Mixed-Spin Pairing Condensates in Heavy Nuclei

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Mixed-spin pairing condensates in heavy nuclei

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We show that the Bogoliubov-de Gennes equations for nuclear ground-state wave functions support solutions in which the condensate has a mixture of spin-singlet and spin-triplet pairing. We find that such mixed-spin condensates do not occur when there are equal numbers of neutrons and protons, but only when there is an isospin imbalance. Using a phenomenological Hamiltonian, we predict that such nuclei may occur in the physical region within the proton dripline. We also solve the Bogoliubov-de Gennes equations with variable constraints on the spin-singlet and spin-triplet pairing amplitudes. For nuclei that exhibit this new pairing behavior, the resulting energy surface can be rather soft, suggesting that there may be low-lying excitations associated with the spin mixing.

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Introduction. The usual pairing found in nuclei is between identical nucleons in the spin-singlet channel. Although the spin-triplet interaction is stronger, the spin-orbit field tends to suppress pairing in the triplet channel[1, 2]. However, spin-triplet pairing becomes favored in nuclei with equal numbers of neutrons N and protons Z when the nucleon number is very large (probably beyond the proton dripline)[3]. In this work we address nuclei with $N \neq Z$ and find some surprising results: a) the domain where spin-triplet pairing dominates extends well off the $N = Z$ line; b) the condensate changes character smoothly between pure spin-triplet on the $N = Z$ line to pure spin-singlet at large neutron excess, c) the mixed-spin nuclei that we find extend below the proton dripline and are thus relevant to experiment.

Context. The expectation that isospin-zero ($T = 0$) neutron-proton pairing should exist comes from the fact that the interaction in the spin-triplet (isospin-singlet) channel, which binds the deuteron, is stronger than the $^1S_0$ interaction that is largely responsible for ordinary identical-particle spin-singlet pairing. It was suggested a long time ago that neutron-proton pairing is important near the $N = Z$ line (see Refs. [4, 5] and works cited therein, as well as Refs. [6, 7] for a discussion of the experimental situation). A number of theoretical works have examined the possibility that nuclei may contain a $T = 0$ spin-triplet neutron-proton ('deuteron-like') condensate when $N = Z$, suggesting that states of high angular momentum might favor $T = 0$ pairing [8–10]. The possibility of mixed-spin condensation, $T = 0$ and $T = 1$, has also been raised in Ref. [5, 11] for $N = Z$ medium-mass nuclei, although no mixed-spin ground states were shown. In this Letter, we present our findings for the existence of mixed-spin solutions to the Bogoliubov-de Gennes equations for the ground-state of large but accessible nuclei off the $N = Z$ line.

Hamiltonian. We use the same Hamiltonian here as was used in Ref. [3]. It contains a one-body and a two-body part represented in Fock space as:

$$\hat{H} = \sum_i \langle i|H_{sp}|j\rangle a_i^\dagger a_j + \sum_{i>j,k>l} \langle ij|v|kl\rangle a_i^\dagger a_j^\dagger a_l a_k \quad (1)$$

where i, j label orbitals in a spherical shell-model basis. The one-body part H_{sp} is taken from the eigenstates of a Wood-Saxon potential of standard form, containing a kinetic energy, a potential well, and a spin-orbit term. The two-body interaction is of contact form:

$$\langle ij|v|kl\rangle = \tfrac{1}{4}\langle ij|(3v_t + v_s + (v_t - v_s)\vec{\sigma}\cdot\vec{\sigma}')\delta^{(3)}(\vec{r} - \vec{r}')P_{L=0}|kl\rangle. \quad (2)$$

where $P_{L=0}$ projects onto the spherically symmetric part of the pair wave function. This Hamiltonian is appropriate for systems with no nuclear deformation, accenting the pairing condensates. There are two interaction strengths, v_t and v_s, corresponding to spin-triplet and spin-singlet, respectively. These were determined by fitting to phenomenological shell-model Hamiltonians. The interaction of Eq. 2 can generate 6 independent condensates counting only spin and isospin quantum numbers. We label these by an index α enumerated in Table I.

α	1	2	3	4	5	6
(S, S_z)	(0,0)	(0,0)	(0,0)	(1,1)	(1,0)	(1,-1)
(T, T_z)	(1,1)	(1,0)	(1,-1)	(0,0)	(0,0)	(0,0)

TABLE I: Spin-isospin channels for pairing condensates.

Finally, we note that the Coulomb interaction is omitted in the above Hamiltonian. The main effect of this is that the calculated nuclei are only physical within the proton dripline. Nevertheless, the pairing phenomena that can be elucidated beyond the proton dripline are interesting on a purely theoretical level. Also, as we shall show, the region where these effects may occur extends into the physical region, below the proton dripline.

BdG theory. The Bogoliubov-de Gennes (BdG) theory is defined by minimizing the Hamiltonian under Bogoliubov tranformations of the Fock-space vacuum, subject to constraints such as the neutron and proton number expectation values. In the notation of [12], the Bogoliubov transformations are parameterized by the matrices U and V giving the definition of the quasiparticle annihilation operator in terms of the Fock-space annihilation and creation operators, respectively. The key equations in the theory are the formulas for ordinary and anomalous densities, $\rho = V^* V^t$ and $\kappa = V^* U^t$, respectively, and the formula for the expection value of the Hamiltonian,

$$H^{00} = \mathrm{Tr}(\varepsilon\rho + \tfrac{1}{2}\Gamma\rho - \tfrac{1}{2}\Delta\kappa^*). \quad (3)$$

As usual, the matrices Γ, Δ are defined through the standard relations $\Gamma_{ij} = \sum_{kl} v_{ikjl}\rho_{lk}$ and $\Delta_{ij} = \frac{1}{2}\sum_{kl} v_{ijkl}\kappa_{kl}$. Here, and in Eq. (4) below, superscripts denote the number of quasiparticle creation and annihilation operators.

Calculational procedure. Traditionally the minimization is carried out using the BdG equations, which are arrived at by setting the variational derivative of the energy with respect to U and V to zero. (Actually the variation must be constrained to preserve the unitarity of the Bogoliubov transformation. This introduces Lagrange multipliers that give the BdG equations their structure as eigenvalue equations for the quasiparticle energies.) The BdG equations are solved for some assumed density, and the solution is used to update the density. This process is iterated to self-consistency. However, to study the energetics with different types of condensates it is necessary to deal with many constraining fields and therefore thoroughly explore the space of allowed Bogoliubov transformations. Under these conditions, the BdG minimization is easier to carry out by the gradient method [12], and we take advantage of that method here. In taking the variational derivative of the Hamiltonian one makes use of the generalized Thouless matrix Z, whose elements are independent of each other. The gradients of the Hamiltonian and the operators to be constrained can then be applied to update a trial set of U, V matrices, using the steepest descent or other numerical methods[13]. The change in the expectation value of a one-body operator Q can be expressed:

$$Q^{00}_{new} = Q^{00}_{old} - \mathrm{Tr}(Q^{20}Z) + \mathcal{O}(Z^2). \quad (4)$$

A similar formula applies to the Hamiltonian, since its expectation value can be expressed in terms of one-body expectation values. To insure that the space of possible Bogoliubov transformations has been adequately explored, we carry out the iteration process repeatedly starting from U, V matrices obtained by transformations from the vacuum or other states by Z transformations. We have used the gradient method to solve the BdG equations with 8 simultaneous constraining fields, 2 for the neutron and proton particle numbers, and 6 for the pairing amplitudes corresponding to the 6 distinct channels of Table I. To be more precise, the 6 constrained amplitudes are

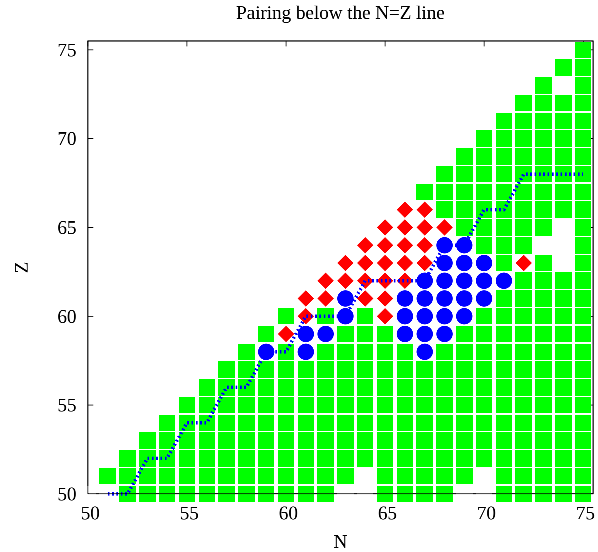

FIG. 1: (color online) Chart of nuclides with $Z \leq N$ for neutron numbers from 50 to 75. Blank squares denote nuclei that exhibit practically no pairing ($E_{corr} < 0.5$ MeV), green squares signify the case where the pairing condensate is mostly spin-singlet, red diamonds are used for the nuclei that exhibit spin-triplet, while blue circles denote nuclei for which the pairing is a mixture of spin-singlet and spin-triplet. The blue dashed line is the proton-drip line from Ref. [14].

computed as $\kappa_\alpha = \mathrm{Tr}(P_\alpha \kappa)$ where the matrices P_α are defined in terms of the quantum numbers $(\ell_k, \ell_{zk}, s_{zk}, t_{zk})$ of the orbitals k as

$$P_{\alpha,ij} = \sqrt{2}\left(\left(\tfrac{1}{2}\, s_{zi}\, \tfrac{1}{2}\, s_{zj} | S(\alpha) S_z(\alpha)\right) \times \right. \quad (5)$$

$$\left. \left(\tfrac{1}{2}\, t_{zi}\, \tfrac{1}{2}\, t_{zj} | T(\alpha) T_z(\alpha)\right) (-)^{\ell_i - \ell_{zi}} \delta_{\ell_i,\ell_j} \delta_{\ell_{zi},-\ell_{zj}}.\right.$$

In the computation, even-A and odd-A nuclei are distinguished by the number parity of the Bogoluibov transformation[13]. For odd-A nuclei, there is a block structure of the Hamiltonian and the odd number parity is imposed on one of the blocks. Each block must be tested to find the global energy minimum.

Results. A quantity that allows us to accurately gauge the relative importance of the pairing condensates is the correlation energy, $E_{corr} = E_0 - E$, where E_0 is the energy of the ground state in the absence of a pairing condensate, i.e. the result of setting all κ_α to zero.

We have mapped out all nuclides with $Z \leq N$ for neutron numbers from 50 to 75 and show the results in Fig. 1. A few nuclei have very small correlation energies (white in Fig. 1), while the majority of nuclei, above and below the proton dripline, are spin-singlet (green squares in Fig. 1). However, a group of nuclei with neutron numbers roughly from 65 to 70 exhibit spin-triplet pairing (red diamonds in Fig. 1), or as discussed below, a

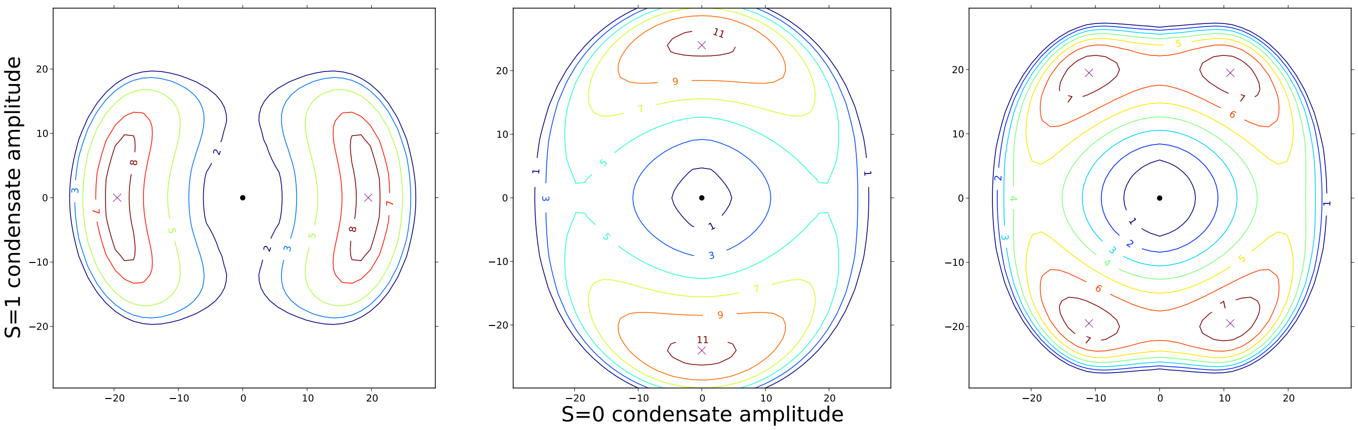

FIG. 2: (color online) Contour plots of the correlation energy in three different $A = 132$ nuclei as a function of the amplitudes of selected spin-singlet and spin-triplet condensates. Left panel: $^{132}_{60}$Nd, mainly spin-singlet pairing, as is common in most nuclei studied to date; middle panel: $^{132}_{66}$Dy, mainly spin-triplet pairing, similarly to what was introduced in Ref. [3]; right panel: $^{132}_{64}$Gd, mixed-spin pairing exemplifying a qualitatively new feature, namely the gradual crossover from spin-singlet to spin-triplet pairing. The numbers show correlation energies in MeV. In all three cases, each peak is marked by an X.

crossover between the two kinds of pairing. The demarcation between the three kinds of pairing is somewhat arbitrary, so we have chosen to call "mixed-spin paired" those nuclei for which the spin-singlet amplitude is between one and three quarters of the total pairing amplitude. Note that the island of mixed-spin paired nuclei (blue circles in Fig. 1) contains many nuclei that lie within the proton dripline. Thus, the predicted mixed-spin pairing may be relevant to experimental investigation.

In an attempt to understand how the pairing condensate changes from from spin-singlet to spin-triplet, we have examined in more detail some nuclei at mass number $A = 132$. Here, the $N = Z$ nucleus $^{132}_{66}$Dy exhibits spin-triplet pairing. Changing the neutron-proton asymmetry, one reaches the region of ordinary spin-singlet pairing when $N - Z > 10$. The nucleus ($^{132}_{60}$Nd) is an example. At the BdG minimum, the only nonzero anomalous densities are the ones for $\alpha = 1, 3$ and they have roughly equal amplitudes. To see how the energy varies as the condensate is changed, we constrain κ_α away from the values at the minimum and examine the energy surface. For a two-dimensional plot we take the x variable to be the amplitude of the neutron-neutron condensate (κ_1) and the y variable the amplitude of the neutron-proton condensate κ_5. The amplitude of the proton-proton condensate κ_3 is taken to be the same as κ_1, all other condensates are set to zero. The resulting correlation energy for $^{132}_{60}$Nd is shown as a contour plot in the left panel of Fig. 2. The peaks near $(x, y) \approx (\pm 20, 0)$ correspond to the unconstrained BdG minimum. The BdG energy does not depend on the phase of the condensate, so the energy surface is symmetric under reflections in both axes. The pure uncorrelated ground state at the center of the graph (black dot) defines the zero level for the condensation energy. Note that the contours are elongated in the vertical direction, indicating that the energy surface is rather soft with respect to forming a spin-triplet condensate.

The middle panel of Fig. 2 shows the energy surface for $^{132}_{66}$Dy on the $N = Z$ line. Here the peaks are at $(x, y) \approx (0, \pm 22)$, i.e. the condensate is spin-triplet. Along the x-axis there the spin-singlet condensatation energy reaches a maximum near $x = \pm 20$, but it is only a saddle point in the two-dimensional space.

We now ask how one condensate changes to the other as $N - Z$ is varied. One could imagine a sudden switch, corresponding to a quantum phase transition, if the saddle point in the middle panel of Fig. 2 became a peak that grew to become the global maximum. This is not what happens. Instead, the peak shifts position, moving smoothly from one axis to the other. A typical case is shown in Fig. 3, $N - Z = 4$, i.e. the nucleus $^{132}_{64}$Gd. The maxima are located at $(x, y) \approx (\pm 11, \pm 20)$, i.e. the condensate has a mixed-spin character. We have examined the form of the pairing in the canonical basis and found that the relationship between paired orbitals $|i\rangle$ and $|\bar{i}\rangle$ is $|\bar{i}\rangle = \tau_z T |i\rangle$, where T is the time reversal operator and τ_z is the Pauli isospin operator. This particular form gives ordinary spin-singlet pairing in the absence of neutron-proton mixing in the orbital $|i\rangle$, but has a spin-triplet component when neutrons and protons are mixed.

Discussion. Trial computations we have performed suggest that the phenomenon of mixed pairing depends on the spin-orbit field in the nucleus. In the absence of spin-orbit splitting, the singlet and triplet interactions would be on an equal footing. There would be a sharp transition at $v_s = v_t$, the SU(4) symmetry point, with pure condensates of one type or the other away from that point. Moreover, the smooth transition between spin-singlet and spin-triplet pairing could not have been anticipated from results such as those in Refs. [8, 9] on the behavior in ^{48}Cr as a function of angular momentum. These authors found that the states of different character do not mix strongly and the character of the yrast state just depends on which is lower in energy. Also, in Ref. [15] the authors report that there is a phase transition as a function of $N - Z$, with the change of character taking place suddenly. However, Ref. [10] on the high spin states in ^{80}Zr found a small degree of mixing. It is important to note, however, that the spin-triplet condensates considered in these references are those in channels $\alpha = 4$ and 6 from our Table I. In fact, we only find a smooth transition to spin-singlet pairing starting from $\alpha = 5$, i.e. spin-triplet with z-projection $S_z = 0$.

We now briefly mention some of the possible physical consequences of the mixed pairing phase. One potential consequence of spin-triplet pairing might be a reduced pairing gap in the odd-even mass differences. In particular, it was found in Ref. [3] that some quasiparticle energies are close to zero, suggesting reduced pairing gaps. To examine the pairing gaps we calculate the second difference of the correlation energies by the formula

$$\Delta_o^{(3)}(n) = E(n) - \tfrac{1}{2}\left[E(n-1) + E(n+1)\right]. \qquad (6)$$

Here n is either the neutron or proton number, taken to be odd, with the other nucleon species held fixed at some even number. Typical values of the gap are 0.7-0.9 Mev in normally paired nuclei. These drop to 0.25 for some of the spin-triplet cases as shown in Fig. 3. One sees all of these nuclei are one unit off the $N = Z$ line. Farther off the line where the pairing becomes mixed, the gaps increase to the larger value. Thus, we find some evidence that the gaps are affected, but the predicted effect does not extend within the drip line.

On a different note, there may be spectral signatures of the triplet pairing and the transition. According to Frauendorf, the spectra of odd-odd nuclei become similar to that of even-even nuclei in the limit of strong spin-triplet pairing ([16], p. 499). condensation. Even in the mixed-spin regime, the softness of the energy surface suggests that there should be low-lying excitations associated with the spin degree of freedom. The mean-field theory has to be extended to deal with broken symmetries including particle number and angular momentum before predictions can be made for spectroscopic quantities. Other observables of interest are two-particle transfer direct reaction cross sections, which in principle can be used to compare correlation strengths in the two spin channels. Here, again, the theory needs to restore good particle number to distinguish between the nuclei participating in the transfer reaction, and this remains for future work. Finally, nuclear deformation can strongly modify pairing behavior, so it is important to extend the calculations to the full Hartree-Fock-Bogoliubov theory in which deformation effects are included. In this Letter, we have focused on the qualitatively new phenomenon of mixed-spin pairing, predicted for nuclei that are experimentally accessible.

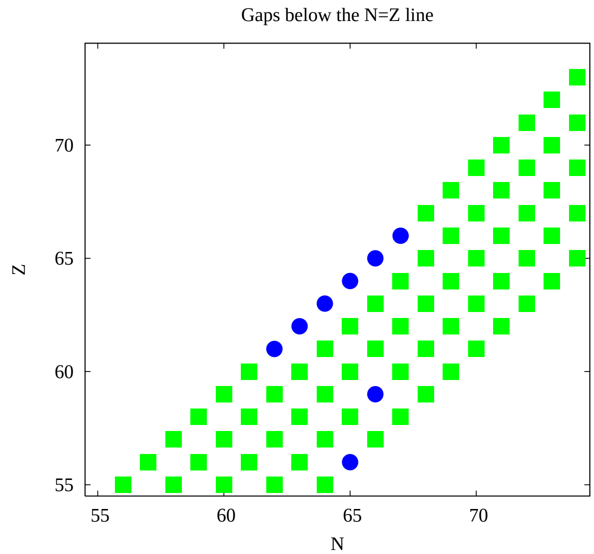

FIG. 3: (color online) Small and large pairing gaps (Eq. 6) for nuclei near the spin-triplet pairing region. Blue circles: $\Delta_o^{(3)}(n) < 0.4$ MeV; green squares: $\Delta_o^{(3)}(n) > 0.4$ MeV.

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