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NUCLEAR STRUCTURE AND PAIRING CORRELATIONS FOR THE HEAVY ELEMENTS

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ABSTRACT

The advent of BCS calculations for deformed nuclei has brought extensive progress in understanding many nuclear properties. With the aid of fast and versatile computer facilities a number of previously-made simplifying assumptions have been tested. (1) By use of delta-force matrix elements between Nilsson eigenfunctions, instead of a constant-G pairing force, some feeling for the nature of fluctuations in Δ_ν values and their variation as the systems are filled is gained. (2) By carrying the usually-neglected $\bar{G}_{\nu\nu'}$ matrix elements of Belyaev a generally uniform lowering of Nilsson levels is observed as the system is filled. (3) The systematic effects on variational energies and average configuration mixing caused by projecting fixed-particle terms from BCS wave functions (PBCS) is studied and (4) the variation has been performed on the fixed-particle expression (FBCS). The FBCS method gives the lowest possible energies for a variational solution of the projected BCS form. The FBCS method is found always to lead to non-trivial solutions no matter how weak the residual force strength; the abrupt transition between superfluid and normal states of the nuclear fluid, predicted by the BCS method, is thus found to be a spurious result. The FBCS method always gives more configuration mixing than PBCS. The PBCS energies are close to

FBCS in the region of high pairing correlation but are worse where pairing correlation is lower. This tendency is reflected strikingly in the odd-even mass differences, where the PBCS method gives differences much too large in the region of low pairing correlation. Most of the simpler methods are found to predict too-high level densities for odd-proton systems, relative to the FBCS method.

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1. Introduction

In pursuing theoretical calculations of alpha decay rates we have found results to be greatly sensitive to configuration mixing in the shell-model wave functions. In the region of mass 242, average decay rate enhancements of three orders of magnitude are caused by introduction of the pairing force.[1,2] It was clear that refinement of the alpha rate theory demanded the closest attention to the pairing force and the increased nucleon-nucleon correlations it brings about. This paper investigates the effects on spectra and eigenfunctions of several modifications to previous detailed calculations for spheroidal nuclei.[3,4,5]

2. BCS Formulas for Ground States of Even Systems

The Hamiltonian of the problem we treat is written in second quantization form as

$$H = \sum_{\nu} \epsilon_{\nu}(b^{+}_{\nu+} b_{\nu+} + b^{+}_{\nu-} b_{\nu-}) - \frac{1}{2} \sum_{\nu\sigma} \langle \nu_1\sigma_1\nu_2\sigma_2 | V\delta(\underset{\sim}{r}_1-\underset{\sim}{r}_2) | \nu_2'\sigma_2'\nu_1'\sigma_1' \rangle b^{+}_{\nu_1\sigma_1} b^{+}_{\nu_2\sigma_2} b_{\nu_2'\sigma_2'} b_{\nu_1'\sigma_1'} \tag{1}$$

where $b^+_{\nu\sigma}$ operating on the vacuum $|0\rangle$ creates a nucleon in state $\nu\sigma$ and $b_{\nu\sigma}$ annihilates it. The notation is that of Belyaev,[6] where the index ν stands for all quantum numbers specifying a given Nilsson orbital and σ for the sign (+ or -) of the projection of particle angular momentum along the nuclear cylindrical symmetry axis. The subscript 1 labels the state of motion of particle 1 and the 2 that of particle 2. The summation $\nu\sigma$ runs over all states inside an arbitrary cut-off energy.

The independent-particle scheme on which the pairing calculations are based is that of Nilsson for nucleons moving in a spheroidal potential (prolate for the actinide nuclei of interest to us). Thus the ϵ_ν are Nilsson-state eigenvalues and the basis states $b^+_{\nu+}|0\rangle$ are Nilsson eigenfunctions and $b^+_{\nu-}|0\rangle$ are conjugates.

The matrix elements of eq. (1) are just the matrix elements of the residual nucleon-nucleon force. A usual approximation is to set all the matrix elements between paired states equal to a constant G, but we shall instead be using the matrix elements of a delta force between Nilsson states.

The number operator which "counts" the number of nucleons in a wave function is

$$N = \sum_\nu (b^+_{\nu+} b_{\nu+} + b^+_{\nu-} b_{\nu-}).$$

We seek simultaneous eigenfunctions of the Hamiltonian and the number operator. For systems where the number of permutations of $N/2$ pairs in the Ω different orbitals (i.e., the binomial coefficient $\binom{\Omega}{N/2}$) is not large it is feasible to solve the problem by exact diagonalization. For larger systems it has proved most valuable to seek variational solutions which specify only the probabilities v^2_ν that the νth orbital is occupied by a pair. In so doing one throws away

some information contained in the $\binom{\Omega}{N/2}$ different coefficients of the exact wave function but achieves a simpler problem in the Ω different thermodynamic average occupation probabilities v_ν^2. Formally, the variational solutions commonly used are of the Bardeen, Cooper, Schrieffer[7] type

$$\psi = \prod_\nu (u_\nu + v_\nu b^+_{\nu+} b^+_{\nu-}) |0\rangle$$

with $u_\nu^2 + v_\nu^2 = 1$ defining the u_ν quantities. The variational treatment seeks stationary values of $H - \lambda N$. The Lagrangian multiplier λ, the chemical potential, is adjustable to give the proper expectation value of the number operator. An alternative method of solving the problem is to introduce the Bogolyubov[8] canonical transformation to quasi-particle operators and demand that u_ν and v_ν all have values that make a certain term in the transformed Hamiltonian (H_{20}) vanish. In either case the resulting solutions are the same and may be found by solving a set of non-linear simultaneous algebraic equations given by Belyaev[6] and involving new parameters Δ_ν and λ.

$$\Delta_\nu = \frac{1}{2} \sum_{\nu'} \frac{G_{\nu\nu'}}{\sqrt{[(\tilde{\epsilon}_{\nu'} - \lambda)^2 + \Delta_{\nu'}^2]}} \Delta_{\nu'} = \sum_{\nu'} G_{\nu\nu'} u_{\nu'} v_{\nu'} \tag{2}$$

$$N = \sum_\nu 2v_\nu^2 \tag{3}$$

$$\tilde{\epsilon}_\nu = \epsilon_\nu - \sum_{\nu'} G_{\nu\nu'} v_{\nu'}^2 \tag{4}$$

$$v_\nu^2 = \frac{1}{2} \left(1 - \frac{\tilde{\epsilon}_\nu - \lambda}{\sqrt{[(\tilde{\epsilon}_\nu - \lambda)^2 + \Delta_\nu^2]}}\right) \tag{5}$$

where the Δ_ν are the pairing-correlation energy parameters of the orbitals.

In the Hamiltonian of eq. (1) the sum over residual-force matrix elements ran separately over all states for each of the four operators appearing. The choice of BCS trial function is restrictive such that matrix elements involving more than two different Nilsson states can make no contribution. Thus, only two types of matrix elements survive. The first type which we denote $G_{\nu\nu'}$ gives rise to the pairing effects and is defined after Belyaev as

$$G_{\nu\nu'} = \langle \nu\ \nu | G | \nu'\ \nu' \rangle = \langle \nu+\ \nu-\ | V\delta | \nu'+\ \nu'- \rangle - \langle \nu+\ \nu-\ | V\delta | \nu'-\ \nu'+ \rangle$$

The second type, which gives rise to terms in the self-consistent field, we denote $\overline{G}_{\nu\nu'}$, and is defined after Belyaev as

$$\overline{G}_{\nu\nu'} = \langle \nu+\ \nu'+ | V\delta |\ \nu+\ \nu'+ \rangle - \langle \nu+\ \nu'+\ | V\delta |\ \nu'+\ \nu+ \rangle +$$

$$\langle \nu+\ \nu'-\ | V\delta |\ \nu+\ \nu'- \rangle - \langle \nu+\ \nu'-\ | V\delta |\ \nu'-\ \nu+ \rangle$$

It is usual to assume that all matrix elements $G_{\nu\nu'}$ are equal and that the $\tilde{\epsilon}_\nu = \epsilon_\nu$. The former assumption simplifies eq. (2), and there results only a single Δ value applying to all orbitals, hence two simultaneous equations in two unknowns. We have instead calculated the matrix elements between various orbitals using a delta force and Nilsson wave functions. The use of a delta force for matrix elements means that we are using an interaction for singlet spin states only. The matrix elements are for pairs of identical fermions and the delta force only acts on s-states of relative orbital motion; hence, use of antisymmetric wave functions causes the interaction in triplet spin states to vanish identically. The delta-force matrix elements are closely related to

certain coefficients entering shell-model alpha decay theory, where also only singlet spin states contribute. The delta-force matrix elements between Nilsson states can be calculated by operating through with the singlet spin projection operator $P_s = \frac{1-\underset{\sim}{\sigma}_1 \cdot \underset{\sim}{\sigma}_2}{\psi}$ and integrating the products of four Nilsson orbital functions over arguments r, θ, ϕ. The angular integrals become integrals over products of four spherical harmonics, expressible as sums over products of four Clebsch-Gordan coefficients. The radial integrals are over products of four associated Laguerre polynomials with an exponential factor. The same integral had earlier been worked out by Mang and Rasmussen[1] for the C_ρ^0 coefficients of alpha decay. The delta-force matrix element is related to its C_ρ^0 coefficients by

$$G_{\nu\nu'} = \frac{V_o}{2} \sum_\rho (-1)^\rho \binom{\rho + \frac{1}{2}}{\rho} 2^\rho C_\rho^0 \left(\frac{M\omega}{2\hbar}\right)^{\frac{3}{2}} \tag{6}$$

A further property of delta-force matrix elements is the identity,

$$G_{\nu\nu'} = \overline{G}_{\nu\nu'} .$$

3. Conservation of Particle Number

As has often been pointed out, the BCS wave functions have the defect that the number of particles is not strictly conserved and this feature may give rise to spurious effects. Kerman, Lawson, and Macfarlane[9] have suggested and used an approach whereby one retains from the BCS wave function just those terms with the number of creation operators exactly equal to the number of nucleons in the problem and then renormalizes. Thus, the BCS solution is only

an intermediate step providing an approximate prescription for obtaining a wave function with all possible terms that conserve the particle number.

Performing calculations of energies and transition probabilities with the projected wave functions is not as formidable as one might suppose. We use the notation of Bayman[10] based on the property

$$\oint \frac{dz}{z^n} = 2\pi i \, \delta_{n1} \quad ,$$

the contour being taken around the origin. Thus, the projected BCS solution with p pairs may be written

$$\psi_P = \frac{\mathcal{N}}{2\pi i} \oint \frac{d\zeta}{\zeta^{p+1}} \prod_\nu (u_\nu + \zeta v_\nu \, b^+_{\nu+} \, b^+_{\nu-}) |0\rangle \tag{7}$$

with $\mathcal{N}$ a normalization constant determined by the condition $\langle \psi_P | \psi_P \rangle = 1$.

For the unprojected solutions the energy of the ground system (E_{BCS}) of an even number of nucleons is just given by evaluating Belyaev's[6] eq. (12) without the λ term

$$E_{BCS} = \sum_\nu 2v_\nu^2 \left(\epsilon_\nu - \frac{1}{2} \sum_{\nu_1} \bar{G}_{\nu\nu_1} v_{\nu_1}^2\right) - \sum_{\nu\nu_1} G_{\nu\nu_1} u_{\nu_1} v_{\nu_1} u_\nu v_\nu \quad . \tag{8}$$

Dietrich, Mang, and Pradal have developed[11] practical formulas for the projection of proper particle-number components from solutions of BCS form. Their energy expression is

$$E_{(\text{projected})} = \langle \psi_P | H | \psi_P \rangle = \langle \psi_{BCS} | H | \psi_P \rangle =$$

$$\frac{\mathcal{N}^2}{2\pi i} \oint \frac{d\zeta}{\zeta^{p+1}} \langle 0 | \prod_{\nu} (u_\nu + v_\nu b_{\nu-} b_{\nu+}) \; | H | \prod_{\nu'} (u_{\nu'} + \zeta v_{\nu'} b^+_{\nu'+} b^+_{\nu'-}) | 0 \rangle =$$

$$\sum_{\nu} (\epsilon_\nu - \frac{1}{2} G_{\nu\nu}) 2v_\nu^2 \frac{R_1^1(\nu)}{R_o^o} - \sum_{\substack{\nu_1 \nu \\ \nu \neq \nu_1}} \bar{G}_{\nu_1 \nu} v_{\nu_1}^2 v_\nu^2 \frac{R_2^2(\nu_1 \nu)}{R_o^o} -$$

$$\sum_{\substack{\nu_1 \nu \\ \nu \neq \nu_1}} G_{\nu_1 \nu} u_{\nu_1} v_{\nu_1} u_\nu v_\nu \frac{R_1^2(\nu_1 \nu)}{R_o^o} \tag{9}$$

The function $R_q^n(\nu_1 \cdots \nu_n)$ is defined as

$$\frac{1}{2\pi i} \oint \frac{dz}{z^{p-q+1}} \prod_{\substack{\nu \\ (\nu \neq \nu_1 \cdots \nu_n)}} (u^2 + z v_\nu^2)$$

Therefore

$$\mathcal{N}^{-2} = R_o^o$$

Note now that there are different ways of employing eq. (9). One may, as done by Kerman et al.[9], solve the ordinary BCS equations first and use the u_ν and v_ν values thus obtained with eq. (9). This method we denote PBCS and the energy E_{PBCS}. A more complicated but more exact variational procedure is to minimize the energy expression of eq. (9) with respect to the v_ν parameters, as done by Dietrich et al.[11]. We denote this method as FBCS, and it must give an energy value lower than that of the PBCS method.

4. Formulas for Odd Systems

For the systems with an odd number of particles there are several different methods of calculation within the BCS framework. The simpler method, outlined by Belyaev[6] and used extensively by Kisslinger and Sorensen[12] and others, is to solve the variational problem as for the BCS ground state of an even system and operate on the eigenfunction with a quasi-particle creation operator. This method leads to the approximation that the excitation energies of the various states in an odd nucleus are simply the quasi-particle energies.

$$E_\nu = \sqrt{[(\tilde{\epsilon}_\nu - \lambda)^2 + \Delta_\nu^2]}$$

The other methods involve "blocking" and require that the energy of each odd particle state be found by recomputing the variational solution as for an even ground state, but omitting the "blocked" orbital populated by the odd nucleon. There are BCS, PBCS, and FBCS solutions possible in the "blocking" framework.

Since we are retaining the usually neglected $\bar{G}$ matrix elements that contribute to the self-energies $\tilde{\epsilon}$, it is necessary to consider carefully their contribution in the blocking calculation.

For the odd system we have the total energy expression

$$E_{BCS} = \sum_{\nu \neq k} (\epsilon_\nu - \frac{1}{2} \sum_{\nu_1 \neq k} \bar{G}_{\nu\nu_1} v^2_{\nu_1}) 2v^2_\nu$$

$$- \sum_{\nu,\nu_1 \neq k} G_{\nu\nu_1} u_{\nu_1} v_{\nu_1} u_\nu v_\nu + \epsilon_k - \sum_{\nu_1 \neq k} \bar{G}_{k\nu_1} v^2_{\nu_1} \tag{10}$$

The BCS wave function which conserves the nucleon number in the odd case has the form

$$\Psi_{p,k} = \frac{\mathcal{N}}{2\pi i} b^+_k \oint \frac{d\zeta}{\zeta^{p+1}} \prod_{\nu \neq k} (u_\nu + \zeta v_\nu b^+_{\nu+} b^+_{\nu-}) |0\rangle, \tag{11}$$

where p is the number of pairs, and the energy is

$$E_{(projected)} = \sum_{\nu \neq k} (\epsilon_\nu - \frac{1}{2} G_{\nu\nu}) 2v^2_\nu \frac{R^2_1 (\nu k)}{R^1_0 (k)}$$

$$- \sum_{\substack{\nu_1,\nu \neq k \\ \nu \neq \nu_1}} \bar{G}_{\nu_1\nu} v^2_{\nu_1} v^2_\nu \frac{R^3_2 (\nu_1 \nu k)}{R^1_0 (k)}$$

$$- \sum_{\substack{\nu_1,\nu \neq k \\ \nu \neq \nu_1}} G_{\nu_1\nu} u_{\nu_1} v_{\nu_1} u_\nu v_\nu \frac{R^3_1 (\nu_1 \nu k)}{R^1_0 (k)} \tag{12}$$

$$- \sum_{\nu \neq k} \bar{G}_{\nu k} v^2_\nu \frac{R^2_1 (\nu k)}{R^1_0 (k)} + \epsilon_k$$

5. Numerical Calculations

Since we desired eigenfunctions for alpha decay calculations, our numerical calculations concentrated on the actinide region. We selected a set of 25 proton orbitals and 40 neutron orbitals covering the actinide region. Our energy values were generally those of Mottelson and Nilsson[13] at an average deformation of $\eta = 5$ but with some upward shifting of the even-parity orbitals for protons and odd-parity levels for neutrons to give better agreement with experimental spectra.

Our delta-force matrix elements were calculated from eigenfunctions of Nilsson[14] or Mottelson and Nilsson[13] at deformation $\eta = 6$. Eigenfunctions are not tabulated for $\eta = 5$, and we wished to avoid interpolation. The over-all strength of the force was adjusted to match, on the average, the experimental odd-even mass difference.

Examination of the delta-force matrix elements showed extensive fluctuation in magnitude, with diagonal matrix elements $G_{\nu\nu}$ and off-diagonal elements between spin-orbit conjugate orbitals being systematically larger than other off-diagonal matrix elements. Table 1 lists for certain proton orbitals the diagonal elements $G_{\nu\nu}$, the average of the 24 off-diagonal elements, and the maximum and minimum off-diagonal elements. The orbitals comprise those tabulated by Stephens, Asaro, and Perlman[15] in their comparison with experimental spectra, plus a few additional nearby orbitals. The matrix elements are tabulated as ratios to a strength parameter g_p. The energy units most frequently appearing are $0.05\ \hbar\omega_o$ (where $\hbar\omega_o \approx 41\ A^{-\frac{1}{3}}$ MeV). In the later numerical work we find a value of $g_p = 5.0$ best matches proton odd-even mass differences.

The observation of the large fluctuation of matrix elements raised the possibility that the solutions of eqs. (2) and (3) might give rise to large fluctuation in the individual Δ_ν correlation parameters. Such results would have serious implications for the usual constant-G approximation.

The BCS eqs. (2) and (3) were solved by a double iterative procedure on the Berkeley IBM-7094 computer.

It is not practical to present the bulk of the numerical results, but we shall try to give enough examples to exhibit the differences arising from (a) use of non-constant $G_{\nu\nu'}$ matrix elements, (b) the retention of self-consistent-field terms $\overline{G}_{\nu\nu'}$, and (c) projecting out fixed particle number, either after (PBCS) or before doing the variation (FBCS).

Figure 1 plots the correlation function (Δ_ν) values as a function of proton number for even proton systems and fig. 2 is the corresponding plot of self-energies $(\tilde{\epsilon}_\nu)$ and the chemical potential λ. We note for orbitals near the Fermi surface that Δ_ν values may scatter by as much as 20%. There is a systematic tendency for an orbital to develop its largest Δ value relative to neighbors just when it is nearest the Fermi surface. This tendency is an obvious consequence of the especially large diagonal matrix elements noted in table 1.

The general trend of overall decrease in Δ with increasing proton number is found here. Such a decrease was found in constant-G calculations of Nilsson and Prior[4] and Veresh, Soloviev and Shiklos[5] and it is a consequence of decreasing single particle level density at the Fermi surface as one goes from proton number 90 to 100. The abrupt change in slope at Z = 96 is a consequence of the rather large Nilsson level spacing between the $\frac{5}{2}$ - (523) and the $\frac{3}{2}$ - (521) orbitals as seen in fig. 2. We do not believe that experimental evidence supports any proton subshell effects at Z = 96, and therefore conclude that our calculations would have been more realistic with Nilsson level spacings not showing such a break. The plot of fig. 2 shows the effect of the retained field terms in $\overline{G}_{\nu\nu'}$. The self energies systematically decrease as the number of nucleons increases. Those orbitals which have larger matrix elements connecting them with the filling orbitals may drop more than others.

Figures 3 - 5 are the corresponding Δ_ν and $\tilde{\epsilon}_\nu$ plots for the 40-orbital even neutron systems. We see in fig. 5 that the retention of the $\bar{G}_{\nu\nu'}$ matrix elements has caused not only a general lowering of $\tilde{\epsilon}_\nu$ with increasing neutron number, but also one actual cross-over.

In the course of this work we came more and more to be concerned with the occasional situation where there existed only a "trivial" solution to the BCS equations. The trivial solutions, where all Δ_ν values equal zero, have no configuration mixing whatsoever and contradict the perturbation theory prediction that there will always be some configuration mixing no matter how weak the residual force. The loss of the non-trivial solution occurs when the Nilsson level spacing near the chemical potential becomes sufficiently large compared to the pairing-force matrix elements. Before final selection of ϵ_ν values we found such solutions for even neutron systems near the 152- neutron "sub-shell". They occurred even more frequently for odd systems with an additional level blocked. Belyaev[6] gave an inequality which must be satisfied for non-trivial solutions. The work published by Soloviev[5] in 1961 showed frequent occurrence of trivial solutions in the two-quasi-particle excited states of even rare earth nuclei. Clearly the projection of fixed-particle-number from the BCS wave function is of no aid in trivial cases, since the trivial solution already conserves the particle number. In the course of comparisons of BCS with exact solutions for model systems (cf. ref. 16) some of us[17], examined analytically the behavior of the FBCS solutions in the region where BCS solutions go trivial. We found that the FBCS method always yields a non-trivial solution at any pairing-force strength, and that the wave functions of FBCS were close to exact over the entire force range, except for some small components in the wave functions. Dietrich has recently been able to prove generally that for an attractive pairing force of any strength, a non-trivial solution exists with lower energy than the trivial solution.[18]

The more sophisticated FBCS method does not yield such simple values as Δ_ν to measure the involvement of an orbital in the pairing correlation. Qualitatively, the features displayed in figs. 1-5 for BCS solutions will also be expected to be valid for the FBCS solutions.

6. Comparison of BCS, PBCS, and FBCS Soutions

6.1 Even Systems

In this section we wish to compare, first of all, the total binding energies of even systems, calculated by three methods: the BCS, where the energy is of a collection of systems with differing numbers of particles; the PBCS, where the energy is of the central component of the collection; and the FBCS, where the variational parameters v_ν are adjusted to minimize the energy of just this component.

Table 2 gives the FBCS total energies and the energy differences to the higher BCS and PBCS energies. The energy units are Nilsson's $0.05\ \hbar\omega_0$ ($\approx$ 0.330 MeV at A = 242). We do not know the exact eigenvalues for these very large systems, but we can certainly appreciate some of the shortcomings of the BCS and PBCS solutions by a study of table 2. The ordinary BCS energies are always higher than FBCS by from $\approx$ 250 keV to $\approx$ 600 keV. Eliminating the spurious particle numbers by the PBCS procedure usually results in substantial reduction of the energy. In general, the errors in both cases increase as pairing correlation decreases with increasing Z or N. The error in PBCS reaches a maximum at N = 152, where the Nilsson levels are spread and the pairing correlation is consequently lowest.

In order to gain insight into the nature of the improvement of solutions in going from PBCS to FBCS we have calculated a quantity D measuring the "diffuseness" of the Fermi surface implied by the various eigenfunctions. This quantity D is

a sum over all orbitals of the square root of the product of the probability that it is occupied times the probability that it is empty. For ordinary BCS solutions we have the simple expression

$$D = \sum_{\nu} u_{\nu} v_{\nu} \tag{13}$$

For PBCS and FBCS this becomes

$$D' = \sum_{\nu} u_{\nu} v_{\nu} \frac{\sqrt{[R_1^1(\nu) R_0^1(\nu)]}}{R_0^0} \tag{14}$$

with whichever set of u_{ν} and v_{ν} values is appropriate. Note that the "diffuseness" D goes to zero for a trivial solution. For the constant-G matrix-element approximation we have $D = \frac{\Delta}{G}$. For ground-to-ground alpha decay rate calculations the average enhancement due to pairing correlations is approximated by the product of the squares of the D values for neutrons and protons. In fact, our unpublished detailed alpha decay rate calculations with these wave functions show fairly good agreement between simple BCS and FBCS, while PBCS wave functions yield substantially lower rates. The plots of D_p and D_n in fig. 6 show the systematically lower diffuseness calculated by PBCS. The presence of the spurious particle-number components in the BCS wave function makes for its greater diffuseness than PBCS, but one sees that the local "scalloping" cusps of PBCS and FBCS are smeared out in BCS. The positions of the cusp-like minima in D correspond to especially low Nilsson level densities over an energy interval comparable to Δ at the Fermi surface, as can be seen by referring back to figs. 2 and 5.

That the apparently good agreement in D between simple BCS and FBCS cannot hold under all conditions becomes clear when we gradually lower the pairing-force strength. Such a calculation has relevance to real nuclei in connection

with the problem of effective moments-of-inertia of high-spin members of rotational bands. Mottelson and Valatin[19] treated the problem in terms of an effective pairing-force strength that is steadily reduced as one goes to higher spin members. It is well known that below some critical pairing-force strength the BCS equations completely fail to give a non-trivial solution (cf. Belyaev's[6] inequality (31)), and this behavior suggested an abrupt change in moment-of-inertia at some critical spin. Yu. T. Grin came to similar conclusions in his theoretical calculations.[20] In fig. 7 we plot for two particular proton numbers the variation of D_p with pairing-force strength-parameter g_p. For $Z = 96$ we see the BCS solution rather sharply going trivial near $g_p = 3.5$, whereas FBCS decreases only gradually. For $Z = 90$ the D_p values for the BCS solution stay large to much weaker pairing force since the $\frac{1}{2}$ - (530) and $\frac{3}{2}$ + (651) levels are almost degenerate and bracket the Fermi energy at low force strength, as seen in fig. 2. There are no abrupt changes in D_p with pairing-force strength when the variational calculation is carried out in the proper manner as in FBCS. The consequences to the question of the nuclear phase transition from "superfluid" to "normal" state are clear. The transition is a gradual and not a sudden phenomenon. One should not expect to find any sudden changes in effective moment-of-inertia at any critical value of the spin, and the experimental data of Diamond, Lark, and Stephens[21] on rotational bands up to $I = 18$ fail to support the notion of a critical spin value.

6.2 Odd Systems

It is usual practice[4,12] in pairing-force calculations to adjust the force-strength to match generally the odd-even mass difference. Because the characteristic Δ_ν values vary from orbital to orbital, it could be rather misleading

to determine odd-even mass differences from difference formulas with more than one nucleus with odd particle-number entering. Furthermore, if we wish to compare the odd-even mass difference with Δ_ν, we should involve only one odd system. For interpolation of the even mass surface it is desirable to do better than a two-point interpolation to approximate the position of the the even mass surface at the odd nucleon number. We therefore use a four-point interpolation on the four neighboring even systems and subtract this interpolated mass from the calculated odd-system mass for our theoretical odd-even mass (energy) differences.

$$\Delta E_{oe}(Z) = E(Z) - \left[-\frac{1}{16}E(Z-3) + \frac{9}{16}E(Z-1) + \frac{9}{16}E(Z+1) - \frac{1}{16}E(Z+3)\right] \qquad (15)$$

These differences were calculated for proton and neutron systems from results of each of the three methods, BCS, PBCS, and FBCS. The experimental differences for comparison were done in similar fashion, using experimental masses of König, Mattauch, and Wapstra[22] with some adjustment (cf. Appendix A). Where the four neighboring even-system masses were not all known, three-point interpolations were used. Usually a given odd-proton (neutron) mass difference could be determined independently for several different neutron (proton) numbers, and the several determinations were averaged, with weighting according to the assigned uncertainties in the masses. Figures 8 and 9 summarize the results for protons and neutrons, respectively. Note that our adjusted pairing-force strengths (kept fixed at $g_p = 5.0$ and $g_N = 3.7$) give satisfactory average agreement between experiment and the FBCS results. Our theoretical mass difference falls somewhat too rapidly with Z compared to experiment, an indication that the true Nilsson orbital energy spacings at the Fermi surface should not be as large at lower Z as the values employed in the calculation.

The ΔE_{oe} of the PBCS method is always larger than that of the FBCS. This behavior is easily understood, since the PBCS error of too-sharp a Fermi surface is more serious in odd systems with an orbital blocked than in adjacent even systems. At 151 neutrons the PBCS method gives a ΔE_{oe} which is about twice greater than the FBCS and experimental values. It is just in these regions of lowest pairing correlation that the BCS and PBCS approaches become unreliable, but they compare much better with FBCS in the regions of largest pairing correlation.

A common procedure in BCS calculations is to adjust the strength of the pairing force to make the Δ value calculated for unblocked systems equal to the experimental odd-even mass difference. In table 3 we give numbers to test how closely the Δ values estimate the odd-even mass difference calculated by our best method (FBCS). The Δ_ν values are for the theoretical ground-state orbitals at the particular odd particle-number, and they are calculated by BCS without blocking and with the average number of particles equal to the odd number in question. Evidently Δ_ν usually overestimates the PBCS odd-even binding energy. The ratio of these energies is near unity for the first entries of both proton and neutron systems. Here the pairing correlation is high. The ratio increases as the pairing correlation falls, though curiously the difference is not a maximum near the 152-neutron subshell, where pairing correlation is the smallest of all.

Other features that can be shown from calculations on the odd systems are the theoretical spectra. The appearance of these spectra depend on rather small energy differences in the systems, and it is not surprising that the different theoretical methods often give rather different spectra.

In figs. 10 and 11 are shown theoretical band-head positions for odd-proton and odd-neutron systems, respectively, calculated by our best method (FBCS). A comparison with an experimental compilation, such as that of Stephens, Asaro, and Perlman,[15] shows a generally correct ordering. Calculations such

as ours which allow no adjustment of deformation or Nilsson level ordering for various nuclei cannot fit experimental odd spectra overall; the shifts in experimental spectra in isotopic series like ${}_{95}Am^{239,241,243}$ or the berkelium isotopes suggest the importance of the neglected n-p interactions. In alpha decay rate calculations which we hope to publish in a subsequent paper we make use of the wave functions from these calculations which result in the spectra of figs. 10 and 11. Thus, these figures may serve as a measure of the specific shortcomings in these wave functions, arising from non-optimum selection of Nilsson energy levels.

Four different methods for calculating the spectra in odd-proton nuclei are compared in fig. 12 (essentially the same as fig. 16 of ref. 11). At the far right for each Z value are the FBCS results which have been given above in fig. 10. The states in fig. 12 are simply labelled by numbers, but the identification with particular Nilsson states can be made by referring to fig. 10.

The leftmost spectra for each Z-value are the simple quasi-particle energies $\sqrt{[(\tilde{\epsilon}_\nu - \lambda)^2 + \Delta_\nu^2]}$ from BCS solutions with λ adjusted to give $\langle N \rangle$ the odd Z value. This method is the one used by Kisslinger and Sorensen[12] and many others.

Next to the quasi-particle energy spectrum is the spectrum from an ordinary BCS blocking calculation, as first done extensively by Soloviev.[5]

The third spectrum comes from projecting the fixed-particle components from the blocking calculations (PBCS with blocking).

One sees generally that the three conventional methods systematically overestimate the level density compared to FBCS. (Z = 91, Pa, is somewhat exceptional in that there is a very high density of levels near ground by all the methods.) The third method (PBCS with blocking compares rather well with

FBCS except for Z = 95 and 97, where the pairing correlation is low, and the blocking method aggravates the PBCS underestimation of such correlation.

7. Comparison with Other Methods

Landé from his study of model systems with exact solutions has suggested[23] that a better approximation for odd systems is to solve the BCS equations without blocking (but with ⟨N⟩ the odd value desired) and then project the fixed-particle components. Our fig. 13 compares this prescription with FBCS, and it is seen throughout to provide a good approximation. Landé's method is certainly simpler than FBCS, and it is thus of interest to try to understand the reasons for its success and also its limitations. We have seen earlier in graphs of diffuseness that the PBCS method systematically errs in giving too-sharp a Fermi surface. For the odd system, by not blocking the level occupied by the odd-particle when solving the ordinary BCS equations we tend to correct this systematic error. The correction is only a compensation of two errors and may fail, relative to FBCS, near closed shells or subshells where the local level density at the Fermi surface falls so low that the unblocked systems fail or nearly fail to give non-trivial solutions. Figure 14 is the neutron analog of fig. 13, comparing Landé's method with FBCS.

A good deal of insight into the effects of blocking and of projection of fixed-particle components is afforded by the analysis of S. G. Nilsson[24] on the uniformly-spaced-level model. In appendix B we examine some of our solutions from the standpoint of his formulation.

We have not made calculations on two-quasi-particle states by the FBCS method. In our preliminary calculations of such states by the BCS method with blocking, we frequently encountered trivial solutions. It would be desirable to study two-quasi-particle systems by the FBCS method.

A new and simpler method of solutions for constant-G systems is that of Mikhailov.[25] Its principal feature is the replacement of G in the BCS equations by a G_{eff} [$= G(1 + 1/\Delta N^2)$]. ΔN^2 is the mean square fluctuation in the number of particles in the BCS solution. Obviously this substitution prevents the loss of a non-trivial solution, for if ΔN^2 tends toward zero, the effective pairing-force strength is increased without limit. This method always gives greater pairing correlation than simple PBCS, and it deserves closer comparison with FBCS solutions.

The methods of Chasman[26] and of Richardson and Sherman[27] also circumvent the poor behavior of ordinary PBCS in the low-pairing-force limit. Chasman's method can probably give better variational solutions than FBCS by introduction of a few additional variational parameters, and Richardson's method in principle can give exact solutions. These methods are not applicable to the general problem with non-constant, non-factorable $G_{\nu\nu'}$ matrix elements. It will take further development to see whether these new methods will be superior to the BCS-type methods for practical calculations. Certainly the BCS-type variational methods are clumsy for determining excited 0+ states of even systems, and better methods are desirable.

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FOOTNOTE AND REFERENCES

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Table 1. Matrix elements for protons (in units of 0.05 $\hbar\omega_o$)

Orbital $\Omega\pi(N\ n_Z\Lambda)$	$\frac{G_{\nu\nu}}{g_p}$	$\frac{G_{\nu\nu'}(\text{ave})}{g_p}$	$\frac{G_{\nu\nu'}(\text{max})}{g_p}$	$\frac{G_{\nu\nu'}(\text{min})}{g_p}$
3/2+ (532)	0.1897	0.0826	0.1597	0.0421
1/2+ (660)	0.2801	0.0710	0.2363	0.0361
11/2- (505)	0.2461	0.0965	0.2399	0.0417
3/2+ (402)	0.2458	0.1040	0.1938	0.0464
1/2+ (400)	0.3692	0.1029	0.1881	0.0407
3/2+ (651)	0.1980	0.0750	0.1959	0.0349
1/2- (530)	0.2925	0.0797	0.1576	0.0381
5/2- (523)	0.1818	0.0852	0.1567	0.0464
5/2+ (642)	0.1731	0.0772	0.1597	0.0361
3/2- (521)	0.1970	0.0846	0.1918	0.0493
7/2+ (633)	0.1643	0.0790	0.1447	0.0398
7/2- (514)	0.1908	0.0883	0.1736	0.0507

Table 2. Total energies of the valence nucleon systems (in units 0.05 $\hbar\omega_o$)

Even Proton Systems (25 orbitals outside Z = 76 Core):

Z	$-E_{FBCS}$	$E_{BCS} - E_{FBCS}$	$E_{PBCS} - E_{FBCS}$
88	277.0711	0.7998	0.0057
90	321.2267	1.0000	0.0836
92	364.6673	1.2108	0.1098
94	407.0065	1.2930	0.1546
96	448.3517	1.6747	0.2169
98	487.3604	1.4963	0.2534
100	524.8801	1.5038	0.2339

Even Neutron Systems (40 orbitals outside N = 106 core):

N	$-E_{FBCS}$	$E_{BCS} - E_{FBCS}$	$E_{PBCS} - E_{FBCS}$
132	650.0979	0.9840	0.0661
134	691.5384	1.0014	0.0714
136	732.4847	1.0472	0.0811
138	772.9128	1.270	0.0954
140	812.7555	1.2499	0.1116
142	851.8462	1.3937	0.1352
144	889.7387	1.3002	0.1589
146	926.7140	1.3044	0.2003
148	962.7512	1.4561	0.2692
150	997.2782	1.3624	0.3288
152	1030.802	1.728	0.443
154	1067.575	1.211	0.246
156	1091.6522	1.0947	0.779
158	1120.9400	0.9982	0.152

Table 3. Comparison of theoretical odd-even binding energy differences with Δ_ν of the ground state.

Z	ΔE_{oe}(FBCS) (keV)	Δ_ν (keV)	$\frac{\Delta_\nu}{\Delta E_{oe}}$	Ground State
91	987	898	0.910	5/2+ (642)
93	710	839	1.182	5/2+ (642)
95	707	799	1.130	5/2- (523)
97	572	738	1.290	3/2- (521)
99	531	706	1.330	7/2+ (633)
N				
135	762	792	1.039	13/2+ (606)
137	765	803	1.050	1/2- (501)
139	747	749	1.003	1/2- (501)
141	661	744	1.126	5/2+ (633)
143	515	660	1.282	7/2- (743)
145	514	629	1.224	1/2+ (631)
147	425	557	1.311	5/2+ (622)
149	402	556	1.383	7/2+ (624)
151	372	463	1.245	9/2- (734)
153	442	489	1.106	1/2+ (620)
155	450	536	1.191	7/2+ (613)

Appendix A

Calculation of Experimental Odd-Even Mass Differences

As a further test for realistic values of our pairing-force strengths g_p and g_N, it was desirable to compare the theoretical odd-even mass differences with experimental values. Since our calculations do not take into account proton-neutron interaction, it is necessary to average over as many odd systems as possible in order to delete effects caused by the even nucleons. The mass data were taken from König, et al.[22] with some adjustment, described later in this appendix, to correct for an apparent systematic error in the mass table.

The odd-even mass difference was calculated for all odd-mass nuclei in the region of interest for which the odd mass and the mass of at least three adjacent members of the even system were tabulated. Where four even masses were available, the four-point interpolation illustrated by eq. (15) was used. The three-point interpolation is illustrated by the equation

$$\Delta E_{oe}(N) = E(N) - [-\tfrac{1}{8} E(N-3) + \tfrac{3}{4} E(N-1) + \tfrac{3}{8} E(N+1)] \qquad (A.1)$$

For each odd-even mass difference ΔE_{oe} the number of the even nucleons is kept fixed. As an example, we list in table A.1 the experimental ΔE_{oe} for odd-mass nuclei of neptunium. The fourth column lists the number of data points used in interpolating the even system. Error limits of the mass data in ref.(22) were squared and summed with appropriate interpolation factors, all signs being taken positive. The reciprocal square root of this sum was multiplied by the number of data points used in interpolating the even system to obtain the weighting factors in the last column. This gives heavier weighting to the four-point interpolations.

Examination of table A.1 immediately reveals a systematic difference between the 4n+1 and the 4n+3 mass families. The weighted average of the ΔE_{oe} values for the 4n+3 mass family is about 200 keV higher than that of the 4n+1 family. Indeed this systematic difference was encountered in all the odd-mass systems studied, and can probably be attributed to an error in the relative masses of the two odd-mass families.

The average difference between mass families was found to be 196 keV for odd-proton systems and 179 keV for odd-neutron systems. A correction factor of half the average difference was therefore applied to the ΔE_{oe} values (fifth column of table A.1) in computing the average ΔE_{oe} values plotted in figs. 8 and 9. The correction was added to the 4n+1 members and subtracted from the 4n+3 members.

Table A.1. Experimental odd-even mass differences for Np (Z = 93)

A	mass family	N	number of even-mass points	ΔE_{oe} (keV)	weight
231	4n+3	138	3	1000	0.0309
233	4n+1	140	3	585	0.0373
235	4n+3	142	4	789	0.0614
237	4n+1	144	4	596	0.0580
239	4n+3	146	3	720	0.0399
241	4n+1	148	3	683	0.0224

weighted average: 728 keV

weighted average of 4n+3 family: 828 keV

weighted average of 4n+1 family: 609

difference: 219

Appendix B

Additional Detailed Properties of the BCS Solutions

It is of some interest to decompose some of the ordinary BCS solutions into their various components. In so doing one may hope to gain a better understanding of the fixed-particle projection procedure (PBCS).

Nilsson has developed and explored a useful expansion for estimating the energy lowering with projection of fixed-particle number. Writing the expansion in more detail and including additional terms his eq. (2) becomes

$$E_{BCS}(n) = E_{PBCS}(n,p)_{p=n} + \left(\frac{\partial E_{PBCS}}{\partial p}\right)\sigma^1 + \frac{1}{2}\left(\frac{\partial^2 E_{PBCS}}{\partial p^2}\right)\sigma^2 + \frac{1}{3!}\left(\frac{\partial^3 E_{PBCS}}{\partial p^3}\right)\sigma^3 + \cdots . \tag{B.1}$$

Here n is the average number of pairs in the BCS wave function, and p is the number of pairs in a particular component of the BCS function. The σ^i are the ith moments of the pair number probability distribution about the average n. The partial derivatives are to be evaluated at $(n, p = n)$. The projected energies E_{PBCS} which we have compared in the main article are always $E_{PBCS}(n, p = n)$; that is, the BCS equations are solved to give the right average number of pairs n and the central component with $p = n$ is projected. In fact, n may be regarded as a continuous variable, and we shall see that lower E_{PBCS} energies could in general be obtained by minimizing with respect to n. The variable p is not a continuous variable but may take integral values only. Expansion (B.1) then is based on the assumption that the discrete values $(\cdots, E_{PBCS}(n,n-1), E_{PBCS}(n,n), E_{PBCS}(n,n+1), \cdots)$ define a continuous function. There is in Nilsson's eq. (2) the further approximation which he has discussed, that the partial derivatives with respect to p may be replaced by derivatives with respect to n. The

first-derivative term in expansion (B.1) vanishes because σ^1 is zero when the expansion is taken at $p = n$. Nilsson assumes that higher derivative terms than the second may be neglected. It is a purpose of this appendix to evaluate the various partial derivatives and moments of the number distribution for our proton systems and to test eq. (B.1). To be sure, we will not be testing directly the "homogeneous model" (constant-G matrix elements, uniformly-spaced ϵ_ν) which Nilsson treats but we may gain a better notion of the validity of the expansion for real nuclei than if we had treated only the homogeneous model.

Let us denote the probability of the component with p pairs in the BCS wave function of n average pairs as $\mathcal{P}(n,p)$. The formal definition of σ^i is then

$$\sigma^i = \sum_p (p-n)^i \, \mathcal{P}(n,p) \tag{B.2}$$

The identity which expansion (B.1) approximates is

$$E_{BCS} = \sum_p E_{PBCS}(n,p) \, \mathcal{P}(n,p) \tag{B.3}$$

The set of $\mathcal{P}(n,p)$ values peak at $p = n$ and fall off on either side. In fig. B.1 we have plotted the probabilities for two even systems, $n = 7$ and 10, and for the odd system ($\frac{5}{2}$ + (642) blocked) with $n = 8$. The points have been connected by a smooth curve, appearing rather Gaussian-like in form.

Now consider the other factor in eq. (B.3), the energy values of the projected and renormalized components, $E_{PBCS}(n,p)$. Table B.1 lists these energy values for our even-proton systems for several values of n and p. Note that the $E_{PBCS}(n,p)$ values in the n-p plane define a sloping surface slightly convex upward in both dimensions.

The expansion (B.1) results when the summations of eqs. (B.2) and (B.3) are approximated by integrals and $E_{PBCS}(n,p)$ is expanded in a Taylor series in powers of $(p - n)$.

One may first check the assumption that $\partial^2E/\partial n^2 \approx \partial^2E/\partial p^2$. Table B.2 gives second differences of the energies of table B.1 in the vertical and in the horizontal directions, and also gives entries for the case of blocking the $\frac{5}{2}$ + (642) orbital. The derivatives are of the same order of magnitude but it is clear that there is a systematic difference. Thus, the substitution of $\partial^2E/\partial n^2$ in eq. (B.2) may underestimate the second-derivative term by about 30%. Actually Nilsson proposes the derivative of the chemical potential $2\partial\lambda/\partial n$ be substituted for the second derivative. The chemical potential λ strictly speaking is $\partial E_{BCS}/\partial n$. We give the first differences of λ for odd values of particle number, and they also undershoot the desired second derivative. Let us now look at numerical values of various terms in expansion (B.1), using for the second and fourth derivatives the second and fourth differences with respect to p. For the third derivative we use the average of the two third differences adjacent to $p = n$. For the moments σ^i, we use values determined from eq. (B.2) with the sum over all terms $0 \leq p \leq 25$, there being 25 orbitals in the system.

Table B.3 lists the moments, the values of the various derivative terms of eq. (B.1), their sum through the fourth derivative, and the actual rigorous values of $E_{BCS} - E_{PBCS}$ for comparison. The third-derivative term is insignificant throughout, but the fourth-derivative term may enter with either sign and can be significant. The failure to obtain exact agreement between the last two columns is probably due to the approximation of replacing a sum by an integral. The simple approximation $(\partial\lambda/\partial n)\sigma^2$ for $E_{BCS}(n) - E_{PBCS}(n,n)$ is for our examples fairly good, with systematic underestimation of $\approx$ 25%.

It should be pointed out that the energy derivatives higher than the second should vanish in the homogeneous model with a large number of levels. These higher

derivatives in our example are a consequence of non-uniform level spacing.

It might at first appear that projection of fixed-particle number should systematically increase the calculated odd-even mass difference compared to BCS with blocking, since σ^2 is greater for the unblocked even systems. However, we have seen in figs. 8 and 9 that $\Delta E_{oe(PBCS)}$ and $\Delta E_{oe(BCS)}$ are usually about the same. The energy lowering of the blocked odd system is comparable to the even system because its greater $\partial\lambda/\partial n$ approximately compensates its smaller σ^2; the energy lowering by projection of the blocked odd system is in some cases greater and some cases less than neighboring even systems. However, in going to the FBCS method there is a systematic lowering of ΔE_{oe} because FBCS lowers the energy more for the odd systems than for the even systems.

Table B.1

PBCS Energies of proton BCS components with different numbers of pairs.

	n^a			
p-n	7	8	9	10
+3	446.5884[b]	485.3804	522.3448	558.0288
+2	406.5678	447.4843	486.2739	523.3800
+1	364.6239	406.9145	448.0846	486.8174
0	321.1431	364.5575	406.8516	448.1346
-1	276.7780	320.8255	364.1137	406.3198
-2	231.8681	276.3483	320.2611	363.3117
-3	186.5584	231.4113	275.7735	319.4712

[a] n is the average number of pairs of the BCS wave function

p is the number of pairs in the projected component.

[b] All energies are negative in sign.

Table B.2. Some second differences of energies

n	$\left(\frac{\partial^2 E_{PBCS}}{\partial n^2}\right)_{p=n}$	$\left(\frac{\partial^2 E_{PBCS}}{\partial p^2}\right)_{p=n}$	$2\frac{\partial \lambda_{odd}}{\partial n}$
No blocking			
7	0.7221	0.8843	0.7358
8	1.1200	1.3750	0.9628
9	1.0118	1.5049	1.2732
10	2.3101	3.1320	-
5/2+ (642) blocked			
7	-	0.9472	-
8	-	2.8221	-
9	-	4.4400	-

Table B.3. Moments of the particle number distribution and terms of the projected energy series expansion.

n	$\frac{\sigma^2}{2}$	$\frac{\sigma^3}{6}$	$\frac{\sigma^4}{24}$	$\frac{1}{2}\left(\frac{\partial^2 E_{PBCS}}{\partial p^2}\right)\sigma^2$	$\frac{1}{6}\left(\frac{\partial^3 E}{\partial p^3}\right)\sigma^3$	$\frac{1}{24}\left(\frac{\partial^4 E}{\partial p^4}\right)\sigma^4$	sum	$E_{BCS} - E_{PBCS}$
No blocking								
7	0.974	- 0.0347	0.476	0.860	- 0.017	+ 0.150	0.993	0.916
8	0.845	- 0.0388	0.366	1.162	- 0.020	- 0.080	1.062	1.101
9	0.702	- 0.0252	0.258	1.057	- 0.024	+ 0.297	1.330	1.138
10	0.557	- 0.0122	0.171	1.744	- 0.006	- 0.505	1.233	1.458
5/2+ (642) blocked								
7	0.740	- 0.0575	0.282	0.702	- 0.079	+ 0.435	1.058	0.872
8	0.492	- 0.0317	0.135	1.388	- 0.058	- 0.106	1.224	1.226
9	0.333	+ 0.0001	0.068	1.480	0.000	- 0.346	1.134	1.287

FIGURE CAPTIONS

Figure 1. Plot of proton correlation functions Δ_ν as a function of proton number. The energy is indicated in units of 0.05 $\hbar\omega_0$ on the left and in keV on the right.

Figure 2. Plot of proton energies $\tilde{\epsilon}_\nu$ in the self-consistent field (abbreviated, self-energies) as a function of proton number.

Figure 3. Plot of neutron correlation functions Δ_ν as a function of neutron number for some neutron orbitals.

Figure 4. Plot of neutron correlation functions Δ_ν as a function of neutron number for some other orbitals.

Figure 5. Plot of neutron self-energies $\tilde{\epsilon}_\nu$ as a function of N.

Figure 6. Plots of diffuseness of the Fermi surface for proton and neutron systems. The three variational methods are plotted with the following symbols: ⊙ BCS, △ PBCS, ⊡ FBCS.

Figure 7. Plots of diffuseness of the Fermi surface for proton systems as a function of decreasing pairing force strength. Open symbols denote 7 pairs (Z = 90), and closed symbols 10 pairs (Z = 96). Circles are for the BCS method, triangles for PBCS, and squares for FBCS.

Figure 8. Odd-even mass differences for proton systems (⊙ BCS, △ PBCS, ⊡ FBCS theoretical and ▲ experimental).

Figure 9. Odd-even mass differences for neutron systems (⊙ BCS, △ PBCS, ⊡ FBCS theoretical and ▲ experimental).

Figure 10. Theoretical (FBCS) energies of various bands in odd-proton nuclei.

Figure 11. Theoretical (FBCS) energies of various bands in odd-neutron nuclei.

Figure 12. Comparison of four theoretical methods for calculating energies of bands in odd-proton nuclei. From left to right the methods are:

Figure 12. (Cont.) Q = quasi-particle energies from unblocked odd-number BCS solutions; B = BCS with blocking; P = PBCS, fixed-particle projection from BCS with blocking; F = FBCS.

Figure 13. Comparison of FBCS spectra (odd-Z), labelled F, with Landé's method (fixed-particle projection from unblocked BCS with $\langle N \rangle$ odd).

Figure 14. Comparison of FBCS Spectra (odd-N), labelled F, with Landé's method (fixed-particle projection from unblocked BCS with $\langle N \rangle$ odd).

Figure B.1. Probability of components with p pairs in a BCS ground state wave function with average pair number n. (● n = 7, wave function for Z = 90; □ n = 10, wave function Z = 96; ▨ n = 8, wave function for Z = 93 with 5/2 + 642 orbital blocked).

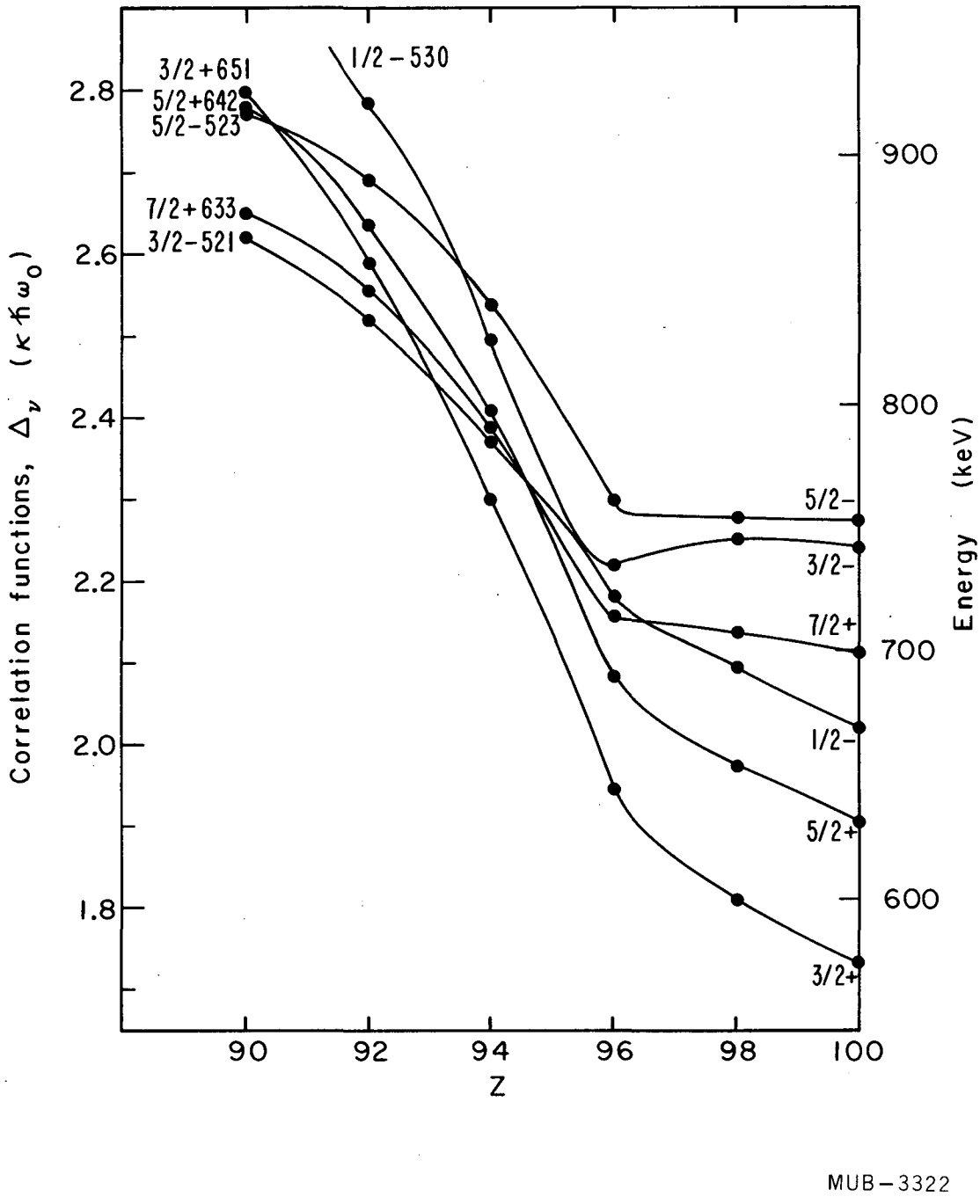
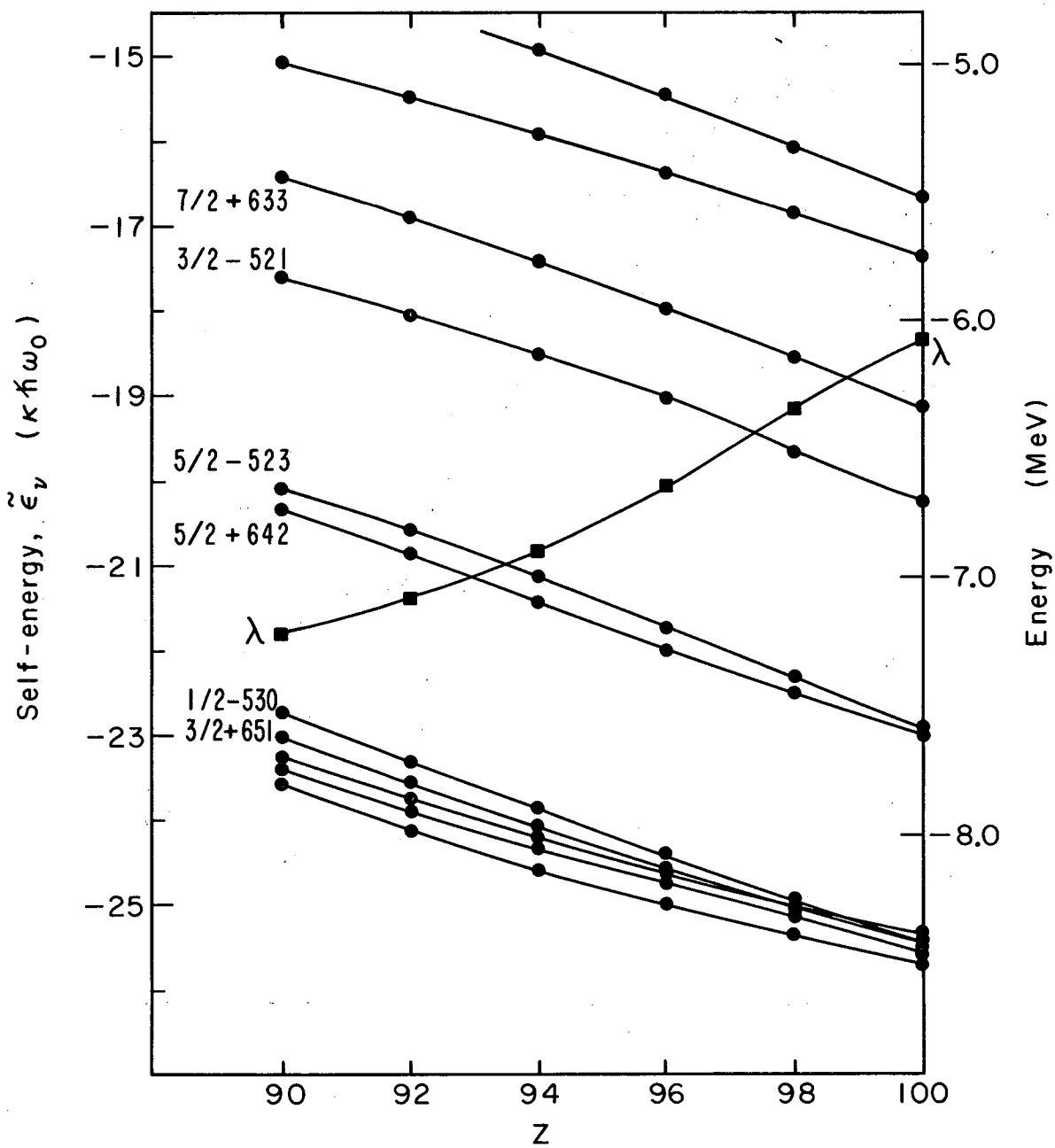
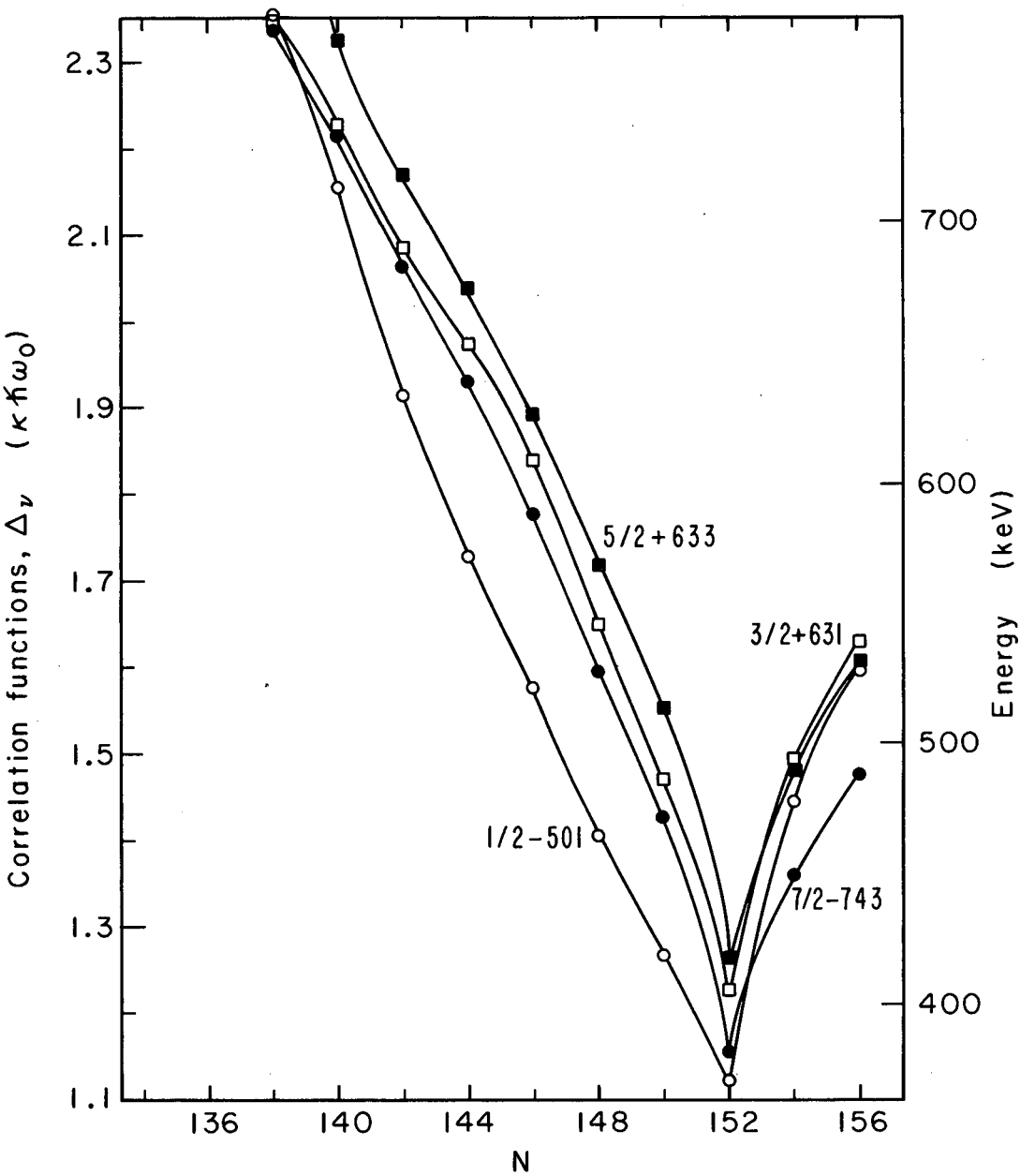

3/2+651
5/2+642
5/2-523
7/2+633
3/2-521
1/2-530
2.8
2.6
2.4
2.2
2.0
1.8
Correlation functions, Δ_ν ($\kappa\hbar\omega_0$)
900
800
700
600
Energy (keV)
5/2-
3/2-
7/2+
1/2-
5/2+
3/2+
90
92
94
96
98
100
Z
MUB-3322

Fig. 1



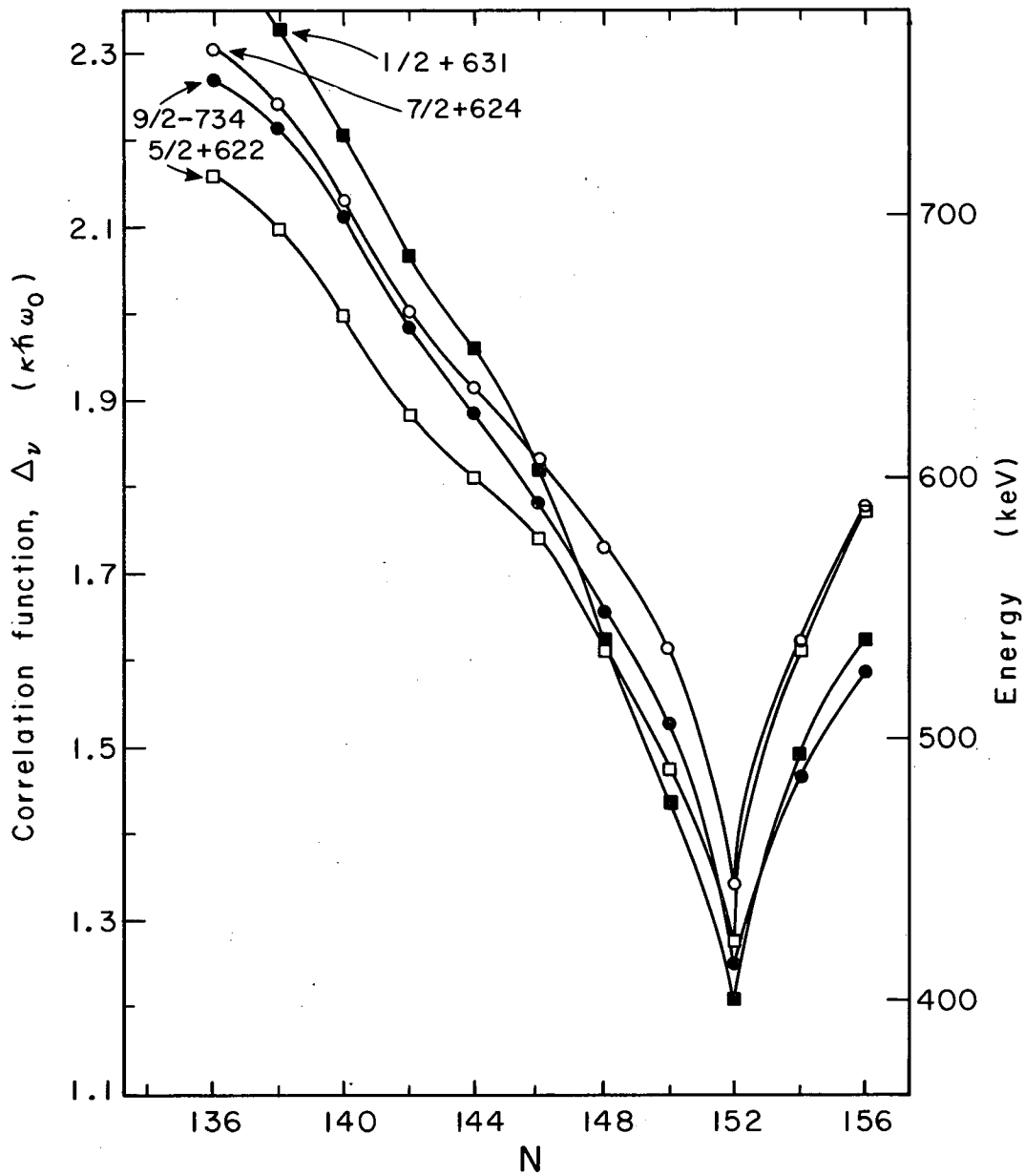
MUB-3324

Fig. 2



MUB-3325

Fig. 3



MUB-3326

Fig. 4

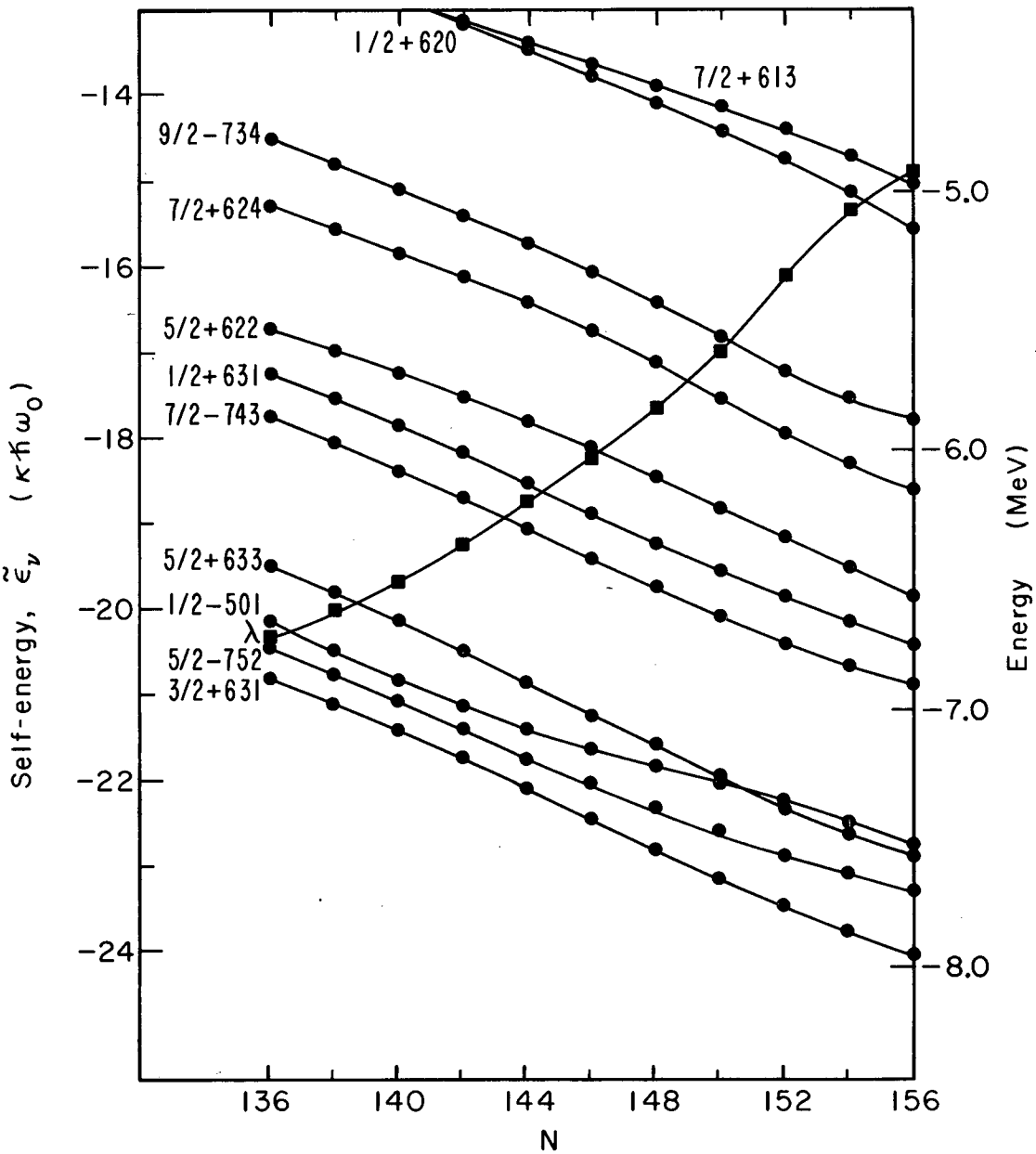
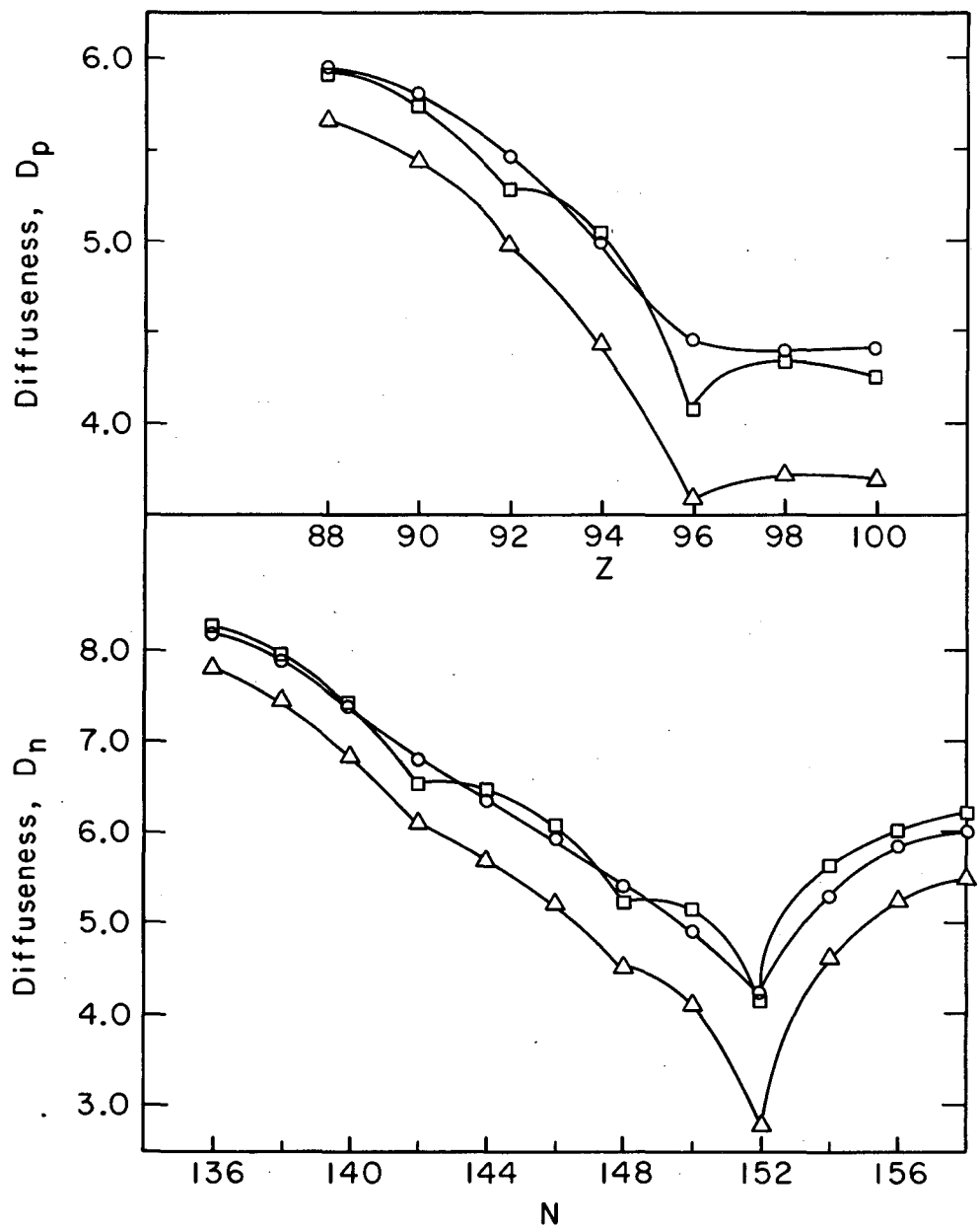
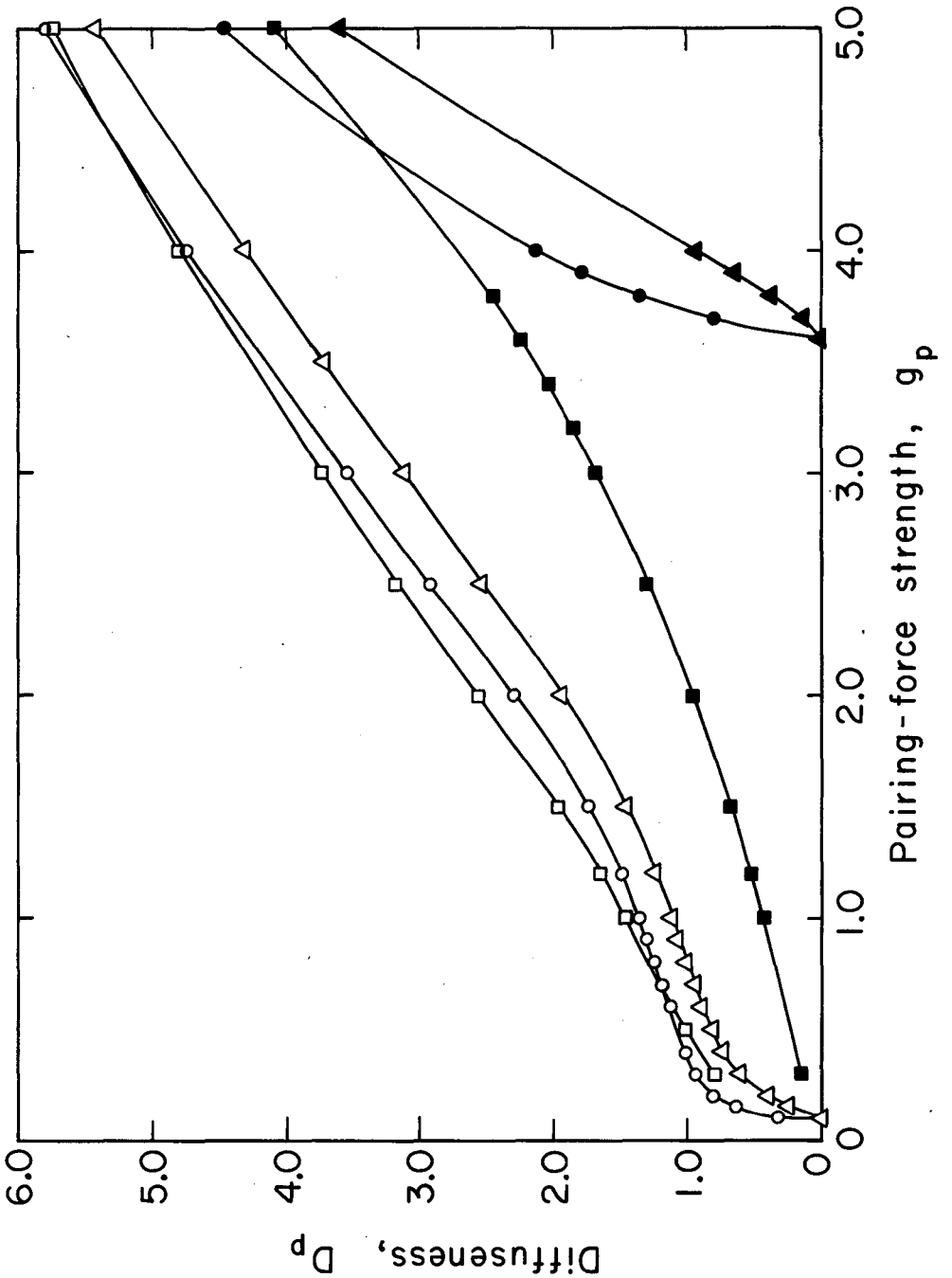

1/2+620
7/2+613
9/2-734
7/2+624
5/2+622
1/2+631
7/2-743
5/2+633
1/2-501
λ
5/2-752
3/2+631
-14
-16
-18
-20
-22
-24
Self-energy, $\tilde{\epsilon}_\nu$ ($\kappa\hbar\omega_0$)
-5.0
-6.0
-7.0
-8.0
Energy (MeV)
136
140
144
148
152
156
N
MUB-3327

Fig. 5



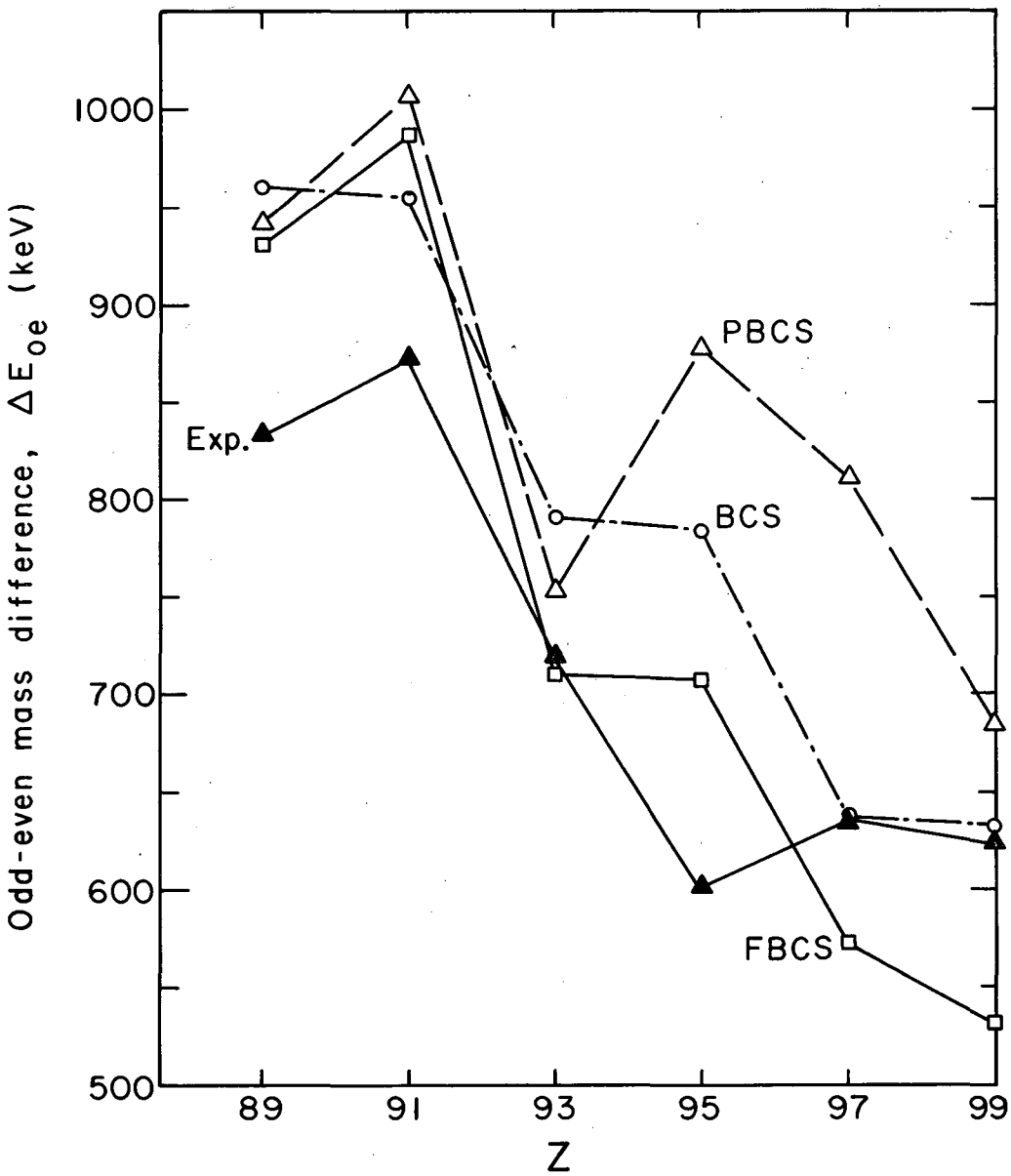
MUB-3328

Fig. 6



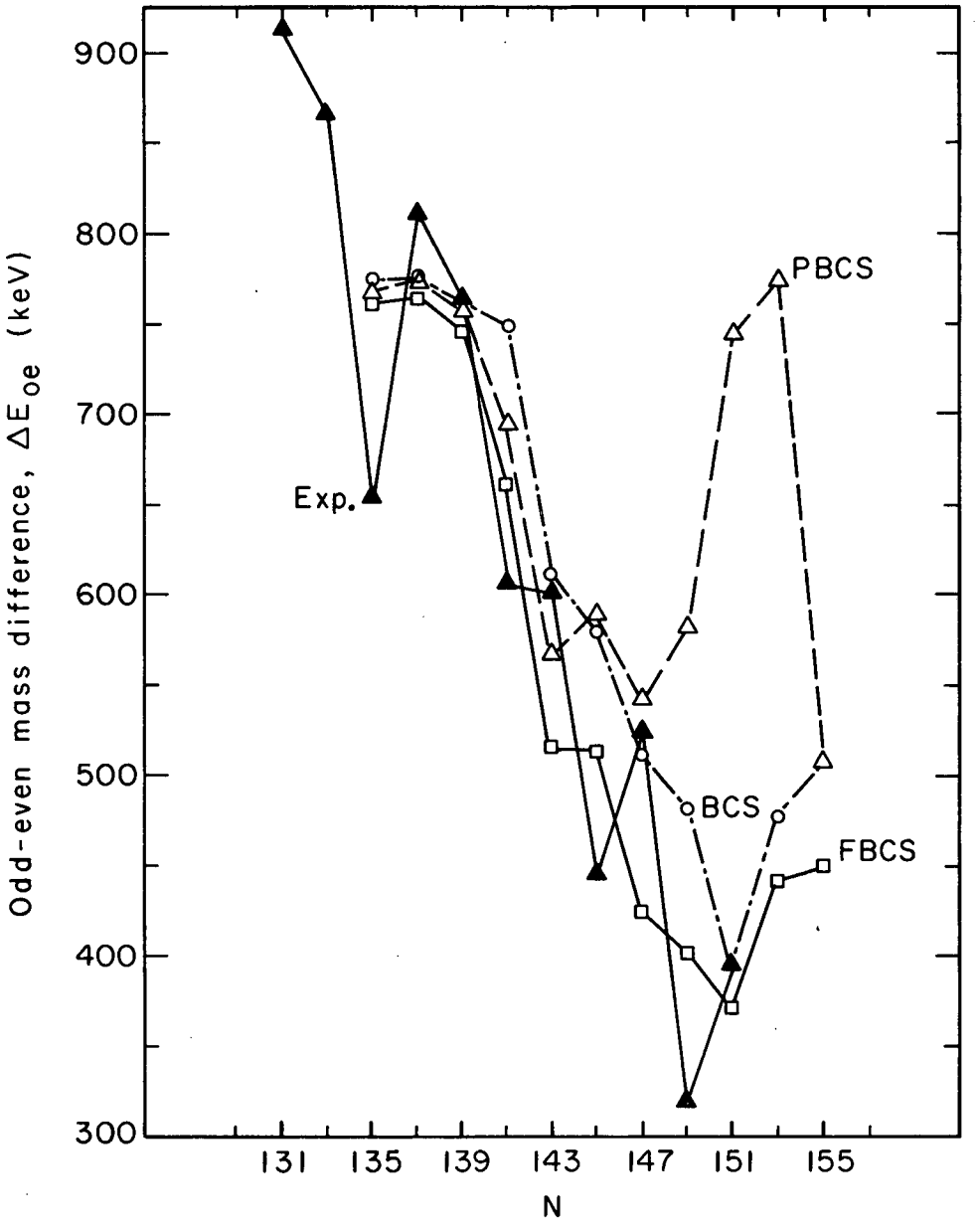
MUB-3329

Fig. 7



MUB-3330

Fig. 8



MUB-3381

Fig. 9

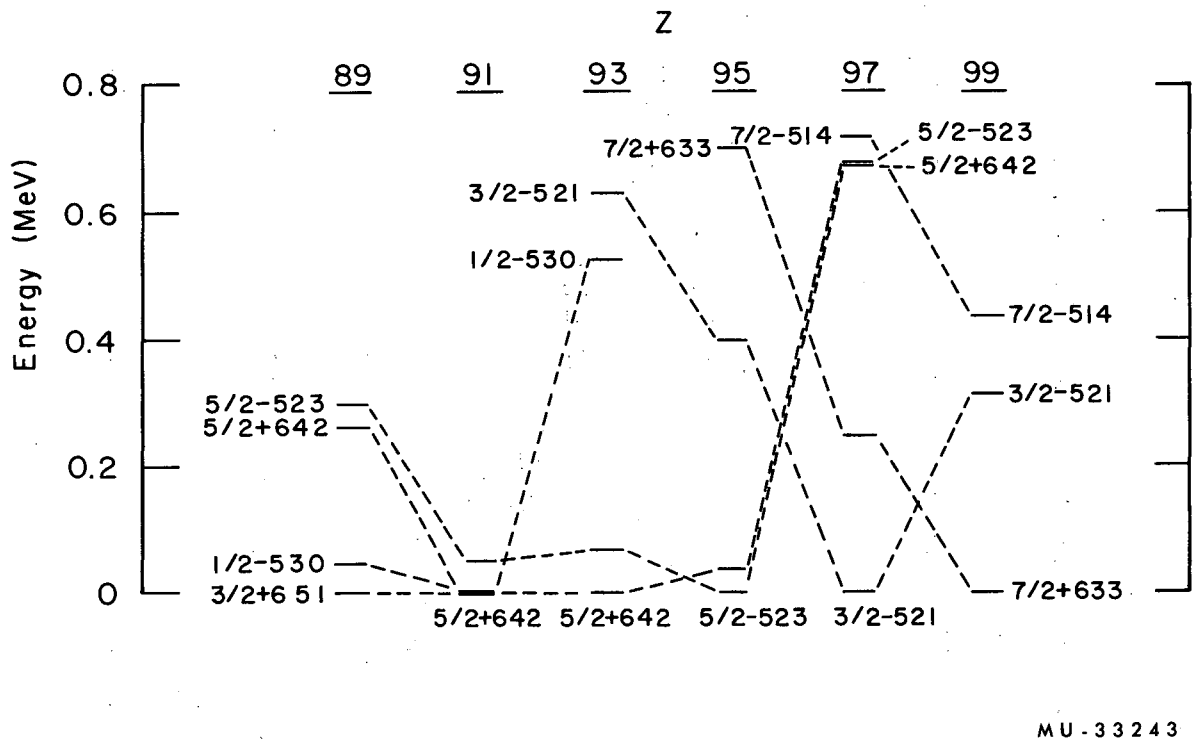
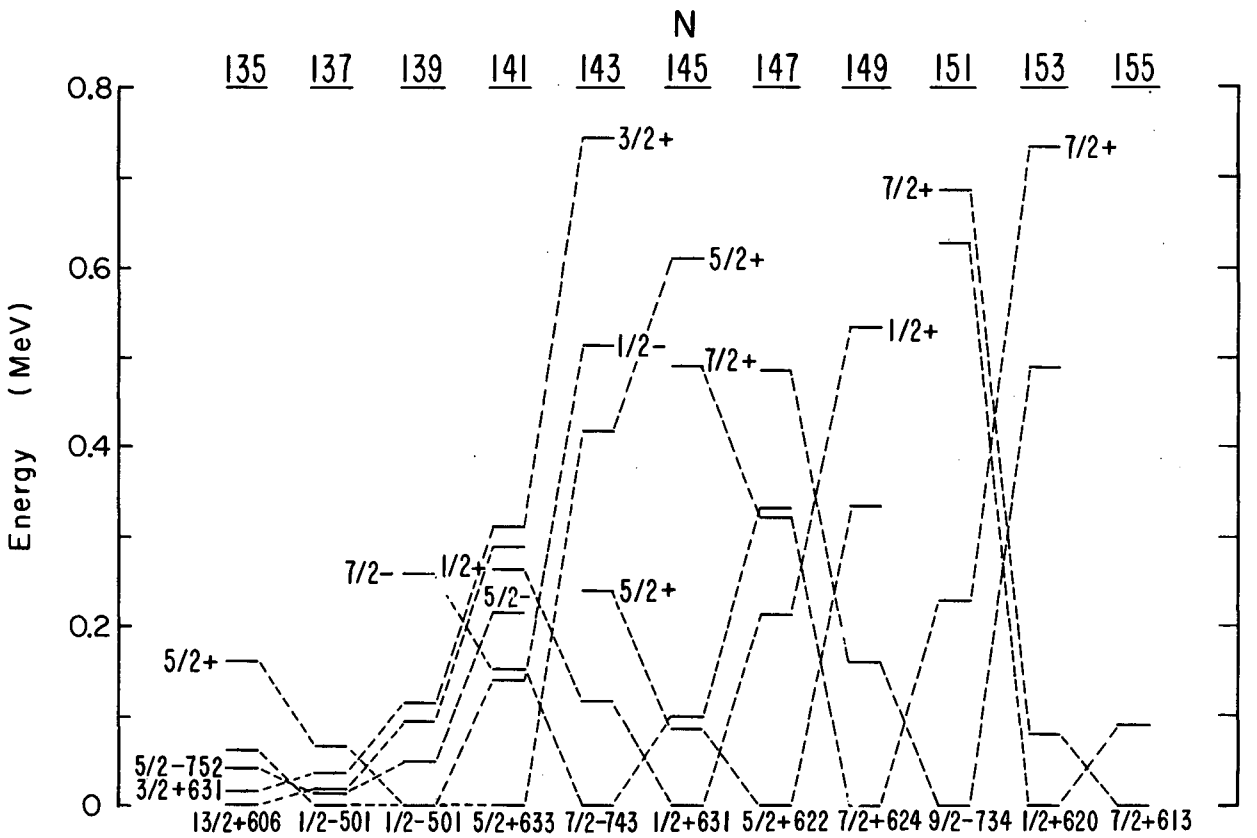

Z
89
91
93
95
97
99
Energy (MeV)
0.8
0.6
0.4
0.2
0
5/2-523
5/2+642
1/2-530
3/2+651
5/2+642
5/2+642
5/2-523
3/2-521
3/2-521
1/2-530
7/2+633
7/2-514
5/2-523
5/2+642
7/2-514
3/2-521
7/2+633
MU-33243

Fig. 10



MUB-3332

Fig. 11

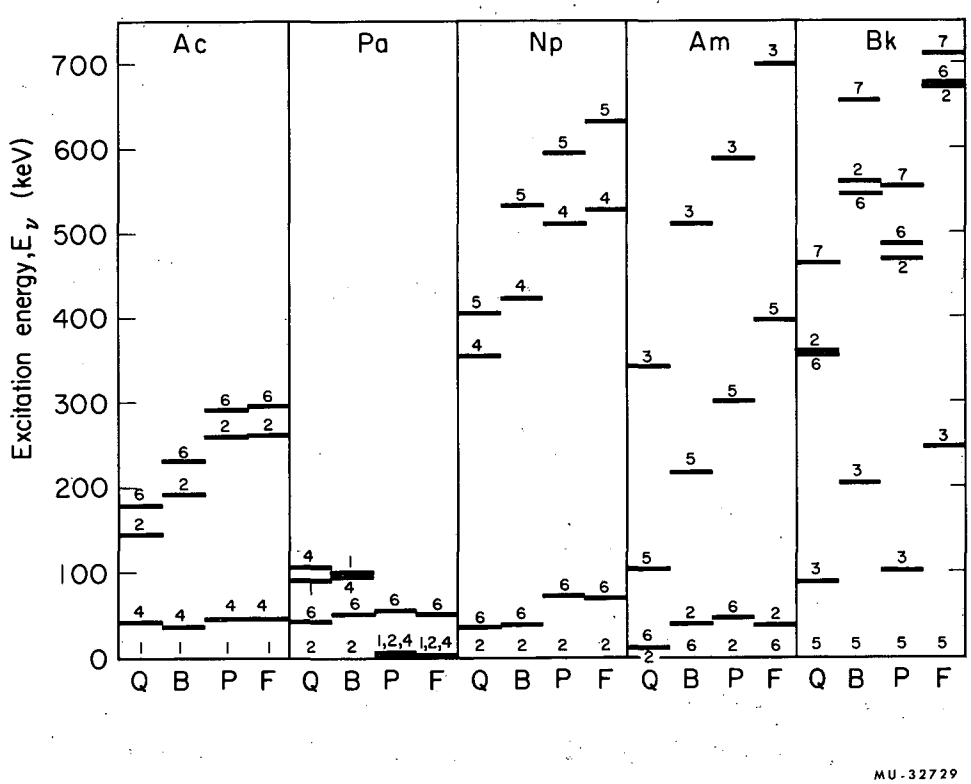

Ac
Pa
Np
Am
Bk
Excitation energy, E_ν (keV)
0
100
200
300
400
500
600
700
Q B P F Q B P F Q B P F Q B P F Q B P F
MU-32729

Fig. 12

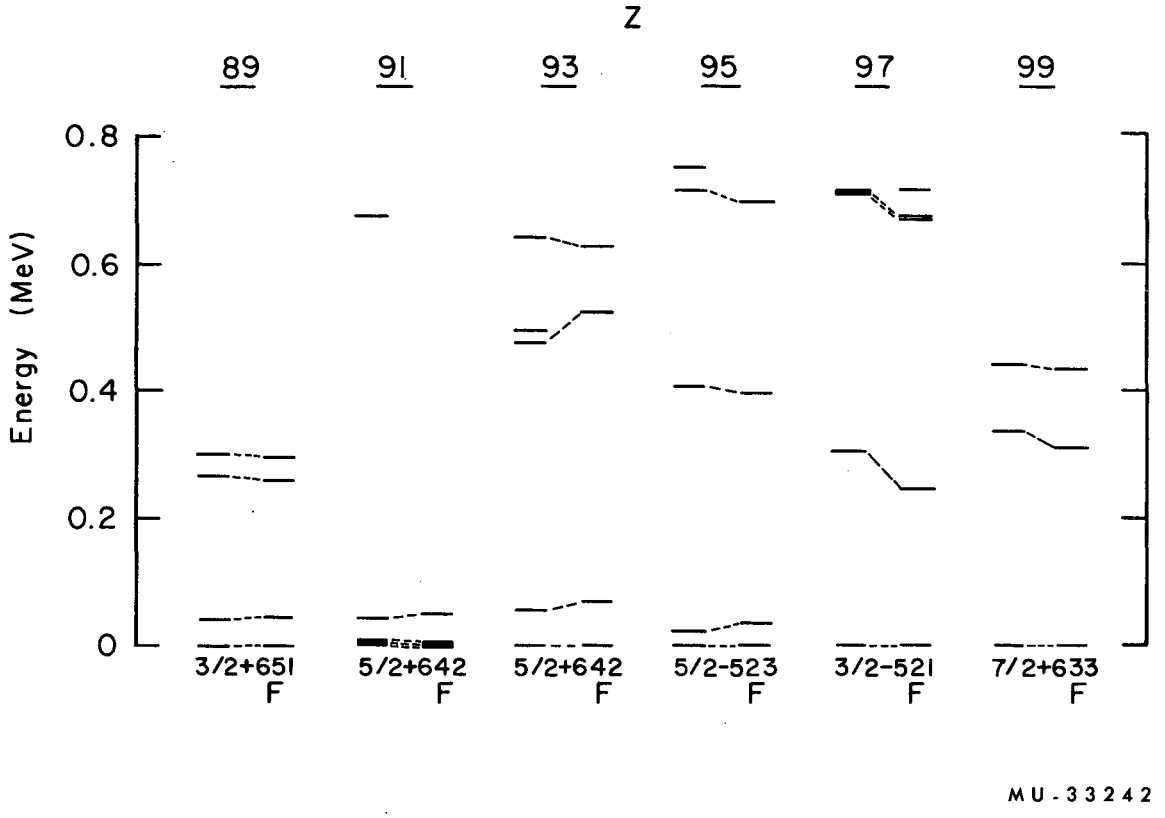
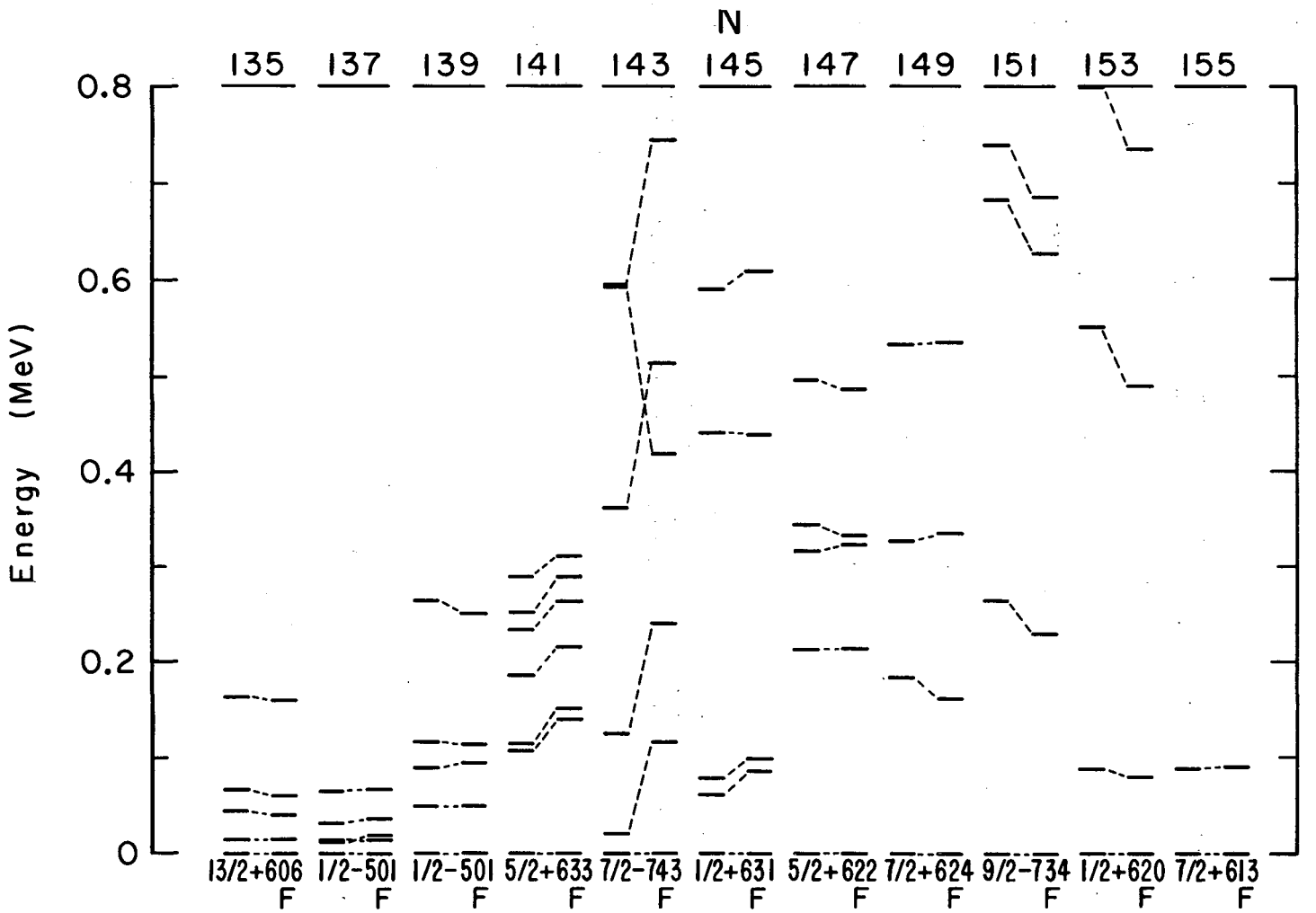
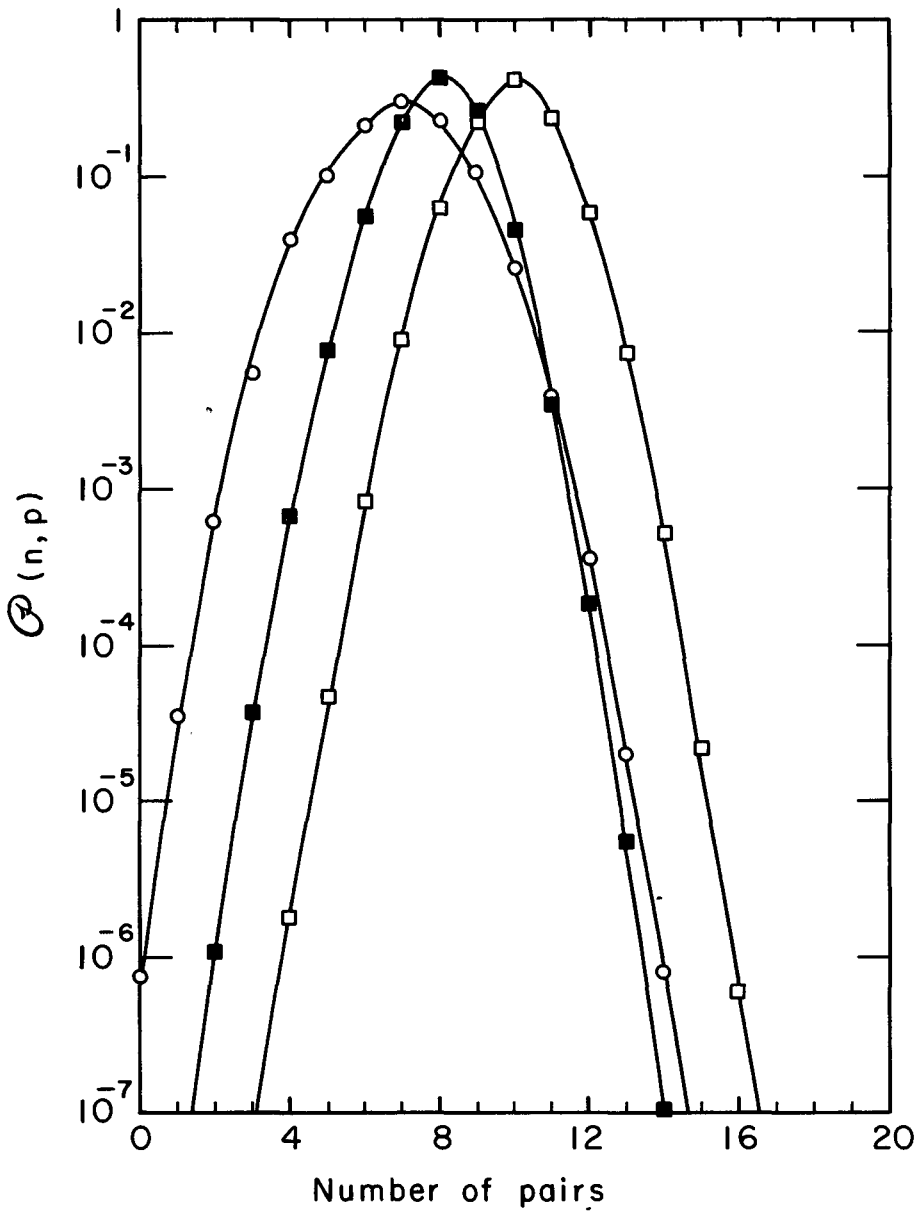

Z
89
91
93
95
97
99
0.8
0.6
0.4
0.2
0
Energy (MeV)
3/2+651
F
5/2+642
F
5/2+642
F
5/2-523
F
3/2-521
F
7/2+633
F
MU-33242

Fig. 13



MUB-3333

Fig. 14



MUB-3323

Fig. B. 1

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