$$

gap parameter

$$\Delta(q)=\sum_j\ G\,\{\Omega_j\}_q0.5$$
$$\times\left(1-\frac{(\varepsilon_j'-\lambda)^2}{(\varepsilon_j'-\lambda)^2+\left[\Delta(q)\dfrac{(\{\Omega_j\}_q}{\Omega_j}\right]^2}\right)^{1/2}, \tag{11}$$

and consequently the gap equation

$$\frac{G}{2}\sum_j\ \frac{\{\Omega_j\}_q^2}{\sqrt{(\varepsilon_j'-\lambda)^2\Omega_j^2+[\Delta(q)\{\Omega_j\}_q]^2}}=1. \tag{12}$$

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

$$\lambda(q)=\lambda+\frac{Gv_j^2\{\Omega_j\}_q}{\Omega_j}(\{\Omega_j\}_q-\Omega_j+1). \tag{13}$$

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

$$E_{BCS}(q)=\sum_{j=1}^m\ [2\varepsilon_j'\,\Omega_j\,v_j^2-G\,v_j^4\{\Omega_j\}_q(\{\Omega_j\}_q-\Omega_j+1)]$$
$$-[\Delta(q)]^2/G. \tag{14}$$

We notice that in a very natural way, the $SU_q(2)$ symmetry introduces in the interaction energy a q dependence which is linked to the j value of the orbit occupied by the zero coupled nucleon pairs.

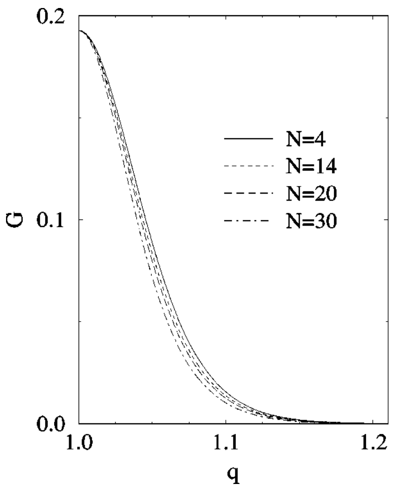

FIG. 1. G versus q for 4,14,20,30 valence nucleons in *sdg* major shell with $\Omega=16$ such that $E_{\rm BCS}(q)=E_{\rm exact}$, $G'=0.187$ MeV, ($\varepsilon_j=0.0$ for all single-particle orbits).

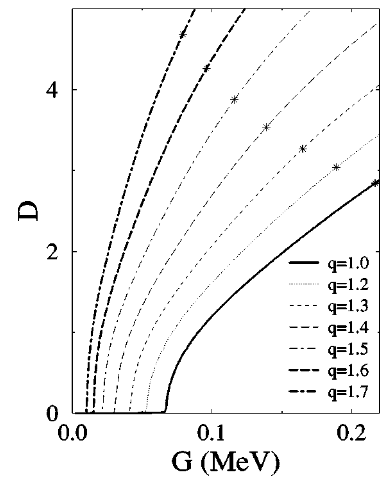

FIG. 2. The calculated pairing correlations function D versus G for $N=20$ and deformation parameter values $q=1.0$, 1.2, 1.3, 1.4, 1.5, 1.6, and 1.7. Stars on the curves mark the (G,q) values that reproduce empirical Δ for ^{120}Sn.

IV. SINGLE ORBIT WITH 2Ω DEGENERATE STATES

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

$$E_{\rm BCS}(q)=\varepsilon_j N-G\{\Omega_j\}_q\frac{N}{4\Omega}\left(2\{\Omega_j\}_q-N+\frac{N}{\Omega}\right), \quad (15)$$

to be compared with the exact energy of the N nucleon zero seniority state [12],

$$E_{\rm exact}=\varepsilon_j N-G'\frac{N}{4}(2\Omega_j-N+2). \quad (16)$$

We notice that we can have $E_{\rm BCS}(q)=E_{\rm exact}$ by choosing q value and pairing strength G such that

$$G=\frac{G'\Omega_j(2\Omega_j-N+2)}{\{\Omega_j\}_q(2\{\Omega_j\}_q-N+N/\Omega)}$$

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 $1d_{5/2}$, $0g_{7/2}$, $2s_{1/2}$, $1d_{3/2}$, and $0h_{11/2}$ orbits, we plot G versus q in Fig. 1 such that $E_{\rm BCS}(q)=E_{\rm exact}(G'=0.187$ MeV, $\varepsilon_j=0.0$ for all levels). The intensity of pairing strength required to reproduce $E_{\rm exact}$ is seen to fall with increasing q and ultimately $G\rightarrow 0$ 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 qBCS 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 $^{100}_{50}$Sn$_{50}$ core. The model space includes $1d_{5/2}$, $0g_{7/2}$, $2s_{1/2}$, $1d_{3/2}$, and $0h_{11/2}$, single particle orbits, with excitation energies 0.0, 0.22, 1.90, 2.20, and 2.80 MeV, respectively. Figure 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 $^{120}_{50}$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 $G<G_c(\sim 0.065$ 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, $G_c\sim 0.04$ MeV for $q=1.3$. We may infer that the qBCS takes us beyond BCS theory.

The sets of G,q values that reproduce the empirical Δ for $^{120}_{50}$Sn$_{70}$, are used to calculate the gap parameter Δ and the ground state BCS energy E_N, for even isotopes $^{114-124}$Sn displayed in Fig. 3. The experimental values of Δ (filled triangles pointing up) are also shown. As far as the gap parameter Δ is concerned all the sets of G,q values fare equally in comparison with the experiment. The ground state energies from qBCS 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 mo-

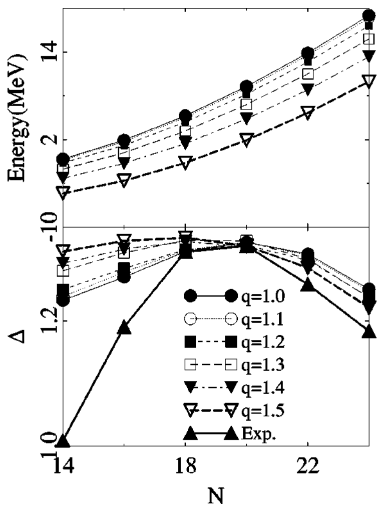

FIG. 3. Calculated (a) Δ vesus N and (b) BCS energy versus N, for $q=1.0,\ 1.1,\ 1.2,\ 1.3,\ 1.4,\ 1.5$ and corresponding G value chosen to reproduce the empirical neutron gap for ^{120}Sn in each case.

mentum nucleon pairs. The study of a realistic case, i.e., Sn isotopes also indicates that there is a well-defined universe of sets of values for pairing strength G and deformation parameter q, for which qBCS converges and has a nontrivial solution. For $^{120}_{50}\mathrm{Sn}_{70}$ we observe that by choosing the pairing strength $G \leqslant 0.217$ MeV a matching value of deformation parameter q can be found such that the experimental pairing gap is reproduced. For the choice $G=0.07$ MeV, for example, a large deformation of $q=1.7$ is needed to reproduce the empirical Δ for $^{120}_{50}\mathrm{Sn}_{70}$. The results of qBCS for Sn isotopes are not much different from BCS as far as the gap parameter Δ 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 [2,8] that the q-deformed pairs with $q>1$ (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 [8]. In general the pairing correlations in N nucleon system, measured by $D=\Delta(q)/\sqrt{G}$, increase with increasing q (for q real) and qBCS 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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