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ABSTRACT

New nuclear structure calculations using a Gaussian residual force in a BCS treatment for the proton system of the 82-neutron nuclei are presented. Comparisons of theoretical binding energies with experimental odd-even mass differences, and trends of alpha decay energies are made. The best agreement with experimental energies is obtained when a force strength ten percent stronger than that deduced from low-energy p-p scattering is used. The wave functions are used for theoretical alpha decay rate calculations, and some insight into the decrease of reduced width near the subshell $Z = 64$ is obtained.

THEORETICAL CALCULATIONS OF PROPERTIES OF RARE-EARTH ALPHA EMITTERS

Introduction

Kisslinger and Sorensen have shown the power of simple pairing-force calculations in understanding single-closed-shell spherical nuclei.[1] It is the purpose of this note to show how these methods can form the basis of understanding alpha decay energy and rate systematics for rare-earth alpha emitters. We confine our attention here to the even-even alpha emitters decaying to 82-neutron closed shell configurations.

Table I summarizes the present best data on alpha disintegration energies and rates for this class of nuclei. The first two entries are energies calculated from mass data, but the other values are from alpha decay measurements. The reduced widths δ^2 are calculated from a previously published barrier-penetrability expression with a diffuse nuclear potential.[2]

BCS Solutions for the Proton System

We have made theoretical calculations of the structure and binding energies of the protons beyond 50 using the Bardeen-Cooper-Schrieffer[3] (BCS) variational methods.

We have gone beyond Kisslinger and Sorensen's first treatment of 82-neutron nuclei[1] by including all proton orbitals within the 50-82 shell and in addition the $h_{9/2}$ orbital. Furthermore, we do not make the simplifying assumption of constant-G pairing-force matrix elements but use matrix elements employing a Gaussian singlet-even force $P_s V_o \exp[-(r_{1/2}/b)^2]$ (P_s is a singlet spin-projection operator, V_o is the well-depth and b the range). If we take a value of V_o = 32.44 MeV, with the range b of 1.755 Fm, we satisfy the low-energy p-p scattering behavior. We also took account of the matrix elements contributing to the self-energy ($\overline{G}_{\nu\nu'}$, in the notation of Belyaev)[4] instead of setting them to zero, as in the usual calculations. A number of different sets of solutions of the Belyaev equation (1) and (2) were carried out on an IBM 7094 computer for various single-particle level spacings and slightly different force strengths.

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

$$N = \sum_\nu 2 V_\nu^2 \tag{2}$$

where

$$V_\nu^{\,2} = \frac{1}{2} \left[1 - \frac{\tilde{\epsilon}_\nu - \lambda}{[(\tilde{\epsilon}_\nu-\lambda)^2+ \Delta_\nu^2]^{1/2}} \right]$$

and

$$\tilde{\epsilon}_\nu = \epsilon_\nu - \sum_{\nu_1} \overline{G}_{\nu\nu_1} V_{\nu_1}^{\,2} .$$

Here N is the total number of valence protons; $V_\nu^{\,2}$ is the probability of the νth orbital being occupied by a pair; Δ_ν is the characteristic pairing energy parameter for the νth orbital; ϵ_ν is the single particle orbital energy in the field of the closed shell nucleons; $\tilde{\epsilon}_\nu$ is the self-energy in the presence of all the nucleons.

Table II lists the Δ_ν and $V_\nu^{\,2}$ values of some solutions with the above force of free-space strength. The orbital energies were chosen as follows: $\epsilon(g_{7/2})$ =-0.6 MeV, $\epsilon(d_{5/2})$ = 0.16 MeV, $\epsilon(h_{11/2})$ = 2.60 MeV, $\epsilon(d_{3/2})$ = 2.9 MeV, $\epsilon(s_{1/2})$ = 3.4 MeV, $\epsilon(h_{9/2})$ = 5.4 MeV. The BCS binding energy (U) is calculated exactly from Belyaev's equation (22).[4]

Note in these calculations the decrease in pairing correlation (Δ_ν values) at the subshell 64.

Binding Energy Comparisons

A first test of such calculations is to compare with experimental odd-even mass differences. Such a comparison essentially tests whether the ratio of pairing force to single-particle energy level separations at the Fermi surface is correctly assumed. The comparison of theory with experiment is graphed in Fig. 1. Our plot is similar to Kisslinger-Sorensen's Fig. 21 except that we use a four-point difference formula with the experimental masses, rather than the three-point formula.

$$P(Z) = \frac{1}{2} [-E(Z + 1) + 3E(Z) - 3E(Z - 1) + E(Z - 2)] .$$

Our theoretical points, like Kisslinger and Sorensen's, are twice the lowest quasi-particle energies ($= \sqrt{(\tilde{\epsilon}_\nu - \lambda)^2 + \Delta_\nu^2}$) for separate BCS solutions setting N equal to the odd number.

The dashed lines give the theoretical odd-even mass differences for the three force strengths; a) Free-space strength pairing V_o, b) 1.1 times V_o, and c) 1.2 times V_o. The experimental masses are taken from the tables of König et al.[5] The comparison of Fig. 1 suggests that the free-space force strength needs to be increased by ten percent to that of our intermediate value for the set of orbitals we took. Inclusion of more distant proton orbitals would call for a lower force strength.

Another use of the BCS binding energies (U) is the comparison of experimental alpha decay energies with theoretical two-proton binding energies. The discontinuity at Z = 64 in the progression of alpha decay energies was noted ten years ago and a proton subshell at 64 suggested.[13] A similar discontinuity in theoretical binding energies comes about if one assumes a sufficient spacing between the $d_{5/2}$ proton orbital and the next higher orbital (here the $h_{11/2}$). The clearest comparison is made by plotting the first difference of the alpha energies of Table I vs. Z and comparing to the second difference of BCS energies (U), as from Table II. Figure 2 gives such a comparison, with theoretical calculations for the same three pairing-force strengths. The magnitude of the theoretical binding-energy discontinuity at 64 is mainly dependent on the ratio of the $d_{5/2}$-$h_{11/2}$ orbital energy separation to the pairing force strength. Again our intermediate force calculations best reproduce the magnitude of the discontinuity.

Alpha Decay Rate Comparison

The next features we examine are the relative reduced alpha transition probabilities of the $N = 84$ even nuclei. The experimental reduced derivative widths δ^2 are tabulated in Table I and plotted vs Z in Fig. 3. The interesting feature is their general constancy except for about a factor of two decrease for the decay from $Z = 66$ into the closed subshell $Z = 64$. The behavior for $Z \geq 66$ is closely analogous to that shown[2] by polonium alpha emitters with $N \geq 128$. The $N = 128$ (Po^{212}) reduced width is a factor of ~0.6 below the next three heavier members, and these three show nearly constant reduced widths.

Our theoretical alpha decay rate calculations are closely related to those of Mang,[14] Harada,[15] and Zeh,[16] in that the alpha decay matrix elements are simply projections of shell model products of two-proton-two-neutron wave functions. We use the approximate factorable form of alpha matrix elements given by Rasmussen,[17] and use the numerical proton radial wave functions of Blomqvist and Wahlborn[18] at 8 Fm.

We further assume that the shell-model wave functions of the 82-neutron and 84-neutron nuclei are purely seniority zero and that the neutron pair wave function is the same for all the 84-neutron nuclei considered.

The calculations here have the complicating feature that the proton numbers are far from the closed shells of 50 and 82, and extensive configuration mixing is implied by the pairing-type proton wave functions. The most general formulation for taking into account configuration mixing has been given by Zeh.[16] Suffice it to say here that the formula we need can be expressed as a generalization of equation (11) of Rasmussen,[17] applied to Po^{212} decay:

$$\delta^2_{pair} = C^2 \left| \left[\sum_{j_p} (-)^{\ell_p} c(j_p)(2j_p + 1)^{1/2} B_p(\ell_p) y^2{}_{j_p}(R) \right] \right. \tag{3}$$

$$\times \quad \left. [\text{similar neutron sum}] \right|^2 .$$

Now, however, the neutron contribution factors out as a constant, and coefficients $c(j_p)$ are to be derived from the BCS proton wave functions from the solutions discussed earlier in this paper.

In second-quantized notation the $c(j_p)$ may be expressed in terms of an operator formed by coupling two proton-annihilation operators a_{jm} to total J of zero (we drop the subscript p)

$$c(j) = (-)^{\ell} \left(f \middle| \sum_m (2j+1)^{-1/2} a_{jm} a_{j-m} \middle| i\right)$$

or in Zeh's notation of the pair annihilation operator A_j, $c(j) = (-)^{\ell}(f|A_j|i)$. If there is no pairing force we have the pure shell-model result of Zeh's Eq. (18) for one orbital j with n pairs in the parent and n-1 pairs in the daughter.

$$c(j) = (-)^{\ell} \langle P_f P \| P_i \rangle = \left[\frac{n(\Omega - n + 1)}{\Omega} \right]^{1/2} \tag{4}$$

where Ω is the pair-degeneracy, $\Omega = j + 1/2$.

Consider now the case of Kisslinger-Sorensen-type product wave functions

$$|i\rangle = \prod_j (u_j + v_j A_j^+)^{\Omega_j} |0\rangle$$

and $|f\rangle$ the same but primes for u_j and v_j. A straightforward calculation using Zeh's commutation relations of the annihilation and creation operators A_j and A_j^+ gives the results below (Zeh's Eq. (35a)):

$$\langle P_f P(j) \| P_i \rangle = \frac{u_j' v_j \Omega_j^{1/2}}{(u_j' u_j + v_j' v_j)} \prod_\nu (u_\nu u_\nu' + v_\nu v_\nu')^{\Omega_\nu} , \tag{5}$$

In Zeh's numerical calculations for the series of even polonium isotopes he modifies the above formula by raising the factor in the denominator to the Ω_j power, in order to achieve exact correspondence with the pure shell model expression in the absence of pairing force.

As is well-known, the simple BCS wave functions do not conserve the number of particles, and there have been some calculations[19,20] supporting the procedure of projecting out the desired fixed-particle component of the BCS wave functions. That is, we take

$$|i\rangle = N_i \mathcal{P}(\tfrac{n}{2}) \prod_j (u_j + z^{1/2} v_j A_j^+)^{\Omega_j} |0\rangle \tag{6}$$

where $\mathcal{P}(\frac{n}{2})$ is a projection operator that selects only terms in $z^{n/2}$, where n is the number of pairs.

$$\mathcal{P}(\tfrac{n}{2})\ (a_o + a_1 z^{1/2} + a_2 z + \ldots + a_n z^{n/2} + \ldots) = a_n$$

N_i is a normalization factor to make $(i|i) = 1$.

$$N_i = [\ \mathcal{P}(n) \prod_j (u_j^2 + z v_j^2)^{\Omega_j}\ ]^{-1/2}. \tag{7}$$

[Mang, Dietrich, and Pradal[21] use the Cauchy integral property in their contour integral notation instead of our projection operator $\mathcal{P}(\frac{n}{2})$, but the difference is only one of notation.] The final state wave function will be similar except that we prime the u_j and v_j and replace n by $n-1$. For the projected BCS wave functions the element $\langle P_f P(j) \| P_i \rangle$ becomes

$$\langle P_f P(j) \| P_i \rangle = \Omega_j^{1/2} u_j' v_j \cdot N_i N_f S(j), \tag{8}$$

where

$$S(j) = \mathcal{P}(n-1) \left[\frac{\prod_i (u_i u_i' + z v_i v_i')^{\Omega_i}}{(u_j u_j' + z v_j v_j')} \right].$$

We have performed relative alpha width ($\delta_\alpha{}^2$) calculations for the 84-neutron nuclei with the three different expressions, Eq. (8), (4), and (5) for $\langle P_f P \| P_i \rangle$ outlined above. The calculations with the projected BCS formulation were performed for three different sets of BCS wave functions—those calculated with the residual-force well depth V_o, a) exactly that for free p-p scattering, b) 1.1 times this depth, and c) 1.2 times this depth.

Figure 4 presents our theoretical calculations with Eq. (8), which used the fixed-particle parts of the BCS wave function. For the weaker force-strengths there is a significant dip of alpha widths at the subshell 64. The dip of points at Z = 66 and 64 may be qualitatively associated with a rate decrease associated with a lowered "core-overlap." The Z = 64 solutions have low Δ_ν values and small configuration mixing, while solutions at Z = 62 and 66 develop larger pairing correlations. No reasonable adjustment of parameters seems capable of reproducing the experimental feature that only the width at Z_{parent} = 66 is depressed and not that at 64. We can only suggest that the theoretical curves of Fig. 4 show a great sensitivity near Z = 64 to the pairing force strength. The experimental data suggest that the alpha daughter ${}_{64}Gd^{146}_{82}$ has a low amount of proton pairing correlation, but the addition of a neutron pair to form ${}_{64}Gd^{148}_{84}$ effects a restoration of proton pairing correlation.

Figure 5 shows the theoretical alpha widths from Eq. (4) for the absence of a pairing force and configuration mixing. It is seen that the $(d_{5/2})^n$ and $(h_{11/2})^n$ proton configurations make the largest intrinsic contributions to alpha decay. The $g_{7/2}$ orbital has a small alpha matrix element because of its relatively small radial wave function in the nuclear surface region.

Figure 6 compares for the free-space force strength wave functions the alpha width calculations using the fixed particle parts (Eq. (8)) and using essentially the whole BCS wave function in Zeh's modification[16] of Eq. (5). It is seen that there is little difference between the calculations except near the closed subshell 64, where the pairing correlation changes rapidly with Z.

Clearly the results are encouraging for these simple BCS calculations neglecting n-p interactions, possible changes of neutron pair configuration with Z, and 4-quasi-particle contributions in ground. Probably alpha widths and spectroscopic factors for (p,t) reactions and other direct interactions involving transfer of nucleon pairs are among the most sensitive experimental probes of the nucleon-nucleon correlations resulting from the pairing force. Further study along these lines should be most valuable in testing theory.

Acknowledgment

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Fig. 1. Comparison of experimental odd-even mass differences (solid squares) for 82-neutron nuclei with three BCS calculations (open symbols). The lowest theoretical curve is with free-space residual force strength, the middle for force increased by a factor 1.1, and the upper with the force increased by factor 1.2.

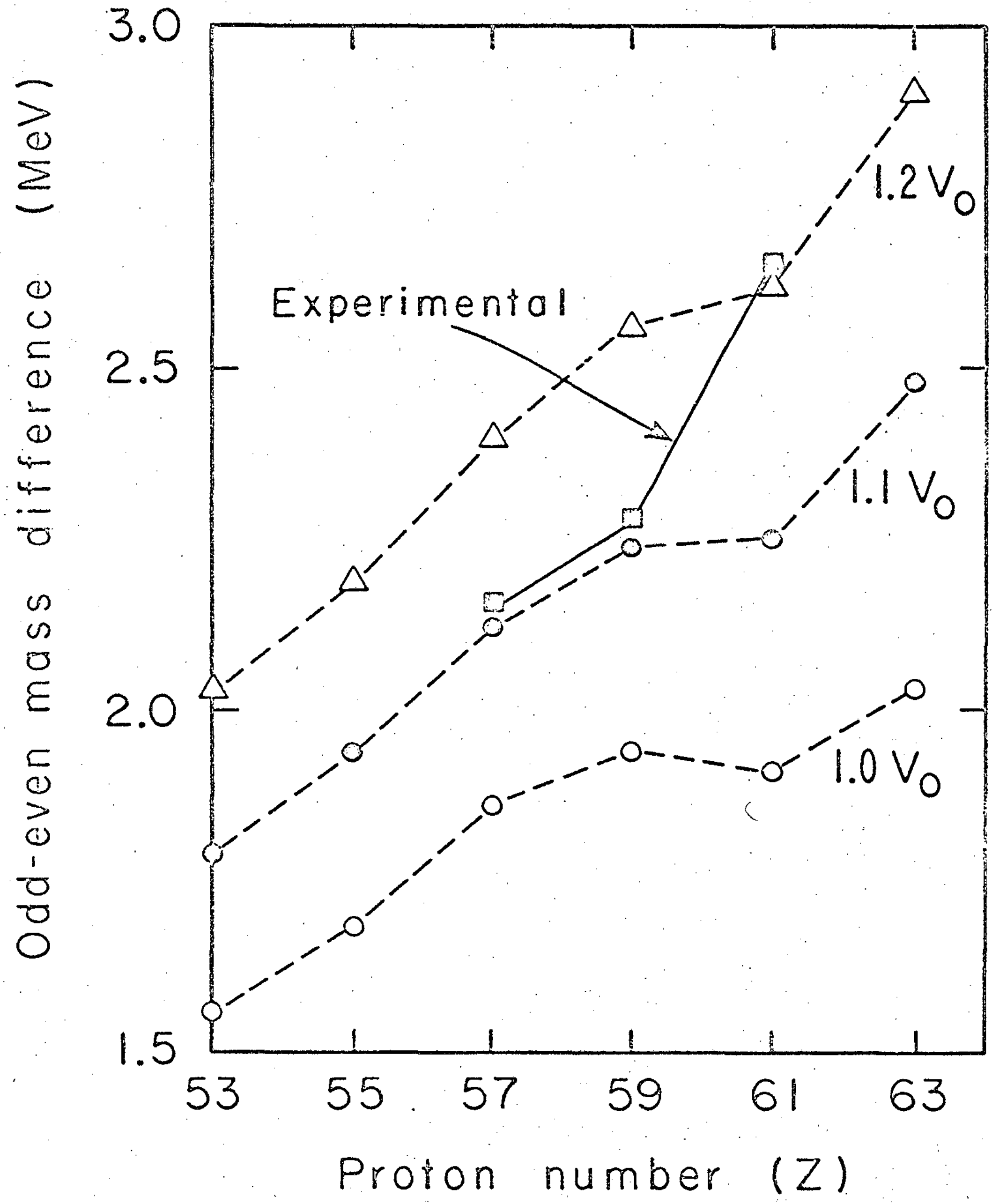
Fig. 2. Comparison of first differences of alpha decay energy of even-mass, 84 neutron nuclides and second differences of theoretical BCS binding energies. The experimental points (crosses, dashed line) have their ordinate (MeV) on the right-hand side, and the three theoretical curves have their ordinate scale on the left. The relative vertical position of the experimental curve has been arbitrarily adjusted to facilitate easiest visual comparision of the magnitude of the Z = 64 discontinuities between experimental and theory. The upper theoretical curve (O) is for free-space residual force strength V_o, and the middle curve ($\bigtriangledown$) refers to the force strengthened to 1.1 V_o, with the lower (Δ) for the force of 1.2 V_o.

Fig. 3. Plot of experimental reduced alpha decay widths vs Z for even 84 neutron alpha emitters.

Fig. 4. Theoretical relative reduced alpha widths using the fixed proton number parts of the BCS wave functions for the three different residual force strength V_o (lowest), 1.1 V_o (middle), 1.2 V_o (upper).

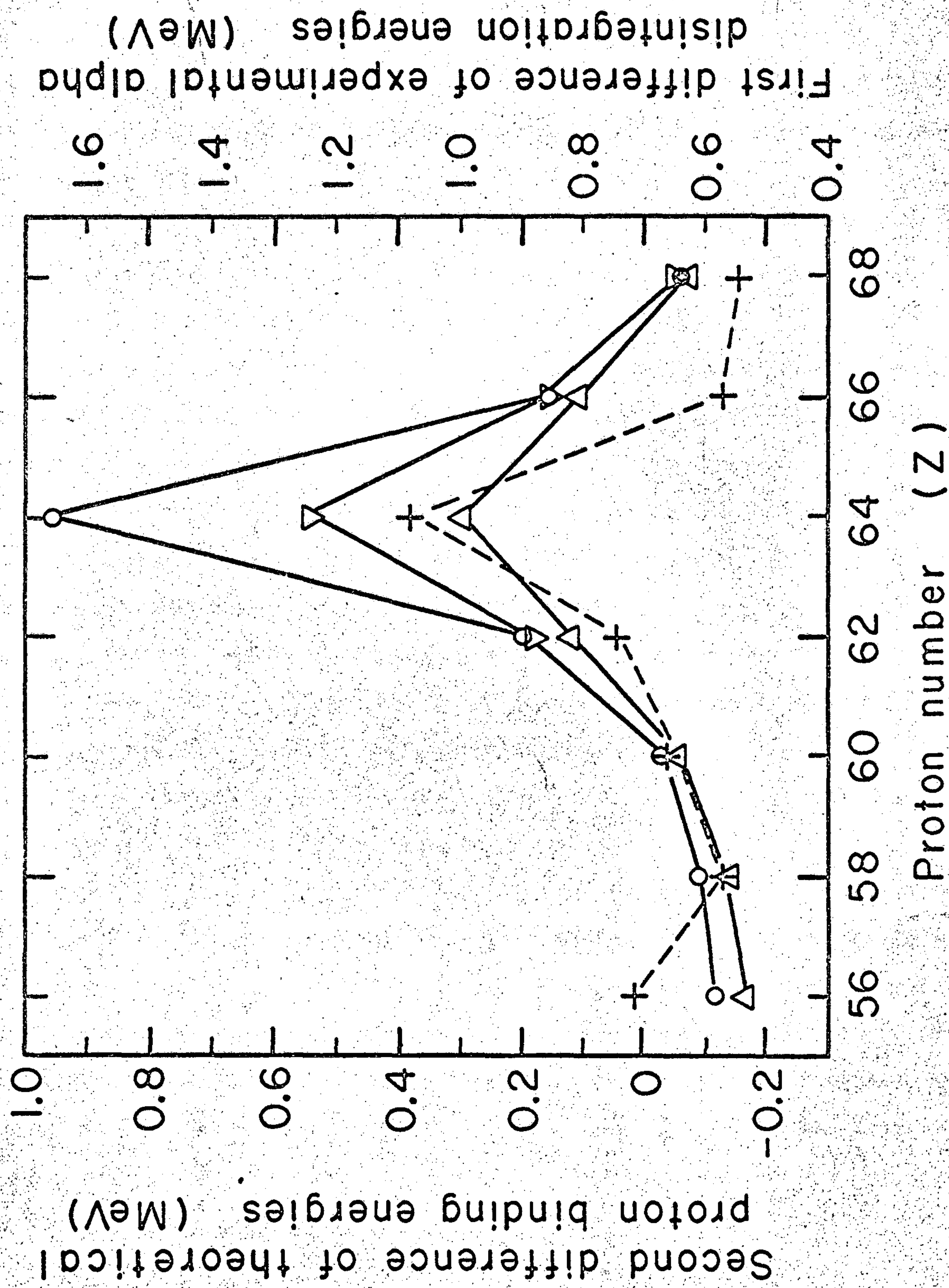
Fig. 5. Pure shell-model relative reduced widths for alpha decay, the limiting result for zero residual force.

Fig. 6. Comparison of the theoretical reduced widths for the same BCS wave functions set (V_o) but in one case using the full BCS wave functions (●) and in the the other case (O) using only the parts of the BCS wave function with correct proton number.



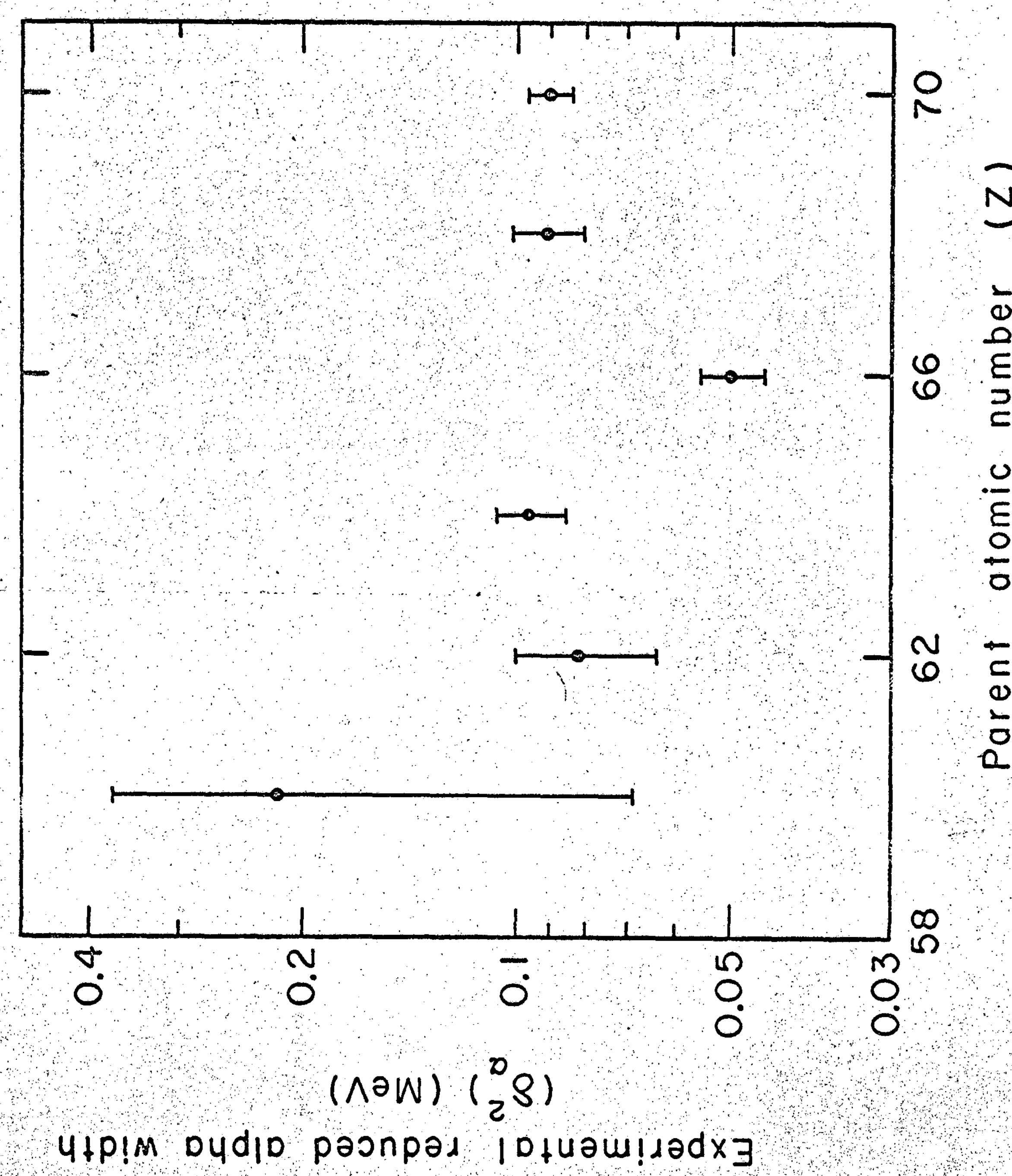
MU-32912

Fig. 1.



MU-32913

Fig. 2.



MU-32914

Fig. 3.

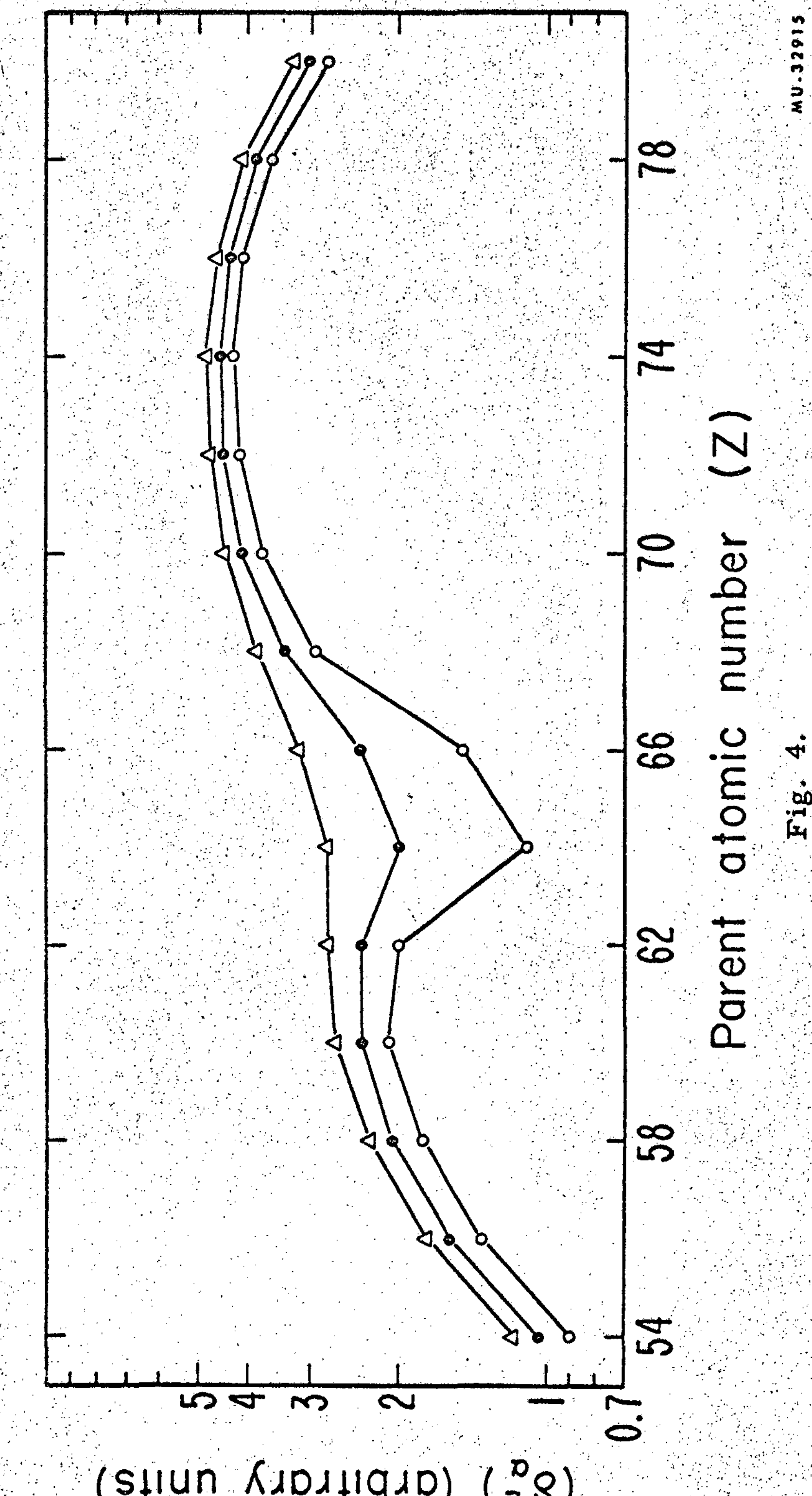

Relative reduced alpha width
(δ_α^2) (arbitrary units)
0.7
1
2
3
4
5
54
58
62
66
70
74
78
Parent atomic number (Z)
MU-32915

Fig. 4.

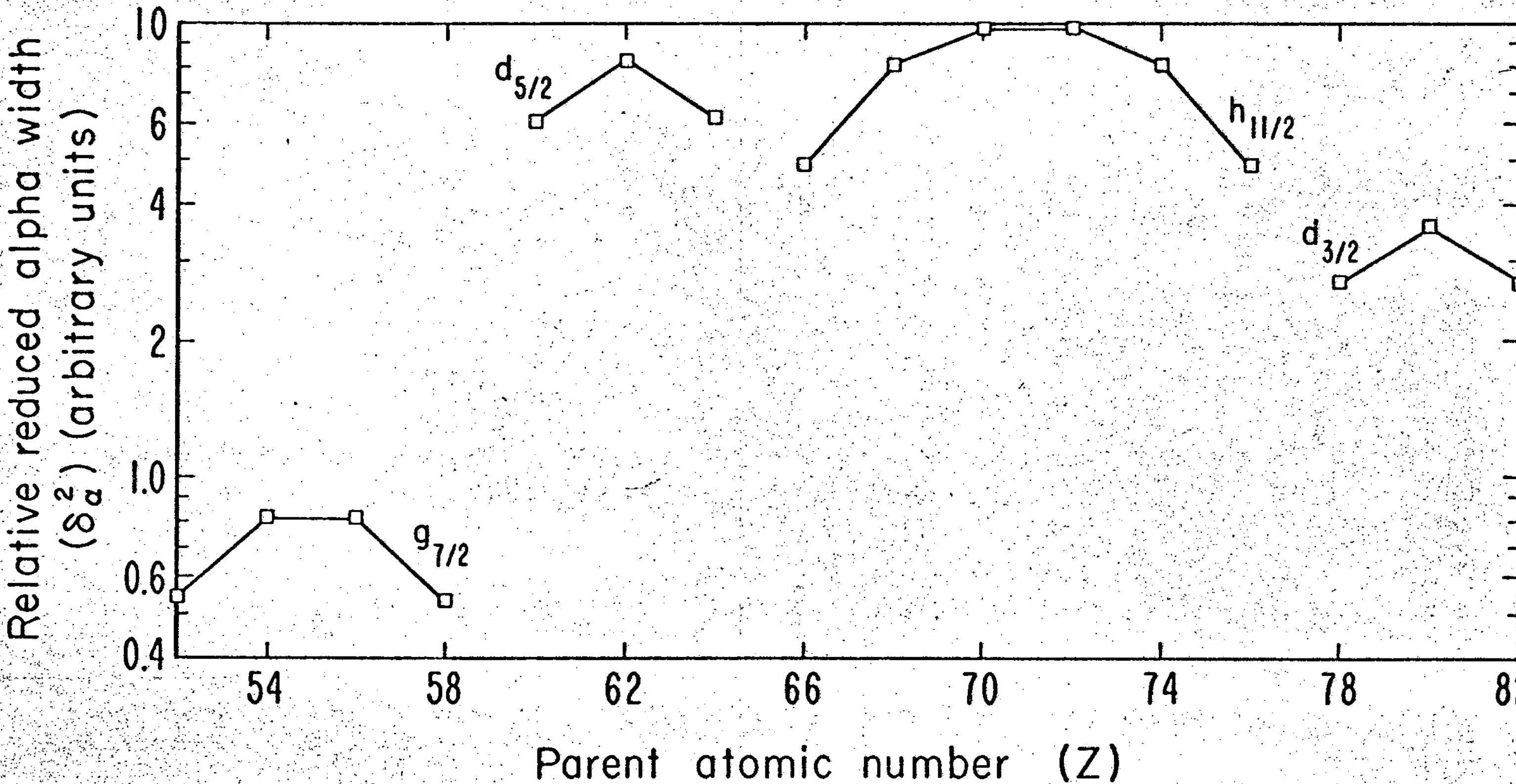


Fig. 5.

MUB-2291

Fig. 6

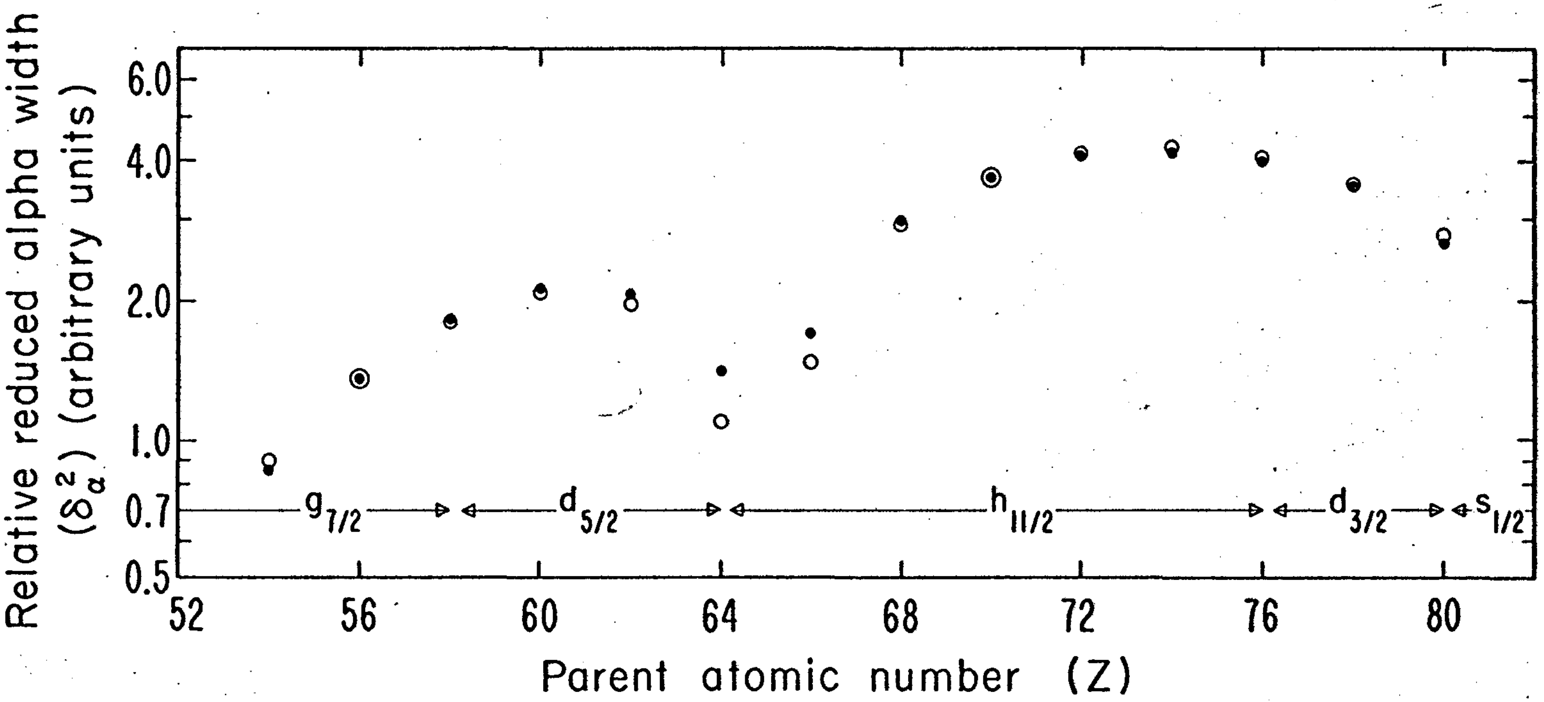


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Fig. 6.

TABLE I

DATA ON 84-NEUTRON EMITTERS

Nuclide	Q_{α}(MeV)	$t_{1/2}(\alpha)$	δ^2(MeV)	Reference
Ba^{140}	0.59 ± 0.05			5
Ce^{142}	1.31 ± 0.10			5
Nd^{144}	1.88 ± 0.03	$(2.4 \pm 0.3)\times10^{15}$y	0.219 ± 0.15	6
Sm^{146}	2.53 ± 0.02	$(1.17 \pm 0.25)\times10^{8}$y	0.082 ± 0.018	7, 8
Gd^{148}	3.27 ± 0.01	84 ± 9 y	0.097 ± 0.01	9
Dy^{150}	4.35 ± 0.02	40 ± 4 min	0.050 ± 0.005	10
Er^{152}	4.93 ± 0.02	11.9 ± 1 sec	0.091 ± 0.01	11
Yb^{154}	5.48 ± 0.02	0.39 sec	0.091 ± 0.005	12

TABLE II

RESULTS OF PAIRING FORCE CALCULATIONS FOR SOME 82-NEUTRON NUCLEI
(Free-space Residual Force Strength)

Z	BCS Binding Energy (U) (MeV)		$g_{7/2}$	$d_{5/2}$	$h_{11/2}$	$d_{3/2}$	$s_{1/2}$	$h_{9/2}$
54	-2.704	Δ_ν	794 keV	703 keV	679 keV	702 keV	564 keV	679 keV
		V_ν^2	.402	.098	.010	.009	.004	.003
56	-5.543	Δ_ν	875 keV	841 keV	757 keV	841 keV	673 keV	757 keV
		V_ν^2	.569	.192	.016	.014	.007	.004
58	-8.501	Δ_ν	895 keV	931 keV	782 keV	930 keV	744 keV	782 keV
		V_ν^2	.706	.327	.020	.021	.010	.005
60	-11.571	Δ_ν	861 keV	956 keV	761 keV	956 keV	768 keV	762 keV
		V_ν^2	.815	.501	.024	.028	.012	.005
62	-14.730	Δ_ν	758 keV	878 keV	677 keV	878 keV	715 keV	677 keV
		V_ν^2	.903	.711	.026	.034	.013	.004
64	-17.924	Δ_ν	506 keV	565 keV	458 keV	564 keV	488 keV	458 keV
		V_ν^2	.979	.948	.025	.034	.011	.002
66	-20.920	Δ_ν	868 keV	892 keV	792 keV	891 keV	828 keV	793 keV
		V_ν^2	.970	.947	.144	.157	.051	.010
68	-22.959	Δ_ν	1027 keV	1038 keV	941 keV	1036 keV	995 keV	942 keV
		V_ν^2	.968	.948	.260	.272	.093	.016