## NUCLEAR PAIRING MODELS

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Abstract: We calculate nuclear pairing gaps for nuclei throughout the periodic system in both the BCS and Lipkin-Nogami pairing models. The energy levels required for the calculations are obtained from the folded-Yukawa single-particle model for ground-state shapes obtained in the macroscopic-microscopic approach by minimizing the total potential energy with respect to  $\epsilon_2$  and  $\epsilon_4$  shape degrees of freedom. For both pairing models we study two proposed forms for the effective-interaction pairing gap that is used to determine the pairing-gap parameter G that enters directly into the pairing equations. By comparing the calculated pairing gaps to experimental odd-even mass differences we determine parameter values for the proposed forms of the effective-interaction pairing gap by least-squares minimization. These comparisons to data lead to a preferred form for the effective-interaction pairing gap and to values of its parameters for both the BCS and Lipkin-Nogami models. From this microscopic study we conclude that no explicit isospin dependence is required for the effective-interaction pairing gap that is used to determine the pairing-gap parameter G.

#### 1. Introduction

Low-energy nuclear-structure properties show a strong dependence on the nuclear pairing force. In calculations of nuclear masses,  $\beta$ -strength functions, low-lying quasi-particle energies and other quantities that depend on the low-energy microscopic structure of the nucleus, it is therefore crucial to consider pairing effects. A sophisticated pairing model and an appropriate choice of pairing-model parameters are both important for obtaining realistic results. In theoretical nuclear-structure studies of large regions of the periodic system, such as nuclear mass calculations and astrophysical nucleosynthesis studies, it is important to have available pairing models and pairing parameters that give reliable results far from the valley of  $\beta$ -stability.

With the aim of obtaining the pairing-model parameters and expressions required for studies of this type, we here investigate both the conventional BCS pairing model[1, 2, 3, 4] and the Lipkin-Nogami (LN) extension[5, 6, 7]. The LN model takes into account the lowest-order correction to the total energy of the system associated with particle-number fluctuation. Specifically we

1. define pairing-model effective-interaction parameters. The effective-interaction parameter that directly enters into both the BCS and LN models is the pairing strength parameter G. Since G depends sensitively on the nuclear region considered and on

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specific details of the pairing calculations it is better to obtain G from a smooth pairing-gap expression by use of eq. (24) than to consider G as the primary parameter of the model. The smooth pairing-gap expression used to calculate G is denoted by  $\Delta_G$  and is referred to as the effective-interaction pairing gap. Thus we consider the parameters in the expression for  $\Delta_G$  to be the pairing-model effective-interaction parameters.

- 2. clarify the distinction between the effective-interaction pairing-gap  $\Delta_G$  used to determine G and the average pairing-gap  $\overline{\Delta}$ . An unfortunate source of confusion is that the model for  $\overline{\Delta}$  is just given by an expression similar or identical to the expression for  $\Delta_G$ . However, in contrast to  $\Delta_G$ ,  $\overline{\Delta}$  is directly compared to experimental pairing gaps, which are assumed to be given by the odd-even mass differences in eqs. (35,36). To further emphasize the distinction between  $\Delta_G$  and  $\overline{\Delta}$  we refer to the former as an expression but to the latter as a model, since the latter is compared directly to experimental data. Earlier, it was assumed that a distinction between  $\Delta_G$  and  $\overline{\Delta}$  was unnecessary. However, we will find below that when small effects, such as whether the pairing gap depends on neutron excess, are investigated, it is necessary to make the above distinction.
- 3. study two proposed models for  $\overline{\Delta}$  and two proposed expressions for  $\Delta_G$ .
- 4. determine the parameters of the two proposed expressions for  $\Delta_G$  by calculating the corresponding pairing strength parameter G, solving the BCS and LN pairing equations and comparing the calculated microscopic pairing gaps to the finite-difference pairing gaps obtained from experimental masses through eqs. (35,36). The calculations are performed for all nuclei for which finite-difference pairing gaps can be determined from experimental masses, for a grid of effective-interaction pairing-gap parameters that is large enough so that the parameters can be determined by least-squares minimization.
- 5. determine the parameters of the two proposed models for the average pairing-gap model  $\overline{\Delta}$ , by comparing  $\overline{\Delta}$  directly to the finite-difference pairing gaps obtained from experimental masses through eqs. (35,36). However, it is of little interest to use macroscopic pairing-gap models for direct *detailed* comparisons with odd-even experimental mass differences. A better approach is to obtain theoretical pairing gaps from microscopic BCS and LN models as indicated above.
- 6. derive the average pairing-energy expressions that are required for nuclear mass calculations. For the LN model such expressions are quite complicated and have never been given before. For the BCS model we present more general expressions than given earlier.
- 7. address the question "does the magnitude of the pairing gap depend on neutron excess?" We show that to answer this question, it has to be made more precise. In addition the fairly large scatter of both experimental and calculated quantities

around possible systematic trends with neutron excess makes it necessary to introduce expressions that are suitable for quantitative statistical analysis to extract trends with neutron excess in a well-defined manner.

Our presentation is organized in the following manner. In Chapter 2 we present the models, notation and expressions used in our study here. In particular, section

- **2.1** presents equations of the BCS model.
- **2.2** presents equations of the LN model.
- 2.3 presents proposed expressions for the effective-pairing gap  $\Delta_G$ , models for the average pairing gap  $\overline{\Delta}$ , and models for the average residual neutron-proton interaction energy  $\delta$ .
- 2.4 presents derivations of average pairing expressions. The material for the LN model is new, and for the BCS model it is more general than before.
- **2.5** presents finite-difference pairing gap expressions, which are expressions for extracting pairing gaps from odd-even experimental mass differences.

In chapter 3 we present model studies and parameter determinations, as well as the statistical models used to study trends in the neutron pairing gap behaviour with increasing neutron excess. In particular, section

- 3.1 presents expressions that are suitable for describing pairing gap trends with neutron excess, as well as statistical methods to analyse the behaviour of these expressions.
- 3.2 presents results of pairing calculations using previous expressions for the effective-interaction pairing gap  $\Delta_G$ . We do not repeat old material here, but instead analyse the old results by use of the new methods presented in section 3.1.
- 3.3 presents determinations of pairing model parameters. Calculated pairing gaps are compared to odd-even experimental mass differences for sufficiently many parameter sets that least-squares minimization can be carried out and optimum theoretical parameter sets determined.
- **3.4** presents figures and discussions of results obtained with the optimum parameter sets.

In Chapter 4 we present a brief summary of the results obtained in the present study. Finally, in the Appendix we present a summary of the most important symbols used here, with information about what equations define the symbols and in what equations the symbols are used.

## 2. Pairing models

Because of its basic simplicity, the BCS pairing model[1, 2, 3, 4] has been the pairing model of choice in most previous nuclear-structure calculations[8, 9, 10, 11]. However, a well-known deficiency of the BCS model is that for large spacings between the single-particle levels at the Fermi surface, no non-trivial solutions exist. These situations occur not only at magic numbers, but also, for example, for deformed actinide nuclei at neutron numbers N=142 and N=152. By taking into account effects associated with particle-number fluctuations, the Lipkin-Nogami approximation[5, 6, 7] goes beyond the BCS approximation and avoids such collapses.

In solving the pairing equations for neutrons or protons in either the BCS or Lipkin-Nogami model, we consider a constant pairing interaction G acting between  $N_2 - N_1 + 1$  doubly degenerate single-particle levels, which are occupied by  $N_{\text{int}}$  nucleons. This interaction interval starts at level  $N_1$ , located below the Fermi surface, and ends at level  $N_2$ , located above the Fermi surface. With the definitions we use here, the levels are numbered consecutively starting with number 1 for the level at the bottom of the well. Thus, for even particle numbers, the last occupied levels in the neutron and proton wells are N/2 and Z/2, respectively.

The level pairs included in the pairing calculation are often chosen symmetrically around the Fermi surface. However, for spherical nuclei it is more reasonable to require that degenerate spherical states have equal occupation probability. This condition cannot generally be satisfied simultaneously with a symmetric choice of levels in the interaction region. We therefore derive the pairing equations below for the more general case of arbitrary  $N_1$  and  $N_2$ .

#### 2.1. BCS PAIRING MODEL

In the BCS pairing model the pairing gap  $\Delta$  and Fermi energy  $\lambda$  are determined from the two coupled nonlinear equations [1, 2, 3, 4, 12]

$$N_{\text{tot}} = 2\sum_{k=N_1}^{N_2} v_k^2 + 2(N_1 - 1)$$
(1)

$$\frac{2}{G} = \sum_{k=N_1}^{N_2} \frac{1}{\sqrt{(e_k - \lambda)^2 + \Delta^2}}$$
 (2)

where the occupation probabilities  $v_k^2$  are

$$v_k^2 = \frac{1}{2} \left[ 1 - \frac{e_k - \lambda}{\sqrt{(e_k - \lambda)^2 + \Delta^2}} \right], \quad k = N_1, N_1 + 1, \dots, N_2$$
 (3)

and  $e_k$  are the single-particle energies. The quasi-particle energies  $E_k$  are given by the expressions

$$E_k = [(e_k - \lambda)^2 + \Delta^2]^{1/2}, \quad k = N_1, N_1 + 1, \dots, N_2$$
 (4)

The odd-even mass differences due to pairing are identified with the pairing gap  $\Delta$  in the above equations.

In order to calculate the potential energy in nuclear mass calculations, one also needs an expression for the pairing correction energy  $E_{\rm pc} - \tilde{E}_{\rm pc}$ . The pairing correlation energy plus quasi-particle energy is given by [2, 4]

$$E_{\rm pc} = \sum_{k=N_1}^{N_2} (2v_k^2 - n_k)e_k - \frac{\Delta^2}{G} - \frac{G}{2} \sum_{k=N_1}^{N_2} (2v_k^4 - n_k) + E_i \theta_{\rm odd, N_{tot}}$$
 (5)

where  $n_k$ , with values 2, 1 or 0, specify the sharp distribution of particles in the absence of pairing. The quasi-particle energy  $E_i$  for the odd particle occupying level i is given by eq. (4) and  $\theta_{\text{odd},N_{\text{tot}}}$  is unity if  $N_{\text{tot}}$  is odd and zero if  $N_{\text{tot}}$  is even. The calculation of the pairing correlation energy  $\widetilde{E}_{\text{pc}}$  for an *average* nucleus is discussed in sect. 2.4.

To solve eqs. (1–3) one must know the pairing strength G. In sect. 2.4 we discuss a powerful method for determining G from a knowledge of the *effective-interaction* pairing gap  $\Delta_G$ . Models for  $\Delta_G$  are introduced in sect. 2.3.

#### 2.2. LIPKIN-NOGAMI PAIRING MODEL

In the Lipkin-Nogami pairing model[5, 6, 7] the pairing gap  $\Delta$ , Fermi energy  $\lambda$ , number-fluctuation constant  $\lambda_2$ , occupation probabilities  $v_k^2$ , and shifted single-particle energies  $\epsilon_k$  are determined from the  $2(N_2 - N_1) + 5$  coupled nonlinear equations

$$N_{\text{tot}} = 2\sum_{k=N_1}^{N_2} v_k^2 + 2(N_1 - 1)$$
(6)

$$\frac{2}{G} = \sum_{k=N_1}^{N_2} \frac{1}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}$$
 (7)

$$v_k^2 = \frac{1}{2} \left[ 1 - \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}} \right], \quad k = N_1, N_1 + 1, \dots, N_2$$
 (8)

$$\epsilon_k = e_k + (4\lambda_2 - G)v_k^2, \quad k = N_1, N_1 + 1, \dots, N_2$$
 (9)

and

$$\lambda_{2} = \frac{G}{4} \left[ \frac{\left(\sum_{k=N_{1}}^{N_{2}} u_{k}^{3} v_{k}\right) \left(\sum_{k=N_{1}}^{N_{2}} u_{k} v_{k}^{3}\right) - \sum_{k=N_{1}}^{N_{2}} u_{k}^{4} v_{k}^{4}}{\left(\sum_{k=N_{1}}^{N_{2}} u_{k}^{2} v_{k}^{2}\right)^{2} - \sum_{k=N_{1}}^{N_{2}} u_{k}^{4} v_{k}^{4}} \right]$$
(10)

where

$$u_k^2 = 1 - v_k^2$$
,  $k = N_1, N_1 + 1, \dots, N_2$  (11)

The quasi-particle energies  $E_k$  of the odd nucleon in an odd-A nucleus are now given by [6]

$$E_k = \left[ (\epsilon_k - \lambda)^2 + \Delta^2 \right]^{1/2} + \lambda_2, \quad k = N_1, N_1 + 1, \dots, N_2$$
 (12)

In the Lipkin-Nogami model it is the quantity  $\Delta + \lambda_2$  that is identified with odd-even mass differences[6].

The pairing correlation energy plus quasi-particle energy in the Lipkin-Nogami model is given by

$$E_{\rm pc} = \sum_{k=N_1}^{N_2} (2v_k^2 - n_k)e_k - \frac{\Delta^2}{G} - \frac{G}{2} \sum_{k=N_1}^{N_2} (2v_k^4 - n_k) - 4\lambda_2 \sum_{k=N_1}^{N_2} u_k^2 v_k^2 + E_i \theta_{\rm odd, N_{tot}}$$
(13)

where  $e_k$  are the single-particle energies and  $n_k$ , with values 2, 1 or 0, specify the sharp distribution of particles in the absence of pairing. The quasi-particle energy  $E_i$  for the odd particle occupying level i given by eq. (12).

We have developed a computer code to solve the Lipkin-Nogami pairing equations, which is now also used in the calculation of nuclear potential-energy surfaces, from which we determine nuclear ground-state masses. Since we often survey large regions of nuclei, an important goal in developing this code was to make it both fast and reliable. In particular, we wanted to avoid crashes that initially occurred due to numerical difficulties. Such difficulties will always arise for sufficiently small values of the pairing matrix element G and large gaps in the single-particle level spectrum at the Fermi surface, where the BCS equations have no non-trivial solution. Thus the statement by Pradhan et al.[7] that "anyone with a computer programme for the usual BCS calculation can readily do the LN calculation" is grossly misleading. However, our current code solves the pairing equations for any reasonable choice of pairing matrix element G.

#### 2.3. EFFECTIVE-INTERACTION PAIRING-GAP MODELS

To solve the pairing equations one needs the pairing matrix element G, along with the single-particle levels  $e_k$ . In some early approaches[8], G was determined by solving the

pairing equations for a region of nuclei and adjusting G so that calculated values of  $\Delta$  optimally reproduced the odd-even mass differences. The disadvantage of this approach is that the value of G depends on the region of nuclei considered and also on the number of levels above and below the Fermi surface that are included in the pairing calculation.

A more powerful approach that is valid throughout the periodic system and for any reasonable choice of the interaction region is to use the effective-interaction pairing gap  $\Delta_G$  as the primary parameter. Then, by considering the properties of an *average* nucleus it is possible to determine G from its relation to the effective-interaction pairing-gap[13, 14] through the equations that are derived in sect. 2.4.

Several recent studies[15, 16, 17] have indicated an explicit isospin dependence of the average pairing gap. This observation led to the conclusion that "the pairing gap decreases with increasing isospin." Below we investigate in detail whether the pairing gaps do indeed exhibit such a decrease with increasing neutron excess. However, this question cannot be answered unless it is made more precise. One ambiguity in the earlier work arises from equating the pairing-gap expression that is used to determine the strength of the pairing matrix element G for microscopic pairing calculations with the macroscopic pairing-gap model that is used to describe average odd-even mass differences. The pairing-gap model has been used both as an odd-even term in liquid-drop models and as the effective-interaction pairing gap that is used to determine G. However, to achieve clarity in the arguments and to obtain optimum parameter choices it is necessary to introduce two distinct concepts, namely an average pairing gap  $\overline{\Delta}$  and an effective-interaction pairing gap  $\Delta_G$ .

The average pairing gap  $\overline{\Delta}$  is a model given by an analytical expression whose parameters are obtained by directly comparing the model expression to odd-even mass differences. It is also often used in models of the liquid-drop type to represent odd-even mass differences. On the other hand, the effective-interaction pairing gap  $\Delta_G$  is used to determine the magnitude of the pairing matrix element G that enters in microscopic pairing models.

Earlier, the average pairing gap  $\overline{\Delta}$  has also been used as a model for the effectiveinteraction pairing gap  $\Delta_G$ . However, the magnitude of a particular experimental pairing gap depends on the specific structure of the single-particle level spectrum of the nucleus, in addition to an overall smooth dependence on proton number Z and neutron number N. If the shell effects on the pairing gap were sufficiently random, their effect would average out over the periodic system and they would not affect the parameter values obtained in a least-squares adjustment of the average pairing gap  $\Delta$  to odd-even mass differences. In practice, the presence of certain correlations does affect the values obtained for the parameters. By selecting nuclear ground states for our studies we have introduced in the data set a bias towards large gaps in the single-particle level spectrum at the Fermi surface. Since these are configurations of high stability, they are automatically favoured at ground-state configurations. The pairing gaps here would be slightly lower, on the average, than pairing gaps at average level densities. There may also be other correlation effects present in the ground state. The effect of the gaps in the single-particle spectrum should be described by the microscopic model itself, rather than through a choice of parameters of the pairing-gap model. Therefore, one cannot use parameters that have been obtained by directly comparing a proposed pairing-gap expression to odd-even mass differences as parameters for the effective-interaction pairing gap  $\Delta_G$ , as has been done

in many earlier calculations.

In earlier studies that suggested[15, 16, 17] that pairing effects decrease with increasing neutron excess, no distinction was made between  $\Delta_G$  and  $\overline{\Delta}$ . In our study here we make this distinction. Specifically, we study here how pairing gaps calculated in the BCS and LN models compare to experimental pairing gaps, estimated by use of eqs. (35,36), for different choices of parameter values for the effective-interaction pairing gap expressions  $\Delta_G$ . This is a much more fundamental approach than a direct comparison between  $\overline{\Delta}$  and eqs. (35,36). However, we here also do the latter comparison, mainly for comparing with previous results and for illustrating the different results that are obtained in the two approaches.

We study here two proposed forms for the average pairing gap  $\overline{\Delta}$  and for the effective-interaction pairing gap  $\Delta_G$ . In the first form, the average and effective-interaction pairing gaps are given by expressions that for certain parameter choices may explicitly decrease with increasing neutron excess[17]:

$$\Delta_{Gn} = \frac{rB_{s}}{N^{1/3}} e^{-sI - tI^{2}}$$

$$\Delta_{Gp} = \frac{rB_{s}}{Z^{1/3}} e^{+sI - tI^{2}}$$
(14)

and

$$\overline{\Delta}_{\rm n} = \frac{rB_{\rm s}}{N^{1/3}} \, {\rm e}^{-sI - tI^2}$$

$$\overline{\Delta}_{p} = \frac{rB_{s}}{Z^{1/3}} e^{+sI - tI^{2}}$$

$$\tag{15}$$

Although the average pairing gap  $\overline{\Delta}$  and effective-interaction pairing gap  $\Delta_G$  are given by the identical expressions, they represent different concepts and, as we will see below, they each have a different optimum parameter set. Here

$$I = \frac{N - Z}{N + Z} \tag{16}$$

is the relative neutron excess and  $B_s$  is the ratio of the surface area of the nucleus at the deformation considered to the surface area of the spherical nucleus. In addition, ref.[17] introduced a new expression for the average residual n-p interaction energy  $\delta$  appearing in the masses of odd-odd nuclei:

$$\delta = \frac{h}{A^{2/3}B_{\rm s}}\tag{17}$$

The four constants r, s, t and h were determined by a least-squares adjustment to experimental pairing gaps obtained from measured masses, which resulted in r = 5.72 MeV, s = 0.118, t = 8.12 and h = 6.52 MeV.

As the other pairing-gap model for our study we choose the conventional pairing-gap expressions

$$\Delta_{Gn} = \frac{c_n}{\sqrt{A}}$$

$$\Delta_{G_{\mathbf{p}}} = \frac{c_{\mathbf{p}}}{\sqrt{A}} \tag{18}$$

and

$$\overline{\Delta}_{n} = \frac{c_{n}}{\sqrt{A}}$$

$$\overline{\Delta}_{p} = \frac{c_{p}}{\sqrt{A}}$$
(19)

The n-p interaction that has been used together with the pairing gap expressions (18,19) is

$$\delta = \frac{d}{A} \tag{20}$$

which do not exhibit any explicit isospin dependence. Although it has been well known for many years that the neutron pairing for heavy nuclei is somewhat weaker than the proton pairing[18], in most investigations  $c_{\rm n}$  and  $c_{\rm p}$  are chosen the same and equal to about 12 MeV. Here we determine more precise values by least-squares minimization.

#### 2.4. AVERAGE PAIRING EXPRESSIONS

The dependence of the pairing strength G on the corresponding effective-interaction pairing gap  $\Delta_G$  is obtained from the microscopic equations by assuming a constant level density for the average nucleus in the vicinity of the Fermi surface. This allows the sums in the equations to be replaced by integrals. The average level density of doubly degenerate levels is taken to be

$$\widetilde{\rho} = \frac{1}{2}\widetilde{g}(\widetilde{\lambda}) \tag{21}$$

where  $\tilde{g}$  is the smooth level density that is obtained in Strutinsky's shell-correction method and  $\tilde{\lambda}$  is the Fermi energy of the smoothed single-particle energy[9, 12]. Thus, we can make the substitution

$$\sum_{k=N_1}^{N_2} f(e_k - \lambda) \Longrightarrow \tilde{\rho} \int_{y_1}^{y_2} f(x) dx \tag{22}$$

where

$$y_1 = \frac{-\frac{1}{2}N_{\text{tot}} + N_1 - 1}{\tilde{\rho}}$$

$$y_2 = \frac{-\frac{1}{2}N_{\text{tot}} + N_2}{\tilde{\rho}}$$
(23)

The gap equation (2) may now be evaluated for an average nucleus, with the result

$$\frac{1}{G} = \frac{1}{2} \tilde{\rho} \int_{y_1}^{y_2} \frac{dx}{\sqrt{x^2 + \Delta_G^2}}$$

$$= \frac{1}{2} \tilde{\rho} \left[ \ln \left( \sqrt{y_2^2 + \Delta_G^2} + y_2 \right) - \ln \left( \sqrt{y_1^2 + \Delta_G^2} + y_1 \right) \right] \tag{24}$$

From this expression, the pairing strength G in the BCS model may be determined in any region of the nuclear chart.

The same expression may also be used in the Lipkin-Nogami case, but some reinterpretations are necessary. It is now the energies  $\epsilon_k$  occurring in eq. (7) that are assumed to be equally spaced. These are not precisely the single-particle energies  $e_k$  but are related to them by eq. (9). Thus, in order for  $\epsilon_k$  to be equally spaced, the single-particle energies  $e_k$ must be shifted downward by the amounts  $(4\lambda_2 - G)v_k^2$ . Since the occupation probability  $v_k^2$  is approximately unity far below the Fermi surface and zero far above, the corresponding single-particle energy distribution is approximately uniform far above and far below the Fermi surface but spread apart by the additional amount  $4\lambda_2 - G$  close to the Fermi surface. Although this decrease in level density near the Fermi surface is accidental, it is in approximate accord with the ground-state structure of real nuclei, since the increased stability associated with ground-state configurations is due to low level densities near the Fermi surface[12, 17].

In the Lipkin-Nogami model, it is the quantity  $\Delta + \lambda_2$  that is associated with oddeven mass differences, whereas in the BCS model it is  $\Delta$  only that should be directly compared to the experimental data. This leads to the expectation that there is a related difference between  $\Delta_G^{\rm LN}$  and  $\Delta_G^{\rm BCS}$ , the effective-interaction pairing gaps associated with the LN and BCS models, respectively. Since we determine the parameters of the model for  $\Delta_G^{\rm LN}$  directly from least-squares minimization, it is not necessary to specify exactly such a relationship. However, the above observation is of value as a rough rule of thumb, and to remind us to expect that the effective-interaction pairing gaps in the BCS and LN models are of somewhat different magnitude.

The expression for the average pairing correlation energy plus quasi-particle energy  $\tilde{E}_{pc}$  in the BCS and Lipkin-Nogami models is obtained in a similar manner as the expression for the pairing matrix element G. The summations in eqs. (5) and (13) are replaced by integrations according to the rule given by eqs. (22) and (23). For the first part of eqs. (5) and (13) we obtain

$$\sum_{k=N_{1}}^{N_{2}} (2v_{k}^{2} - n_{k})e_{k} - \frac{\Delta_{G}^{2}}{G}$$

$$= \sum_{k=N_{1}}^{N_{2}} 2v_{k}^{2}(e_{k} - \lambda) - \sum_{k=N_{1}}^{N_{2}} n_{k}(e_{k} - \lambda) - \frac{\Delta_{G}^{2}}{G}$$

$$= \tilde{\rho} \int_{y_{1}}^{y_{2}} \left( x - \frac{x^{2}}{\sqrt{x^{2} + \Delta_{G}^{2}}} \right) dx - 2\tilde{\rho} \int_{y_{1}}^{0} x dx - \frac{\Delta_{G}^{2}}{G}$$

$$= \tilde{\rho} \left[ \frac{y_{2}^{2}}{2} - \frac{y_{2}\sqrt{y_{2}^{2} + \Delta_{G}^{2}}}{2} + \frac{\Delta_{G}^{2}}{2} \ln\left(\sqrt{y_{2}^{2} + \Delta_{G}^{2}} + y_{2}\right) \right]$$

$$- \tilde{\rho} \left[ \frac{y_{1}^{2}}{2} - \frac{y_{1}\sqrt{y_{1}^{2} + \Delta_{G}^{2}}}{2} + \frac{\Delta_{G}^{2}}{2} \ln\left(\sqrt{y_{1}^{2} + \Delta_{G}^{2}} + y_{1}\right) \right] + 2\tilde{\rho} \frac{y_{1}^{2}}{2} - \frac{\Delta_{G}^{2}}{G}$$
 (25)

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For the second part of eqs. (5) and (13) we obtain

$$-\frac{G}{2} \sum_{k=N_1}^{N_2} (2v_k^4 - n_k)$$

$$= -\frac{G}{2} \sum_{k=N_1}^{N_2} \left\{ \frac{1}{4} \left[ 1 - \frac{e_k - \lambda}{\left[ (e_k - \lambda)^2 + \Delta_G^2 \right]^{1/2}} \right]^2 - n_k \right\}$$

$$= -\frac{G}{4} \tilde{\rho} \int_{y_1}^{y_2} \left[ 1 + \frac{x^2}{x^2 + \Delta_G^2} - \frac{2x}{\left(x^2 + \Delta_G^2\right)^{1/2}} \right] dx + G \tilde{\rho} \int_{y_1}^{0} x \, dx$$

$$= -\frac{G}{4} \tilde{\rho} \left[ 2y_2 - 2\sqrt{y_2^2 + \Delta_G^2} - \Delta_G \tan^{-1} \left( \frac{y_2}{\Delta_G} \right) \right]$$

$$+ \frac{G}{4} \tilde{\rho} \left[ 2y_1 - 2\sqrt{y_1^2 + \Delta_G^2} - \Delta_G \tan^{-1} \left( \frac{y_1}{\Delta_G} \right) \right] - G \tilde{\rho} y_1$$
(26)

Adding the various terms together leads to the following expression for the average pairing correlation energy plus quasi-particle energy in the BCS model:

$$\widetilde{E}_{pc} = \frac{1}{2}\widetilde{\rho} \left[ (y_2 - G) \left( y_2 - \sqrt{y_2^2 + \Delta_G^2} \right) + (y_1 - G) \left( y_1 + \sqrt{y_1^2 + \Delta_G^2} \right) \right] 
+ \frac{1}{4} G \widetilde{\rho} \Delta_G \left[ \tan^{-1} \left( \frac{y_2}{\Delta_G} \right) - \tan^{-1} \left( \frac{y_1}{\Delta_G} \right) \right] + \overline{\Delta} \theta_{\text{odd}, N_{\text{tot}}}$$
(27)

To obtain the average pairing correlation energy in the Lipkin-Nogami model we need to evaluate additional terms. For the third part of eq. (13) we find

$$-4\lambda_2 \sum_{k=N_1}^{N_2} u_k^2 v_k^2$$

$$= -\lambda_2 \sum_{k=N_1}^{N_2} \frac{\Delta_G^2}{(E_k - \lambda)^2 + \Delta_G^2}$$

$$= -\lambda_2 \tilde{\rho} \int_{y_1}^{y_2} \frac{\Delta_G^2}{x^2 + \Delta_G^2} dx$$

$$= -\lambda_2 \tilde{\rho} \Delta_G \left[ \tan^{-1} \left( \frac{y_2}{\Delta_G} \right) - \tan^{-1} \left( \frac{y_1}{\Delta_G} \right) \right]$$
(28)

The value  $\lambda_2$  of  $\lambda_2$  for the *average* nucleus is obtained from eq. (10) by converting the sums in that expression to integrals with the substitution in eq. (22). Four different sums have to be evaluated. For the first sum in eq. (10) we obtain

$$\sum_{N_{1}}^{N_{2}} u_{k}^{3} v_{k}$$

$$= \frac{1}{4} \tilde{\rho} \int_{y_{1}}^{y_{2}} dx \left[ 1 + \frac{x}{\sqrt{x^{2} + \Delta_{G}^{2}}} \right]^{3/2} \left[ 1 - \frac{x}{\sqrt{x^{2} + \Delta_{G}^{2}}} \right]^{1/2}$$

$$= \frac{1}{4} \tilde{\rho} \int_{y_{1}}^{y_{2}} dx \left[ \frac{\Delta_{G}}{\sqrt{x^{2} + \Delta_{G}^{2}}} + \frac{x \Delta_{G}}{x^{2} + \Delta_{G}^{2}} \right]$$

$$= \frac{1}{4} \Delta_{G} \tilde{\rho} \left[ \ln \left( \sqrt{y_{2}^{2} + \Delta_{G}^{2}} + y_{2} \right) + \frac{1}{2} \ln \left( y_{2}^{2} + \Delta_{G}^{2} \right) \right]$$

$$- \frac{1}{4} \Delta_{G} \tilde{\rho} \left[ \ln \left( \sqrt{y_{1}^{2} + \Delta_{G}^{2}} + y_{1} \right) + \frac{1}{2} \ln \left( y_{1}^{2} + \Delta_{G}^{2} \right) \right] \tag{29}$$

The second sum is very similar, yielding

$$\sum_{N_1}^{N_2} u_k v_k^3$$

$$= \frac{1}{4} \tilde{\rho} \int_{y_1}^{y_2} dx \left[ 1 + \frac{x}{\sqrt{x^2 + \Delta_G^2}} \right]^{1/2} \left[ 1 - \frac{x}{\sqrt{x^2 + \Delta_G^2}} \right]^{3/2}$$

$$= \frac{1}{4} \Delta_G \tilde{\rho} \left[ \ln \left( \sqrt{y_2^2 + \Delta_G^2} + y_2 \right) - \frac{1}{2} \ln \left( y_2^2 + \Delta_G^2 \right) \right]$$

$$- \frac{1}{4} \Delta_G \tilde{\rho} \left[ \ln \left( \sqrt{y_1^2 + \Delta_G^2} + y_1 \right) - \frac{1}{2} \ln \left( y_1^2 + \Delta_G^2 \right) \right] \tag{30}$$

For the third sum we obtain

$$\sum_{N_{1}}^{N_{2}} u_{k}^{4} v_{k}^{4}$$

$$= \tilde{\rho} \int_{y_{1}}^{y_{2}} dx \left[ \frac{1}{4} \left( 1 + \frac{x}{\sqrt{x^{2} + \Delta_{G}^{2}}} \right) \left( 1 - \frac{x}{\sqrt{x^{2} + \Delta_{G}^{2}}} \right) \right]^{2}$$

$$= \frac{\Delta_{G}^{4}}{16} \tilde{\rho} \int_{y_{1}}^{y_{2}} \frac{dx}{\left( x^{2} + \Delta_{G}^{2} \right)^{2}}$$

$$= \frac{1}{16} \tilde{\rho} \left[ \frac{\Delta_{G}^{2}}{2} \frac{y_{2}}{y_{2}^{2} + \Delta_{G}^{2}} + \frac{\Delta_{G}}{2} \tan^{-1} \left( \frac{y_{2}}{\Delta_{G}} \right) \right]$$

$$- \frac{1}{16} \tilde{\rho} \left[ \frac{\Delta_{G}^{2}}{2} \frac{y_{1}}{y_{1}^{2} + \Delta_{G}^{2}} + \frac{\Delta_{G}}{2} \tan^{-1} \left( \frac{y_{1}}{\Delta_{G}} \right) \right] \tag{31}$$

Finally, we obtain the expression for the last sum from eq. (28).

Collecting the various expressions together we find the following expressions for the average pairing quantities in the Lipkin-Nogami model. The limits  $y_1$  and  $y_2$  and the pairing strength G in the final expressions below are given by eqs. (23) and (24). The expression for  $\tilde{\lambda}_2$  for an average nucleus is fairly lengthy. It is given by

$$\tilde{\lambda}_2 = \frac{G}{4} \left( \frac{A - C}{B - C} \right) \tag{32}$$

where

$$A = \left(\frac{\tilde{\rho}\Delta_G}{4}\right)^2 \left\{ \left(\frac{2}{G\tilde{\rho}}\right)^2 - \left[\ln\left(\frac{\sqrt{y_2^2 + \Delta_G^2}}{\sqrt{y_1^2 + \Delta_G^2}}\right)\right]^2 \right\}$$

$$B = \frac{\Delta_G^2 \tilde{\rho}^2}{16} \left[\tan^{-1}\left(\frac{y_2}{\Delta_G}\right) - \tan^{-1}\left(\frac{y_1}{\Delta_G}\right)\right]^2$$

$$C = \frac{\tilde{\rho}\Delta_G}{32} \left[\Delta_G\left(\frac{y_2}{y_2^2 + \Delta_G^2} - \frac{y_1}{y_1^2 + \Delta_G^2}\right) + \tan^{-1}\left(\frac{y_2}{\Delta_G}\right) - \tan^{-1}\left(\frac{y_1}{\Delta_G}\right)\right]$$
(33)

For the average pairing correlation energy plus quasi-particle energy in the Lipkin-Nogami model we then obtain

$$\widetilde{E}_{pc} = \frac{1}{2}\widetilde{\rho} \left[ (y_2 - G) \left( y_2 - \sqrt{y_2^2 + \Delta_G^2} \right) + (y_1 - G) \left( y_1 + \sqrt{y_1^2 + \Delta_G^2} \right) \right] 
+ \frac{1}{4} (G - 4\widetilde{\lambda}_2) \widetilde{\rho} \Delta_G \left[ \tan^{-1} \left( \frac{y_2}{\Delta_G} \right) - \tan^{-1} \left( \frac{y_1}{\Delta_G} \right) \right] + \overline{\Delta} \theta_{\text{odd}, N_{\text{tot}}}$$
(34)

Since the odd-even mass difference in the Lipkin-Nogami model is given by the sum  $\Delta + \lambda_2$  it would be most consistent to use an average odd-even mass-difference expression for  $\overline{\Delta}$  above that is the sum  $\overline{\Delta}^{\text{LN}} + \overline{\lambda}_2$ . However, this would lead to the use of three  $\lambda_2$ -like quantities, namely  $\lambda_2$ ,  $\widetilde{\lambda}_2$  and  $\overline{\lambda}_2$ . Fortunately, this can be avoided by observing that in the expression for the total potential energy the average odd-even mass difference is first subtracted out through the term  $\widetilde{E}_{\text{pc}}$  in the pairing correction energy  $E_{\text{pc}} - \widetilde{E}_{\text{pc}}$  and then added back through the macroscopic energy. Because the specific form of  $\overline{\Delta}$  only affects the value of the shell correction, which is not an experimentally measurable quantity, and not the calculated total potential energy we use here the same definition as in the BCS expression. The identical odd average-paring term must be present both in the macroscopic model and in the BCS or Lipkin-Nogami average-pairing correlation-energy expression in order to provide a consistent definition of the microscopic shell-plus-pairing corrections.

One should observe that the expression for  $\tilde{\lambda}_2$  in eq. (32) goes to infinity as  $\Delta_G^{\text{LN}}$  decreases to a small but finite value. With the functional forms and parameter values that we finally select for  $\Delta_G^{\text{LN}}$ , this critical value is not approached for nuclei inside the neutron drip line. When the original parameter values[17] were used in eq. (14) the expression did diverge for a few nuclei with Z below 20, close to the neutron drip line.

In most of our calculations, where we use the diffuse-surface folded-Yukawa single-particle potential [9, 19, 10], we choose  $N_2$  to correspond to either the last bound single-particle level or the last level within an energy interval of 5 MeV above the sharp Fermi surface, whichever is higher. We include an equal number of levels below the Fermi surface, which determines  $N_1$ . However, the equations are general enough to allow any choice of  $N_1$  and  $N_2$ .

In table 1 we show the stability of BCS pairing-model calculations with respect to changes in the details of the microscopic calculations when the above methods for defining average pairing quantities are used. The calculations were performed for Nilsson-model[8] proton single-particle levels corresponding to  $\kappa_{\rm p}=0.0800$ ,  $\mu_{\rm p}=0.300$  and  $\epsilon_{\rm 2}=0.20$  for the nucleus <sup>94</sup>Sr. The first three lines are calculations with an equal number of levels below and above the Fermi surface; the remaining lines represent non-symmetric choices. Compare, for example, line 7 to line 2, where an increase of  $N_2$  to 39 with a simultaneous corresponding adjustment of G has resulted in a change of  $\Delta_{\rm p}$  to 1.615 MeV, or a change of only 5%. This should be compared to the value  $\Delta_{\rm p}=2.12$  MeV, an increase of 38%, that is obtained if G is not readjusted according to eq. (24) but is instead held fixed at G=0.3028 MeV. These results demonstrate that the method that we use here to determine G from the properties of an average nucleus yields results that are very stable with respect to changes in the details of the calculations, except when the number of levels above and below the Fermi surface are very different, as is the case on lines 4 and 6.

#### 2.5. FINITE-DIFFERENCE PAIRING-GAP EXPRESSIONS

The magnitude of the neutron and proton pairing gaps can be determined only indirectly from experimental data. A commonly used method is to estimate the pairing gaps

Table 1

Effect of changing the summation interval in a BCS pairing calculation for protons in <sup>94</sup>Sr. The number of particles is 38, so that the last occupied level is number 19.

$N_1$	$N_2$	G (MeV)	$\Delta_{\rm p}$ (MeV)	$E_{\rm pc}$ (MeV)	$\widetilde{E}_{ m pc}$ (MeV)	$E_{\rm pc} - \tilde{E}_{\rm pc} $ (MeV)
13	26	0.3532	1.581	-1.80	-0.70	-1.10
10	29	0.3028	1.540	-1.78	-0.75	-1.03
6	33	0.2666	1.519	-1.78	-0.79	-0.99
6	26	0.2923	1.453	-1.57	-0.74	-0.83
13	36	0.2923	1.630	-2.04	-0.78	-1.26
13	46	0.2679	1.711	-2.31	-0.81	-1.50
10	39	0.2655	1.615	-2.04	-0.80	-1.24
6	43	0.2431	1.600	-2.04	-0.82	-1.22

from experimental odd-even mass differences. Several different finite-difference formulas have been used for this purpose. An in-depth discussion of the properties of these expressions is given in ref.[17]. To avoid the ambiguities that are associated with the lower-order finite-difference expressions, we use the fourth-order expressions from this work. Thus, for the neutron pairing gap we use

$$\Delta_{n}^{\text{even-even}} = -\frac{1}{8}[M(Z, N+2) - 4M(Z, N+1) + 6M(Z, N) \\
-4M(Z, N-1) + M(Z, N-2)]$$

$$\Delta_{n}^{\text{odd-neutron}} = \frac{1}{8}[M(Z, N+2) - 4M(Z, N+1) + 6M(Z, N) \\
-4M(Z, N-1) + M(Z, N-2)]$$

$$\Delta_{n}^{\text{odd-proton}} = -\frac{1}{8}[M(Z, N+2) - 4M(Z, N+1) + 6M(Z, N) \\
-4M(Z, N-1) + M(Z, N-2)] + \delta$$

$$\Delta_{n}^{\text{odd-odd}} = \frac{1}{8}[M(Z, N+2) - 4M(Z, N+1) + 6M(Z, N) \\
-4M(Z, N-1) + M(Z, N-2)] + \delta$$
(35)

Correspondingly, for the proton pairing gap we use

$$\Delta_{\rm p}^{\text{even-even}} = -\frac{1}{8}[M(Z+2,N) - 4M(Z+1,N) + 6M(Z,N) \\
-4M(Z-1,N) + M(Z-2,N)]$$

$$\Delta_{\rm p}^{\text{odd-neutron}} = -\frac{1}{8}[M(Z+2,N) - 4M(Z+1,N) + 6M(Z,N) \\
-4M(Z-1,N) + M(Z-2,N)] + \delta$$

$$\Delta_{\rm p}^{\text{odd-proton}} = \frac{1}{8}[M(Z+2,N) - 4M(Z+1,N) + 6M(Z,N) \\
-4M(Z-1,N) + M(Z-2,N)]$$

$$\Delta_{\rm p}^{\text{odd-odd}} = \frac{1}{8}[M(Z+2,N) - 4M(Z+1,N) + 6M(Z,N) \\
-4M(Z-1,N) + M(Z-2,N)] + \delta$$
(36)

The residual n-p interaction energy  $\delta$  appearing in some of the above equations can be estimated from [17]

$$\delta^{\text{even-even}} = \frac{1}{4} \{ 2[M(Z, N+1) + M(Z, N-1) + M(Z-1, N) \\ + M(Z+1, N)] - [M(Z+1, N+1) + M(Z-1, N+1) \\ + M(Z-1, N-1) + M(Z+1, N-1)] - 4M(Z, N) \}$$

$$\delta^{\text{odd-neutron}} = -\frac{1}{4} \{ 2[M(Z, N+1) + M(Z, N-1) + M(Z-1, N) \\ + M(Z+1, N)] - [M(Z+1, N+1) + M(Z-1, N+1) \\ + M(Z-1, N-1) + M(Z+1, N-1)] - 4M(Z, N) \}$$

$$\delta^{\text{odd-proton}} = \delta^{\text{odd-neutron}}$$

$$\delta^{\text{odd-proton}} = \delta^{\text{even-even}}$$
(37)

The difference expressions in eqs. (35–37) depend on whether the center nucleus is even-even, odd-neutron, odd-proton or odd-odd, as indicated by the superscripts. The finite-difference equations used to extract estimates of pairing gaps from experimental masses are derived under the assumption that there are no non-smooth contributions to the masses apart from pairing effects. However, this assumption is often not fulfilled. For example, for N = Z there is a cusp in the mass surface, usually described in terms of the Wigner term W|I|. At magic numbers there are other irregularities in the mass surface.

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Thus, expressions (35–37) cannot be used for nucleon numbers that span such singularities in the mass surface. Therefore, we exclude the following nuclei from consideration, for the reasons given in parentheses:

For the neutron pairing-gap expression (35) we exclude nuclei with

• 
$$N + 1, N \text{ or } N - 1 = 8, 14, 20, 28, 50, 82, 126$$
 (magic-number cusps)

• 
$$Z = 8, 14, 20, 28, 50, 82$$
 ( $\delta$  undefined for odd  $Z$ )

• 
$$Z = N + 1$$
,  $Z = N$  or  $Z = N - 1$  (Wigner cusp)

• Z or N < 8

Correspondingly, for the proton pairing-gap expression (36) we exclude nuclei with

• 
$$Z + 1, Z \text{ or } Z - 1 = 8, 14, 20, 28, 50, 82$$
 (magic-number cusps)

• 
$$N = 8, 14, 20, 28, 50, 82, 126$$
 ( $\delta$  undefined for odd  $N$ )

• 
$$Z = N + 1$$
,  $Z = N$  or  $Z = N - 1$  (Wigner cusp)

• Z or N < 8

For the neutron-proton residual pairing-gap expression (37) we exclude nuclei with

• 
$$Z$$
 or  $N = 8, 14, 20, 28, 50, 82, 126$  (magic-number cusps)

• 
$$Z = N$$
 (Wigner cusp)

• Z or N < 8

When  $\delta$  is not needed to estimate the proton pairing gap, we could, in principle, have included the nuclei that are on the second line of the proton pairing-gap exclusions, but we have chosen to exclude these cases for all four proton pairing-gap expressions. Keeping the cases that could be retained would still only let us include every second nucleus in the magic isotope chains, which would leave these chains unsuitable for some of the analyses we carry out later. For neutrons  $\delta$  does not enter the even-Z chains, so these chains could have been retained, but to keep the expressions similar for both protons and neutrons, we exclude these nuclei also for neutrons. In the remaining cases where  $\delta$  is undefined we only exclude precisely the neutron and proton pairing gaps where  $\delta$  is needed for the estimates.

In addition to the traditional magic numbers we have also excluded nucleon number 14, because there is a strong discontinuity in the experimental shell corrections at this nucleon number. One could argue that other sub-shell closures and possibly some deformed semi-magic numbers should also be excluded. Although we exclude only the cases listed above, we must in comparisons between calculated and experimental pairing gaps bear in mind that the finite-difference expression must also be expected to be inaccurate at other sub-shells and in regions where significant deformation changes occur between the nuclei in the finite-difference expressions.

#### 3. Calculations

From earlier calculations of nuclear ground-state masses in the macroscopic-microscopic approach we have available the ground-state single-particle level spectra calculated with the folded-Yukawa single-particle potential for 8979 nuclei ranging from the proton drip line to the neutron drip line. By using these levels as the starting point for a microscopic pairing calculation, we can quickly calculate microscopic pairing quantities for all these nuclei corresponding to any available model of interest for the effective-interaction pairing gap. Our searches for optimum parameter sets below typically involve solving the pairing equations for these 8979 nuclei for 25 different parameter sets with each new model. The calculations for one group of 25 parameter sets require about 15 minutes of CRAY-1 computer time.

When the number of particles is odd, we still include all of the single-particle levels between  $N_1$  and  $N_2$  rather than blocking (omitting) the half-filled level, as is sometimes done. We have also investigated the effect of blocking, and have found that the pairing gaps calculated with blocking contain an odd-even staggering that is not present in the experimental odd-even mass differences.

Our calculations here will focus on comparing calculated and experimental pairing gaps. We assume the experimental gaps are given by the fourth-order mass differences in eqs. (35–37). It would then seem natural to use the same fourth-order mass differences applied to calculated masses for the theoretical pairing gaps. Such an approach in principle has the advantage that the errors in the mass differences that result from non-smooth contributions, such as deformation changes between neighbouring nuclei, would be equally present in both the experimental and theoretical pairing gaps and consequently not affect a comparison of these quantities. However, this is true only if the theoretical model is sufficiently accurate. In practice, the theoretical model has its greatest uncertainties in the transition regions between spherical and deformed regions of nuclei. These errors have contributions from shell-correction terms and other non-pairing terms in the model. The transition regions have some of the largest changes in deformation between neighbouring nuclei, and it would therefore seem that in these regions, it would be particularly advantageous to use the above method. However, since the mass-model uncertainties are largest here, their adverse effects outweigh the advantage that the deformation-change errors are similar in the theoretical pairing-gap model and in the model used to extract the pairing gap from experiment. Therefore, we only use the calculated mass differences in a few of the comparisons, for illustrative purposes. In all other cases, we use the theoretical pairing gaps obtained by solving the microscopic pairing equations. For the propose of relating our results to previous work we also compare the macroscopic average-pairing gap models for  $\overline{\Delta}$  to data.

As an important consequence of the effects discussed above, there will be remaining discrepancies in a comparison between the experimental pairing quantities and the quantities that are obtained by solving the microscopic pairing equations even if the theoretical pairing model were a perfect one. One can expect these discrepancies to be largest for the lightest nuclei, where it is unlikely that five adjacent nuclei, which are required to estimate the experimental pairing gap, are devoid of non-smooth contributions to the mass. This is a difficulty over and above the expectation that mean-field approaches such

as the macroscopic-microscopic model or Hartree-Fock models should work less well for lighter nuclei because such concepts as average field and nuclear surface no longer apply. A more complete picture may be obtained by studying other pairing-dependent properties of nuclei, such as rotational band-head energies and band crossings at high spin. Such studies are outside the scope of the present investigation.

#### 3.1. EXPRESSIONS DESCRIBING TRENDS WITH NEUTRON EXCESS

One goal of this investigation is to establish whether the pairing gap decreases with increasing neutron excess. However, even the traditional expression  $\Delta_G = 12 \text{ MeV}/\sqrt{A}$  has this property. We also noted earlier that it is necessary to distinguish between the effective-interaction pairing gap and the average pairing gap. A more precise statement of the goal of our study is therefore that we want to establish whether pairing gaps that we obtain in microscopic calculations with various proposed expressions for the effective-interaction pairing gap  $\Delta_G$  accurately reproduce the trend of the experimental pairing gap with increasing neutron number. In particular, we want to determine a preferred expression for the effective-interaction pairing gap and values of the expression parameters.

To develop a well-defined method of analysis, it is natural to start by introducing the difference D(Z, N) between the calculated and experimental pairing gaps. Thus

$$D(Z, N) = \Delta(Z, N)_{\text{exp}} - \Delta(Z, N)_{\text{calc}}$$
(38)

For each element Z this difference can be determined only for certain N values, namely those for which the experimental pairing gaps can be determined.

To study how well various models reproduce the trend of the experimental pairing gaps with increasing neutron excess, one should study the behaviour of the error term D(Z, N) as N increases. To do this in a systematic and quantitative manner, we introduce the quantities S(Z, N),  $n_-$  and  $n_+$ , where

$$S(Z, N) = D(Z, N) - D(Z, N - 1)$$
(39)

with (Z, N) designating any proton-neutron combination for which the above expression is defined,

$$n_{-} = \sum_{Z,N} \Theta(-S(Z,N)), \quad S(Z,N) \neq 0$$
 (40)

and

$$n_{+} = \sum_{Z,N} \Theta(S(Z,N)), \quad S(Z,N) \neq 0$$
 (41)

The theta function  $\Theta(x)$  is 1 for x > 0 and 0 for x < 0. Neutron-proton combinations for which  $S(Z, N) \equiv 0$  are not counted in either group.

These three quantities have a straightforward interpretation. Suppose we plot the difference between calculated and experimental pairing gaps as a function of neutron number N, and for each Z value connect neighbouring isotopes by straight lines, as is done in fig. 1, for a single isotopic chain. For a particular nucleus  $n_+$  gets a contribution

+1 if the function described by this line increases towards the next neutron number. If the function decreases there is no contribution to  $n_+$  but instead a contribution of +1 to  $n_-$ . When the double sums have been carried out,  $n_+$  shows how many upward-sloping line segments there are and  $n_-$  shows how many downward-sloping line segments there are. If the theory correctly describes the trend of the pairing gap with increasing neutron excess, there should be about an equal number of upward- and downward-sloping segments, so that  $n_+ \approx n_-$ . Also, the line connecting different isotopes of the same element would be approximately horizontal on the large scale over the total range of neutron numbers, although the line would have a saw-tooth appearance on the small scale of a few neutron numbers, that is, S(Z, N) would be about 0, on the average. On the other hand, if  $n_+$  is considerably larger than  $n_-$  this means that the calculated pairing gap decreases faster than the experimental pairing gap with increasing neutron excess, and vice versa.

However, if some unexpected correlation exists, such that, for example, the upward-sloping segments go up further than the downward-sloping segments go down, the error could be quite different for a neutron-deficient nucleus compared to a neutron-rich nucleus, even if  $n_+ \approx n_-$ . It is to guard against such correlations that we have introduced the quantity S(Z, N), in addition to the counters  $n_-$  and  $n_+$ . In the absence of such correlations one would draw similar conclusions from studying the behaviour of S(Z, N) or the behaviour of the counters  $n_-$  and  $n_+$ , but it is from studying the slope S(Z, N) of the segments of the error term D(Z, N) that one is able to draw the most definitive conclusions about the trends of the different models with neutron excess, compared to experimental data. To establish whether the behaviour of a model with neutron excess follows the trends of the data, one determines if the slope S(Z, N) is 0 on the average, or whether it is significantly different from 0. One simple and informative way to do this is to assume that for each combination (Z, N), S(Z, N) is an observation of a random variable  $v \in N(m, \sigma^2)$ , that is, a random variable with a normal distribution described by the distribution function

$$f_v(x, m, \sigma^2) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma} e^{-(x-m)^2/2\sigma^2}$$
 (42)

One can analyze the agreement between models and experiment without the assumption of a normal distribution. However, we show below that the assumption of a normal distribution is extremely well fulfilled, as can be expected, since the number of observations usually exceeds 500. For this reason and because the assumption of a normal distribution easily allows for the interpretation of the results in terms of familiar concepts, we retain this assumption in most of our analyses.

One can now estimate the mean m and standard deviation  $\sigma$  of the distribution function (42) through the well-known expressions

$$m^* = \frac{1}{N_{\text{data}}} \sum_{Z,N} S(Z,N)$$

$$\sigma^* = \left[ \frac{1}{N_{\text{data}}} \sum_{Z,N} (S(Z,N) - m^*)^2 \right]^{1/2}$$
(43)

Table 2 Trend with neutron excess of the difference between experimental and calculated neutron pairing gaps for different  $\overline{\Delta}$  and  $\Delta_G$ .

$\overline{\Delta} \text{ or } \Delta_G \ (\text{MeV})$	Pairing model	$\Delta_{\mathrm{micr}}$ model	$n_{-}$	$n_+$	$N_{ m data}$	$m^*$ (MeV)	$\sigma_m^*$ (MeV)	$\sigma^* $ (MeV)
$\frac{\overline{\Delta}}{\Delta} = 12.18/\sqrt{A}$ $\overline{\Delta} = rB_{\rm s}e^{-sI-tI^2}/N^{1/3}$	Macro Macro	Macro Macro	356 273	289 365	641 641	-0.0098 $0.0130$	0.0023 0.0024	0.0579 0.0600
$\Delta_G = 12.0/\sqrt{A}$ $\Delta_G = rB_{\rm s}e^{-sI - tI^2}/N^{1/3}$	BCS BCS	MD MD	353 268	283 371	641 641	-0.0036 $0.0311$	0.0039 0.0053	0.0980 0.1333
$\Delta_G = 12.5/\sqrt{A}$ $\Delta_G = rB_{\rm s}e^{-sI - tI^2}/N^{1/3}$	BCS BCS	BCS BCS	314 244	310 362	631 611	0.0011 0.0195	0.0035 0.0035	0.0879 0.0863
$\Delta_G = 9.0/\sqrt{A}$ $\Delta_G = rB_s e^{-sI - tI^2}/N^{1/3}$	LN LN	LN LN	329 231	308 406	641 641	-0.0017 $0.0196$	0.0023 0.0024	0.0586 0.0608

where  $N_{\text{data}}$  is the number of terms in the sums, that is the number of proton-neutron combinations (Z, N) for which we have data points. We use the notation  $m^*$  and  $\sigma^*$  to indicate that these quantities are estimates of the true parameters m and  $\sigma$  of the distribution function (42). Obviously the accuracy in our estimate depends on the number of observations  $N_{\text{data}}$ . In fact  $m^*$  is itself an observation of a random variable, and it is well-known that an estimate of the standard deviation  $\sigma_m$  of this variable is given simply by  $\sigma_m^* = \sigma^*/\sqrt{N_{\text{data}}}$ . It is extremely important to observe that it is  $\sigma_m^*$  rather than  $\sigma^*$  that represents the uncertainty in our estimate of the mean slope m of a segment of the error term D(Z, N). The quantity  $\sigma$ , on the other hand, is the standard deviation of the slope of a single segment  $S_k$  around the average slope value.

# 3.2. PROPERTIES OF PREVIOUS MODELS OF $\Delta_G$ and $\overline{\Delta}$

We now use the methods developed in the last section to study calculated pairing gap trends with neutron excess when previous models for  $\Delta_G$  or  $\overline{\Delta}$  are used. In the latter case it is  $\overline{\Delta}$  that is directly compared to data. In the former case G is determined from  $\Delta_G$  by use of eq. (7) and the theoretical pairing gap is obtained as a solution to the BCS or LN pairing equations. In tables 2 and 3 we summarize the results of this study of the trend with neutron excess of the calculated neutron and proton pairing gaps relative to experimental data. The experimental masses used here and elsewhere are taken from ref.[20]. As is seen in tables 2 and 3 two radically different forms are studied for each of  $\overline{\Delta}$  and  $\Delta_G$ . The parameters used for  $\overline{\Delta}$  in lines 1 and 2 and for  $\Delta_G$  in lines 4, 6, and 8 of

Table 3

Trend with neutron excess of the difference between experimental and calculated proton pairing gaps for different  $\overline{\Delta}$  and  $\Delta_G$ .

$\overline{\Delta} \text{ or } \Delta_G \  ext{(MeV)}$	Pairing model	$\Delta_{\mathrm{micr}}$ model	$n_{-}$	$n_+$	$N_{ m data}$	$m^*$ (MeV)	$\sigma_m^*$ (MeV)	$\sigma^* $ (MeV)
$\frac{\overline{\Delta}}{\overline{\Delta}} = 13.66/\sqrt{A}$ $\overline{\Delta} = rB_{\rm s}e^{+sI-tI^2}/Z^{1/3}$	Macro Macro	Macro Macro	270 213	231 284	502 502	-0.0058 $0.0119$	0.0027 0.0028	0.0606 0.0630
$\Delta_G = 12.0/\sqrt{A}$ $\Delta_G = rB_{\rm s}e^{+sI - tI^2}/Z^{1/3}$	BCS BCS	MD MD	247 204	252 297	502 502	0.0051 $0.0275$	0.0044 $0.0057$	0.0994 $0.1268$
$\Delta_G = 12.5/\sqrt{A}$ $\Delta_G = rB_{\rm s}e^{+sI - tI^2}/Z^{1/3}$	BCS BCS	BCS BCS	222 183	256 305	483 491	0.0124 $0.0280$	0.0047 0.0041	0.1033 0.0913
$\Delta_G = 9.0/\sqrt{A}$ $\Delta_G = rB_s e^{+sI - tI^2}/Z^{1/3}$	LN LN	LN LN	273 215	226 284	502 502	-0.0035 $0.0150$	0.0030 0.0031	0.0666 0.0683

tables 2 and 3 are taken from ref.[17]. The choice on line 3 is the choice made in the mass calculation[10, 11] that we investigate here. The parameters on lines 5 and 7 were chosen by adjusting the parameters to obtain approximate agreement between experimental and calculated pairing gaps for a few actinide nuclei. The aim in this case was to quickly be able to compare the properties of the conventional form of the effective pairing gap to the isospin-dependent form.

Tables 2 and 3 show that the isospin-dependent form[17] results in calculated microscopic-model pairing gaps  $\Delta_{\text{micr}}$  that decrease relative to the experimental data with increasing neutron excess. This result is very clear, since the mean slope  $m^*$  is different from 0 by more than five standard deviations  $\sigma_m^*$ . For the conventional form with  $\Delta_G = \text{constant}/\sqrt{A}$  the result is equally clear that the calculated results follow the experimental trend as the neutron number increases; the estimate  $m^*$  of mean slope m is never different from 0 by more than about one standard deviation, apart from the one exception in line 5 in table 3.

The first two lines of tables 2 and 3 give the results obtained when the expressions in column 1 are compared directly to experimental data. In this case we note that neither the isospin-dependent model nor the conventional model give correct trends with neutron excess. The pairing gap in the isospin-dependent model decreases faster than the experimental pairing gap with neutron excess, whereas the conventional pairing model results in the opposite behaviour. The effect is four standard deviations in three of the four cases and two standard deviations in the remaining case.

The results labelled MD in column 3 of tables 2 and 3 are obtained by using theoretical mass differences to calculate the theoretical pairing gaps. Contributions from the large

errors in the calculated masses in the transition regions is probably the reason that the uncertainty  $\sigma^*$  in the trend is usually larger in this model than in the other models. However, since the quantities we study here are calculated from mass differences, it is not the absolute error in the masses that gives rise to errors in the pairing gaps calculated from theoretical mass differences, but instead is the change in the error between neighbouring nuclei. This change is much smaller than the error in the calculated masses. Specifically, we find that the rms deviation between calculated and experimental pairing gaps corresponding to line 3 in table 2 is 0.247 MeV. Comparing instead the pairing gaps obtained from the BCS calculation with experimental odd-even mass differences, we obtain an rms deviation of 0.224 MeV for the non-optimized parameter value used here.

Summarizing, we find from tables 2 and 3 that the indication of a decrease with isospin of the experimental pairing gaps obtained from odd-even mass differences does not necessarily mean that the effective-interaction pairing gap has an explicit isospin dependence. Instead, it is possible that the decrease seen is the result of microscopic structure effects and does not have to be imposed as an explicit isospin dependence of the effective-interaction pairing gap. The isospin-dependent pairing-gap expression with the parameter set determined earlier[17] seems unsuitable as a model for the effective-interaction pairing gap. Thus, to find the parameters of the effective interaction one cannot simply compare a macroscopic expression to experimental data. Instead, we must perform full microscopic calculations and compare pairing gaps obtained for different microscopic parameter sets to odd-even mass differences.

## 3.3. DETERMINATION OF $\Delta_G$ PARAMETER VALUES

To determine the optimum parameter values of the two forms of the effective-interaction pairing gap  $\Delta_G$  given in eqs. (14) and (19) we solve the microscopic pairing equations for several sets of parameter values and obtain the optimum set by least-squares minimization of the difference between the odd-even mass differences and calculated microscopic pairing gaps. Thus, the expression that is minimized is

$$L = \sqrt{\frac{\sum_{Z,N} [\Delta_{\text{exp}} - \Delta_{\text{th}}(\Delta_G)]^2}{N_{\text{data}}}}$$
(44)

where  $\Delta_{\text{exp}}$  is obtained by use of the appropriate expressions in eqs. (35,36),  $\Delta_{\text{th}}$  is a solution to the BCS or LN pairing equations, and  $\Delta_G$  is given by eq. (14) or eq. (18). The least-squares minimization is carried out over the parameters r and t of eq. (14) or the parameter c of eq. (18).

To determine the optimum parameter set for the average pairing-gap model  $\overline{\Delta}$  the expression for  $\overline{\Delta}$  is directly compared to odd-even mass differences and the parameters of the model are determined by least-squares minimization. Thus, the expression that is minimized in this case is

$$L = \sqrt{\frac{\sum_{Z,N} (\Delta_{\exp} - \overline{\Delta})^2}{N_{\text{data}}}}$$
 (45)

Table 4

Results of least-squares determinations of parameters occurring in  $\overline{\Delta}$  and  $\Delta_G$ .

Relative to the general expressions in eqs. (14,15) we have set s=0, as discussed in the text. In the macroscopic model studies we also set  $B_s=1$ .

$\overline{\Delta}$ or $\Delta_G$	Pairing model	m rms $ m (MeV)$	$c \pmod{\mathrm{MeV}}$	$r \pmod{MeV}$	t	$m^*$ (MeV)	$\begin{array}{c} \sigma_m^* \\ (\text{MeV}) \end{array}$	Nucleon species
$\frac{\overline{\Delta}}{\overline{\Delta}} = c/\sqrt{A}$ $\overline{\Delta} = c/\sqrt{A}$	Macro Macro	0.210 0.174	12.2 13.6	_	_	-0.0097 $-0.0057$	0.0023 0.0027	Neutrons Protons
$ \overline{\Delta} = re^{-tI^2}/N^{1/3} $ $ \overline{\Delta} = re^{-tI^2}/N^{1/3} $	Macro Macro	0.177 0.212	_	5.64 4.75	6.94	0.0099 $-0.0089$	0.0023 0.0023	Neutrons Neutrons
$\frac{\overline{\Delta}}{\Delta} = re^{-tI^2}/Z^{1/3}$ $\overline{\Delta} = re^{-tI^2}/Z^{1/3}$	Macro Macro	0.153 0.181	_	5.46 4.80	5.23	0.0042 $-0.0125$	0.0028 $0.0027$	Protons Protons
$\Delta_G = c/\sqrt{A}$ $\Delta_G = c/\sqrt{A}$	BCS BCS	0.216 $0.248$	12.8 13.4	_	_	0.0066 $0.0132$	0.0034 $0.0045$	Neutrons Protons
$\Delta_G = rB_s e^{-tI^2} / N^{1/3}$ $\Delta_G = rB_s e^{-tI^2} / N^{1/3}$	BCS BCS	0.179 0.179		5.05 4.93	0.89	0.0017 $-0.0004$	0.0032	Neutrons Neutrons
$\Delta_G = rB_s e^{-tI^2} / Z^{1/3}$ $\Delta_G = rB_s e^{-tI^2} / Z^{1/3}$	BCS BCS	0.209 $0.210$	_	4.83 4.67	1.29	0.0095 0.0059	0.0041 0.0042	Protons Protons
$\Delta_G = c/\sqrt{A}$ $\Delta_G = c/\sqrt{A}$	LN LN	$0.201 \\ 0.213$	8.5 9.2	_	_	-0.0019 $-0.0034$	0.0023 $0.0030$	Neutrons Protons
$\Delta_G = rB_{\rm s}e^{-tI^2}/N^{1/3}$ $\Delta_G = rB_{\rm s}e^{-tI^2}/N^{1/3}$ $\Delta_G = rB_{\rm s}e^{-tI^2}/Z^{1/3}$	LN LN LN	0.169 $0.170$ $0.165$		3.47 3.32	1.80 0 3.00	0.0015 $-0.0016$ $-0.0018$	0.0023 0.0023 0.0030	Neutrons Neutrons
$\Delta_G = rB_{\rm s}e^{-tI^2}/Z^{1/3}$ $\Delta_G = rB_{\rm s}e^{-tI^2}/Z^{1/3}$	LN	0.169		3.53 3.28	0	-0.0018 $-0.0078$	0.0030	Protons Protons

where  $\Delta_{\text{exp}}$  is obtained by use of the appropriate expressions in eqs. (35,36) and  $\overline{\Delta}$  is given by eq. (15) or eq. (19). The least-squares minimization is carried out over the parameters r and t of eq. (15) or the parameter c of eq. (19).

To determine the parameters of the residual n-p interaction we minimize

$$L = \sqrt{\frac{\sum_{Z,N} (\delta_{\text{exp}} - \delta)^2}{N_{\text{data}}}}$$
 (46)

where  $\delta_{\text{exp}}$  is obtained by use of the appropriate expressions in eq. (37) and  $\delta$  is given by eq. (17) or eq. (20). The least-squares minimization is carried out over the parameter h of eq. (17) or the parameter d of eq. (20).

Some of the studied L functions are shown in figs. 2–5.

One may optimally reduce the influence of experimental mass uncertainties on the parameter values obtained in least-squares minimization by use of appropriate statistical

Table 5
Results of least-squares determinations of parameters occurring in  $\overline{\Delta}$  and  $\Delta_G$ .
Relative to the general expressions in eqs. (14,15) we have set s=0, as discussed in the text. In the macroscopic model studies we also set  $B_s=1$ .

$\overline{\Delta}$ or $\Delta_G$	Pairing model	$ m rms \ (MeV)$	$c \pmod{\mathrm{(MeV)}}$	$r \pmod{MeV}$	t	$m^*$ (MeV)	$\sigma_m^*$ (MeV)	Nucleon species
$\overline{\Delta} = c/\sqrt{A}$	Macro	0.194	12.6	_	_	-0.0082	0.0022	Neutrons
$\overline{\Delta} = c/\sqrt{A}$	Macro	0.154	14.1			-0.0059	0.0027	Protons
$\overline{\Delta} = r e^{-tI^2} / N^{1/3}$	Macro	0.176		5.73	7.81	0.0111	0.0022	Neutrons
$\overline{\Delta} = r e^{-tI^2} / N^{1/3}$	Macro	0.213		4.73	0	-0.0075	0.0022	Neutrons
$\overline{\Delta} = r e^{-tI^2} / Z^{1/3}$	Macro	0.143		5.61	6.26	0.0058	0.0027	Protons
$\overline{\Delta} = r e^{-tI^2} / Z^{1/3}$	Macro	0.179		4.78	0	-0.0116	0.0027	Protons
$\Delta_G = c/\sqrt{A}$	BCS	0.191	13.3			0.0091	0.0033	Neutrons
$\Delta_G = c/\sqrt{A}$	BCS	0.220	13.9			0.0136	0.0041	Protons
$\Delta_G = rB_{\rm s} \mathrm{e}^{-tI^2}/N^{1/3}$	BCS	0.176		5.55	1.38	0.0040	0.0032	Neutrons
$\Delta_G = rB_{\rm s} \mathrm{e}^{-tI^2}/N^{1/3}$	BCS	0.177		4.93	0	0.0006	0.0032	Neutrons
$\Delta_G = rB_{\rm s} \mathrm{e}^{-tI^2}/Z^{1/3}$	BCS	0.203		4.97	1.99	0.0135	0.0041	Protons
$\Delta_G = rB_{\rm s} \mathrm{e}^{-tI^2} / Z^{1/3}$	BCS	0.205		4.70	0	0.0079	0.0042	Protons
$\Delta_G = c/\sqrt{A}$	LN	0.159	8.6			-0.0018	0.0023	Neutrons
$\Delta_G = c/\sqrt{A}$	LN	0.157	9.9	_		-0.0024	0.0030	Protons
$\Delta_G = rB_{\rm s}\mathrm{e}^{-tI^2}/N^{1/3}$	LN	0.150		3.71	3.02	0.0030	0.0022	Neutrons
$\Delta_G = rB_{\rm s} \mathrm{e}^{-tI^2}/N^{1/3}$	LN	0.153		3.44	0	-0.0014	0.0022	Neutrons
$\Delta_G = rB_{\rm s}e^{-tI^2}/Z^{1/3}$	LN	0.139		3.71	3.45	-0.0003	0.0030	Protons
$\Delta_G = rB_{\rm s} \mathrm{e}^{-tI^2} / Z^{1/3}$	LN	0.145	_	3.39	0	-0.0065	0.0030	Protons

methods. However, an earlier study[17] found an effect of only 0.002% on the r parameter when accounting for experimental mass uncertainties. We can therefore avoid the additional complexity that would arise if experimental mass uncertainties were accounted for. The results of these least-squares minimization are given in table 4. To test the stability of the results with respect to the region of nuclei considered, we have repeated the calculations with light nuclei excluded, taking into account instead only nuclei with N>28. The results from this study are given in table 5.

For the isospin-dependent model we have taken the parameter s=0 in order to limit ourselves to a two-parameter search. There are several justifications for this simplification. First, in the original studies of the isospin-dependent model for  $\overline{\Delta}$ , s was found to be about two orders of magnitude smaller than t, and, in fact, not significantly different from zero. However, since one of the important results of this investigation is that the parameters

obtained for  $\overline{\Delta}$  do not necessarily carry over to the effective-interaction pairing gap  $\Delta_G$ , s could conceivably be significantly different from zero in the model for  $\Delta_G$ . However, the results of our studies in this section will show that in a search for optimum parameters r and t with s=0 we obtain results that are consistent with t=0. This makes it highly plausible that  $s\approx 0$ , since otherwise t would have assumed a value significantly different from zero to simulate the effect of the neglected parameter s. In addition, we will see below that the trend of the pairing gaps with isospin calculated for s=0 and t=0 is usually correct. Thus, the studies below will be a justification, a posteriori, of our initial assumption that  $s\approx 0$ .

In the case of the conventional pairing-gap model  $c/\sqrt{A}$  we solve the pairing equations for 10 different values of the parameter c, in steps of 0.5 MeV. In fig. 2 the least-squares deviations corresponding to lines 1, 7, and 13 in table 4 are plotted as functions of c.

For the isospin-dependent pairing model we solve the pairing equations for 25 different pairs of values for r and t. In the Lipkin-Nogami model, we solve for t = -3 (3) 9 and r = [2.0 + 0.2t + (i-1)/2] MeV, for i = 1 (1) 5. The complicated choice for r is motivated by the fact that r and t are highly correlated. For the BCS and macroscopic models, different grid choices are made to assure that the optimum parameter set is included in the search. In figs. 3–5 the least-squares deviations corresponding to lines 3, 9 and 15 in table 4 are plotted as functions of r and t.

Results obtained by directly comparing the expressions in column 1 to experimental odd-even mass differences are shown in the top six lines of tables 4 and 5. In these macroscopic studies we set  $B_s = 1$ . The remaining 12 lines show the results when the expressions in column 1 are used as models for the effective-interaction pairing gap. In this case it is the pairing gaps obtained as solutions to the BCS and Lipkin-Nogami pairing equations that are compared to experimental odd-even mass differences. We immediately notice that the values obtained for t in the models for t in the first six lines and for t in the last 12 lines are markedly different. In fact, in the microscopic case there is no significant difference in the rms deviation if t is set to zero compared to allowing t to vary. The change in the rms deviation is only 0.5% in three of the four cases and 2% in the remaining case. In contrast, in the macroscopic case we find a change of about 20% in the rms deviation when t is set to zero compared to allowing t to vary.

It is also of interest to observe that in the Lipkin-Nogami model the effective-interaction pairing gap is considerably smaller than in the BCS model, which is a result we anticipated above. The Lipkin-Nogami model gives a lower rms deviation than does the BCS model, with the improvement about 5% for neutrons and 20% for protons. For both models the conventional pairing-gap expression  $c/\sqrt{A}$  results in a 20% higher rms deviation. The derivation[17] of the isospin-dependent model implies that the parameters of the pairing-gap model are the same for neutrons and protons. It was to test this assumption that we carried out the rms minimization separately for neutrons and protons in tables 4 and 5. The results in the tables show that one does obtain very similar values for the parameters of the isospin-dependent model for both neutrons and protons in the macroscopic model and in the Lipkin-Nogami model. In the Lipkin-Nogami model the difference in the values of r obtained for neutrons and protons is only 1%, whereas the difference in the values of the parameters obtained in the isospin-dependent model for neutrons and protons are

Table 6
Final model constants.

Pairing model	rms (MeV)	$r \pmod{MeV}$	t
Macro	0.167	5.55	6.07
Macro	0.198	4.77	
BCS	0.195	4.96	1.23
BCS	0.196	4.80	
LN LN	$0.167 \\ 0.169$	3.50 3.30	2.36

more similar than the parameters in the conventional model.

By comparing tables 4 and 5 we learn about the stability of the results for changes in the parameter-determination procedure. The values of r and c are as much as 3% larger in table 5 than in table 4. Since it can be seen in the figures that the calculated pairing gaps below N=28 are all too high, it is easy to understand the direction of change in the values between tables 4 and 5. For a 1-MeV pairing gap, the difference between using the values in the two tables results in a difference of about 0.03 MeV in the calculated pairing gaps. This is an acceptable stability since the rms deviation between calculated and experimental pairing gaps is about 0.2 MeV.

From tables 4 and 5 we see that in the BCS and Lipkin-Nogami models an effective interaction of the form constant/ $Z^{1/3}$  and constant/ $N^{1/3}$  results in rms deviations that are about 20% lower than the conventional form constant/ $\sqrt{A}$ . Although rms deviation is not the sole criterion for choosing the effective interaction, the difference is sufficiently large that we select the former model as our preferred model. As a final step, we perform for neutrons and protons taken together a least-squares minimization of the deviations between the calculated and experimental pairing gaps in the macroscopic, BCS and Lipkin-Nogami pairing models. The results are given in table 6. In the microscopic models the rms deviations at the true minima are only 1% lower than those at t=0. Therefore, there is little convincing rationale for retaining the full exponential form given in eq. (14). Thus we obtain the following final expressions for the preferred effective-interaction pairing-gap model:

$$\Delta_{G_{\rm n}} = \frac{rB_{\rm s}}{N^{1/3}}$$

$$\Delta_{G_{\rm p}} = \frac{rB_{\rm s}}{Z^{1/3}} \tag{47}$$

where r is given in lines 4 and 6 of table 6. For the residual n-p interaction  $\delta$  we use

$$\delta = \frac{h}{A^{2/3}B_s} \tag{48}$$

The parameter h is determined from a least-squares adjustment to 831 odd-even mass differences of the form given by eq. (37). We obtain

$$h = 6.6 \text{ MeV} \tag{49}$$

with an rms deviation of 0.1597 MeV. The rms deviation is fairly insensitive to the value of h, rising to only 0.1598 MeV for h = 6.5 MeV, for example. In these adjustments we set  $B_{\rm s} = 1$ . For the conventional form of the n-p residual interaction given by eq. (20), we obtain d = 24.4 MeV with an rms deviation of 0.1756 MeV.

By choosing t=0 we seem to obtain a slightly erroneous trend with increasing neutron number for the proton pairing gap in the LN model, as is seen in the last line of table 4. The mean slope is different from zero by about 2.5 standard deviations. However, had we retained the value of t obtained in the least-squares minimization we would have instead obtained an erroneous mean slope of the proton pairing gap in the BCS model. This minor deficiency of the pairing-gap trend with neutron excess is the only deficiency in the trend with neutron excess that remains in the final BCS and Lipkin-Nogami models. Figures 7 and 9 show that the trend with neutron excess of the proton pairing gap is highly correlated within localized regions of nuclei and that it depends on whether the BCS or Lipkin-Nogami model is used. The result that our final effective-interaction pairing-gap model yields a slightly erroneous trend with neutron excess for the proton pairing gap calculated in the Lipkin-Nogami model may therefore be an accident due to these large-scale correlations and not indicate a true error in the trend with neutron excess.

#### 3.4. GRAPHICAL PRESENTATION OF RESULTS

In figs. 6–9 we compare pairing gaps calculated with our final form of  $\Delta_G$  to experimental odd-even mass differences. In the BCS model we observe a few collapsed cases corresponding to non-magic numbers. The large deviations at neutron number  $N\approx 90$  in figs. 6 and 8 are due to contributions from  $\delta$  obtained from experimental masses and are probably caused by a single, poorly determined experimental mass. Some of the fluctuations in the discrepancy for the neutron pairing gaps are located at neutron numbers with special significance. For example, there are large deviations at N=56, which is a significant spherical sub-shell. Other fluctuations occur at  $N\approx 132$ , where there is a significant effect on the nuclear mass surface due to mass-asymmetric octupole deformations, and in the region between N=142 and N=152, where there are large gaps in the deformed actinide single-particle spectra. These fluctuations in the experimental odd-even mass differences may therefore partly have origins other than pairing effects.

In the Lipkin-Nogami model it is, as pointed out in sect. 2.2, the sum  $\Delta + \lambda_2$  that should be compared to the odd-even mass differences. Figures 10 and 11 show the individual quantities  $\Delta$  and  $\lambda_2$  for neutrons and protons, respectively. For consistency, these figures

are plotted using the identical nuclei as in figs. 6–9, even though the quantities in figs. 10 and 11 are defined also at magic numbers. One observes that as  $\Delta$  decreases towards magic numbers, there is an increase of  $\lambda_2$ , so that the sum of these two quantities shows fairly small irregularities at the magic numbers.

To further interpret our results and relate them to earlier investigations, we plot  $\ln(\Delta_n N^{1/3}/\text{MeV})$  versus relative neutron excess for experimental odd-even mass differences and for our final model in figs. 12 and 13, respectively. Figure 12 corresponds to fig. 11 of ref.[17], with some minor differences. First, we use a more recent experimental mass table here. Second, we plot the pairing gaps also for the cases in which  $\delta$  enters in the mass-difference expressions, which approximately doubles the number of nuclei included in the figure. Finally, we use different symbols to distinguish between the light region with N < 82 and the heavy region with N > 82. The figures show that there is very little overlap between these two regions. The calculated pairing gaps in fig. 13 show a clear trend with isospin, even though the effective-interaction pairing gap has no explicit isospin dependence. Although the trend with isospin seems much stronger in the experimental data in fig. 12, the difference is somewhat illusory.

The experimental neutron gaps shown in, for example, the top part of fig. 8 dip down to about 0.55 MeV in the actinide region. In the absence of a dip the experimental pairing gaps would be about 0.75 MeV here, if they were following the general trend over a larger region. Lowering a pairing gap from 0.75 to 0.55 MeV lowers a circle from 1.35 to 1.05 in fig. 12. In fact, about half of the circles below 1.35 in fig. 12 correspond to actinide nuclei, and the other points below 1.35 correspond to other dips in the plots of the experimental neutron pairing gaps, for instance the dip in the rare-earth region around N = 100. Out of the 45 nuclei with N < 82 that are located below 1.35, 39 are located in a single, connected region defined by  $52 \le N \le 59$  and  $35 \le Z \le 41$ . The logarithmic nature of the plot and the multiplication by  $N^{1/3}$  has the effect of magnifying small dips in the pairing-gap curve, particularly at large N. Thus, the apparent strong dependence of the neutron pairing gap in this plot is due partly to the magnification of small irregularities in the odd-even mass differences that may be related to difficulties in extracting the true pairing gap from the experimental masses, when the mass-difference expressions span nuclear sub-shells or a transition region. The remaining dependence, as seen in fig. 13, is well described by microscopic calculations with an isospin-independent effective-interaction pairing gap.

In sect. 3.1 we introduced a method for studying the trend of the deviation between calculated and experimental pairing gaps with increasing neutron excess in terms of the slope  $S_k$  of the error term, which was assumed to follow a normal distribution. We are now in a position to study the distributions of  $S_k$  and we show two cases. In fig. 14 we show the distribution of  $S_k$  corresponding to line 8 in table 2, and in fig. 15 we show the distribution corresponding to line 6 in table 6. The solid lines show the Gaussians that are obtained for the parameters given by eq. (43) when all data points are used in the calculations, including even points outside the figure areas. For fig. 14 the parameters  $\sigma^*$  and  $m^*$  of the solid Gaussian are given on line 8 of table 2. The arrow in each figure gives the location of the mean of the data points and the solid Gaussian. The significance of the values obtained for  $m^*$  has been discussed in detail above; here we only address the shape of the distribution. Clearly the Gaussian approximations given by the solid

lines in figs. 14 and 15 seem too wide relative to the distribution of the points. One may suspect that this results from a few points with very large values of the slope  $S_k$  that do not follow a normal distribution. One could perform an analysis with the assumption that the distribution is the sum of a normal distribution and a small contribution from a rectangular distribution. The latter distribution would account for the few points that are randomly scattered from about  $S_k = -1$  to  $S_k = +1$ . We have not performed a detailed analysis according to this assumption, but have instead determined the Gaussians given by the dashed lines using only points in the interval  $|S_k - m^*| < 3\sigma^*$ . From figs. 14 and 15 it is clear that the points follow the dashed Gaussians extremely well, scattering around these lines with roughly the expected amplitude of the square root of the frequency.

### 4. Summary and Conclusions

We have pointed out that a meaningful discussion of nuclear pairing gaps must distinguish between two pairing-gap concepts. One concept is the average pairing gap  $\overline{\Delta}$ , which is a macroscopic model, given by a simple analytical expression that is directly compared to the experimentally *observed* pairing gap, determined from odd-even mass differences. In this model the underlying assumption is that the observed pairing gap can be described in its average properties by such a simple model. This model is often used in macroscopic liquid-drop models.

However, just as nuclear masses exhibit correlated structures over large regions that have to be described by going beyond the liquid-drop model to microscopic theories, the pairing gap is also affected by similar large-scale correlations. To analyze the detailed structure of the experimental pairing gaps one should therefore compare them to pairing gaps obtained from microscopic calculations. In the models studied here such calculations require as a parameter the pairing matrix element G. This parameter can be determined in any region of nuclei from the second pairing-gap concept, the effective-interaction pairing gap  $\Delta_G$ . By solving the microscopic pairing equations for more than 1400 nuclear ground states for sufficiently many effective-interaction pairing-gap parameter sets to perform least-squares minimization, we have determined a preferred form for the effective-interaction pairing gap and values of its parameters for both the BCS and Lipkin-Nogami pairing models. Our final effective-interaction pairing-gap model is a simple, one-parameter expression with no explicit dependence on neutron excess. To provide the complete pairing-model framework necessary for nuclear mass calculations, we have also derived the average pairing-energy expressions that are required.

There are remaining discrepancies between the microscopically calculated pairing gaps and the odd-even mass differences. From our extensive investigation here we conclude that it is probably not possible to substantially decrease these remaining differences through an improved effective-interaction pairing-gap model. We have observed above that the odd-even mass differences may contain non-smooth effects in addition to those arising from pairing gaps, such as contributions from deformation changes and spherical and deformed sub-shells. For further work to be meaningful one should compare experimental odd-even mass differences to the corresponding calculated mass differences. This requires some improvement of the mass models in the transitional regions. One must also consider

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going beyond the simple approximation of a constant pairing matrix element to a more realistic pairing force. It was our aim here to provide a firm basis and starting point for such further work by exhaustively exploring some currently used pairing models to find the limits of their applicability. Simultaneously, our study also provides current users of these models with optimized parameter sets and the expressions required for the pairing part of potential-energy calculations.

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## Appendix A

In this appendix we list the most common symbols used, with references to the equations where the symbols are introduced and used. For each symbol a short discussion of the symbol and its relation to other symbols is also given. As a general rule we put the symbol  $\tilde{\ }$  above quantities that are obtained by averaging over a single-particle spectrum in the Strutinsky sense, and  $\bar{\ }$  over symbols that model average behaviour over Z and N.

	, , , , , , , , , , , , , , , , , , ,
$\overline{\Delta}$	Name:
	Obtained from equations:
	Used in equations:
	Comments:
$\Delta_G$	Name: Effective-interaction pairing gap.
	Obtained from equations:
	Used in equations:
	Comments:
Δ	Name: Microscopic pairing gap.
	Obtained from equations: $$
	Used in equations:
	Comments: Determined from microscopic BCS or LN models. This is a calculated quantity that is obtained by solving microscopic BCS or Lipkin-Nogami pairing equations. The value obtained depends on the expression used for $\Delta_G$ and on the calculated single-particle levels $e_k$ . Gaps

in the single-particle spectrum lead in general to lower-than-average values.

 $\Delta_n^{\rm even-even}$ 

In our investigation here we minimize the least-squares deviation between the calculated microscopic pairing gap and the finite-difference pairing gap discussed in the next item, by varying the parameters in the expression for the effective-interaction pairing gap  $\Delta_G$ . In this way the optimum parameters of the expression for  $\Delta_G$  are determined.

Name: ..... Finite-difference pairing gap.

	Obtained from equations:
	Used in equations:
	Comments:
G	Name:
	Obtained from equation:
	Used in equations:
	Comments: Obtained from expression for $\Delta_G$ . The parameter $G$ enters directly in the BCS and Lipkin-Nogami pairing equations. By determining $G$ from the primary parameter $\Delta_G$ we obtain a primary model parameter that is insensitive to the exact details of the calculations and varies smoothly over the periodic system.
δ	Name:
	Obtained from equations:
	Used in equation:
	Comments:Macroscopic model for residual n-p interaction.

	scopic models and the microscopic BCS and Lipkin-Nogami models. In contrast, for the much smaller neutron-proton interaction $\delta$ , we use only a macroscopic approach.
$\delta^{\mathrm{even-even}}$	Name: Finite-difference residual n-p interaction energy.
	Obtained from equation:
	Used in equation:
	<b>Comments:</b> Residual n-p energy obtained from experimental masses. Our discussion here refers to any one of the expressions in eq. (37). The comments made above for $\Delta_n^{\text{even-even}}$ apply here also.
$\lambda$	Name: Pairing-model Fermi energy.
	Obtained from equations:1-3,6-11
	Used in equations:
	Comments:
$\widetilde{\lambda}$	Name: Fermi energy of smoothed single-particle levels.
	Obtained from: Strutinsky shell-correction method.
	Used in equation:
	Comments:
$\lambda_2$	Name:
	Obtained from equations:6–11
	Used in equations:
	Comments:
$\widetilde{\lambda}_2$	Name: Number-fluctuation constant of smoothed single-particle levels.
	Obtained from equation:

For the neutron and proton pairing gaps we study in this paper macro-

	Used in equation:
	Comments:
$e_k$	Name: Single-particle energy.
	Obtained from:
	Used in equations:
	Comments:
$\epsilon_k$	Name:Lipkin-Nogami shifted single-particle energy.
	Obtained from equations:6–11
	<b>Used in equations:</b>
	Comments:
$E_k$	Name:Quasi-particle energy.
	Obtained from equations:
	Used in equations:
	Comments:
$E_{ m pc}$	Name: Pairing correlation plus quasi-particle energy.
	Obtained from equations:
	<b>Used in:</b> Calculation of the nuclear potential energy of deformation.
	<b>Comments:</b>
$\widetilde{E}_{ m pc}$	Name: Average pairing correlation plus quasi-particle energy.

**Used in:** .....Calculation of the nuclear potential energy of deformation.

## Appendix B

The following integrals appear in the expressions for the effective-interaction pairing model:

$$\int \frac{dx}{\sqrt{x^2 + \Delta^2}} = \ln\left(\sqrt{x^2 + \Delta^2} + x\right)$$

$$\int \frac{xdx}{\sqrt{x^2 + \Delta^2}} = \sqrt{x^2 + \Delta^2}$$

$$\int \frac{x^2 dx}{\sqrt{x^2 + \Delta^2}} = \frac{x\sqrt{x^2 + \Delta^2}}{2} - \frac{\Delta^2}{2} \ln\left(\sqrt{x^2 + \Delta^2} + x\right)$$

$$\int \frac{dx}{x^2 + \Delta^2} = \frac{1}{\Delta} \tan^{-1}\left(\frac{x}{\Delta}\right)$$

$$\int \frac{x dx}{x^2 + \Delta^2} = \frac{1}{2} \ln\left(x^2 + \Delta^2\right)$$

$$\int \frac{x^2 dx}{x^2 + \Delta^2} = x - \Delta \tan^{-1}\left(\frac{x}{\Delta}\right)$$

$$\int \frac{dx}{(x^2 + \Delta^2)^2} = \frac{1}{2\Delta^2} \frac{x}{x^2 + \Delta^2} + \frac{1}{2\Delta^3} \tan^{-1}\left(\frac{x}{\Delta}\right)$$
(50)

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## Figure Captions

- Fig. 1. Difference between pairing gaps obtained from odd-even mass differences and pairing gaps calculated in the BCS approximation, with parameters corresponding to line 6 of table 2. The figure also shows definitions of variables that are subject to statistical analysis in the text. The function S(Z, N) is the change in the value of the difference when going from (Z, N-1) to (Z, N),  $n_+$  is a counter for the number of upward-sloping segments and  $n_-$  a counter for the number of downward sloping segments.
- Fig. 2. Root-mean-square deviations between experimental pairing gaps obtained from eq. (35) and calculated pairing gaps. For the macroscopic model the calculated pairing gap is simply  $\Delta_{\rm th} = \overline{\Delta} = c/A^{1/2}$ . For the other two curves  $\Delta_{\rm th}$  is obtained by solving the BCS and LN pairing equations. These have been solved for a set of pairing strength parameters G that were in turn obtained from  $\Delta_G = c/A^{1/2}$ , for 10 different values of c, by use of eq. (24). The similarities between the dashed and dot-dashed curves provide an explanation of why earlier no distinction was made between the two concepts  $\overline{\Delta}$  and  $\Delta_G$ . A comparison of figs. 3 and 4 below show that when  $\overline{\Delta}$  and  $\Delta_G$  are of another functional form, one obtains quite different results in the corresponding cases.
- Fig. 3. Root-mean-square deviations between experimental pairing gaps obtained from eq. (35) and pairing gaps given by the macroscopic model  $\Delta_{\text{macr}} = \overline{\Delta}$ , with  $\overline{\Delta}$  given by the expression on line 3 of table 4. The values given on this line for the two parameters r and t are determined from this figure.
- Fig. 4. Root-mean-square deviations between experimental pairing gaps obtained from eq. (35) and pairing gaps calculated in the BCS model. The pairing gap parameter G is determined from  $\Delta_G$  by use of eq. (24) with  $\Delta_G$  in turn given by the expression on line 9 of table 4. The values of the two parameters r and t determined from this figure are fairly different from those obtained in the macroscopic study. Observe the difference between the x and y axes here and in fig. 3. The scales of the graphs are identical but the locations in r-t space of the windows through which we look at the contour surfaces are different.
- Fig. 5. Root-mean-square deviations between experimental pairing gaps obtained from eq. (35) and pairing gaps calculated in the LN model. The pairing gap parameter G is determined from  $\Delta_G$  by use of eq. (24) with  $\Delta_G$  in turn given by the expression on line 15 of table 4. The values of the two parameters r and t determined from this study are quite different from those obtained in figs. 3 and 4. Observe the difference between the x and y axes here and in figs. 3 and 4. The scales of the graphs are identical but the locations in r-t space of the windows through which we look at the contour surfaces are different.

- Fig. 6. Comparison of experimental neutron pairing gaps determined from odd-even mass differences with results calculated in a BCS model. The lines connecting nuclei with the same proton number are broken at neutron numbers where experimental gaps cannot be extracted. It is clear that the BCS method sometimes collapses also away from magic numbers. Note the particularly large deviations in the  $N\approx 56$  region and compare with the results from the Lipkin-Nogami model in fig. 8.
- Fig. 7. Comparison of experimental proton pairing gaps determined from odd-even mass differences with results calculated in a BCS model. The lines connecting nuclei with the same neutron number are broken at proton numbers where experimental gaps cannot be extracted. Note the particularly large deviations in the  $Z\approx 50$  region and compare with the results from the Lipkin-Nogami model in fig. 9.
- Fig. 8. Comparison of experimental neutron pairing gaps determined from oddeven mass differences with results calculated in the Lipkin-Nogami model. The lines connecting nuclei with the same proton number are broken at neutron numbers where experimental gaps cannot be extracted. Note the particularly large deviations in the  $N \approx 56$  region and compare with the results from the BCS model in fig. 6.
- Fig. 9. Comparison of experimental proton pairing gaps determined from odd-even mass differences with results calculated in the Lipkin-Nogami model. The lines connecting nuclei with the same neutron number are broken at proton numbers where experimental gaps cannot be extracted. Compare the deviations in the  $Z\approx 50$  region with those calculated from the BCS model in fig. 7.
- Fig. 10. Relative importance of the pairing gap  $\Delta_n$  and number-fluctuation constant  $\lambda_{2n}$  in the Lipkin-Nogami model, for neutrons. Close to magic numbers where  $\Delta_n$  decreases,  $\lambda_{2n}$  increases. It is the sum  $\Delta_n + \lambda_{2n}$  that should be compared to odd-even mass differences.
- Fig. 11. Relative importance of the pairing gap  $\Delta_{\rm p}$  and number-fluctuation constant  $\lambda_{\rm 2p}$  in the Lipkin-Nogami model, for protons. Close to magic numbers where  $\Delta_{\rm p}$  decreases,  $\lambda_{\rm 2p}$  increases. It is the sum  $\Delta_{\rm p} + \lambda_{\rm 2p}$  that should be compared to odd-even mass differences.
- Fig. 12. Dependence of the quantity  $\ln(\Delta_n N^{1/3}/\text{MeV})$  upon relative neutron excess. The experimental neutron pairing gaps are determined from odd-even mass differences. This figure is similar to fig. 11 of ref.[17], but we use a more recent experimental mass table here and also include neutron pairing gaps for odd-proton nuclei. The data seem to indicate an isospin dependence of the neutron pairing gap, and similar data were used in ref.[17] to determine values of the parameters s and t in eq. (15).

- Fig. 13. Similar to fig. 12, but with neutron pairing gaps calculated in the Lipkin-Nogami model. There is a decrease of the plotted quantity with increasing isospin, even though the effective-interaction pairing gap does not depend explicitly on the relative neutron excess.
- Fig. 14. Distribution of the slopes S(Z, N) for neutron pairing gaps calculated with the pairing-gap model of ref.[17], corresponding to line 8 of table 2. The filled circles show the actual distribution of S(Z, N), whereas the solid curve is the Gaussian that is obtained from a maximum-likelihood estimate, and the dashed curve is an estimate with distant data points discarded. The arrow gives the location of the mean of the complete distribution.
- Fig. 15. Distribution of the slopes S(Z, N) for neutron pairing gaps calculated with the final pairing-gap model derived in this paper, corresponding to line 6 of table 6. The filled circles show the actual distribution of S(Z, N), whereas the solid curve is the Gaussian that is obtained from a maximum-likelihood estimate, and the dashed curve is an estimate with distant data points discarded. The arrow gives the location of the mean of the complete distribution.