ANISOTROPIC HARMONIC OSCILLATOR WAVE FUNCTIONS

THE USE OF ANISOTROPIC HARMONIC OSCILLATOR WAVE FUNCTIONS IN A CYLINDRICAL REPRESENTATION FOR SPECTROSCOPIC CALCULATIONS

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SCOPE AND CONTENTS:

This work is concerned with the derivation of general analytical formulae for the matrix elements, in an M representation, of an effective two-nucleon interaction. The anisotropic harmonic oscillator wave equation is solved in cylindrical coordinates and the subsequent wave functions used to find the desired matrix element expressions. Since these expressions are in a form conducive to rapid machine computation this representation is well suited for spectroscopic calculations for deformed nuclei. This is illustrated by the calculation of the relative binding energies, by means of a limited Hartree-Fock method, of several nucleonic configurations in the 2s-1d shell.

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CHAPTER 1: INTRODUCTION

In nuclear spectroscopy it is always necessary to assume a particular form for the wavefunction which is to represent the motion of a single nucleon in the nucleus. Since the inception of the shell model in 1949, extensive use has been made of harmonic oscillator orbitals, including the spheroidal harmonic oscillator orbitals of Nilsson (N55).

The original reason for the popularity of such orbitals is that the analytic properties of these functions add a good deal of simplification to shell-model calculations as well as the fact that they reproduce level ordering with a reasonable degree of faithfulness.

An attempt to add a more formal justification to the weight of a decade of reasonably successful use led Newton (NE59) to examine the consistency of an oscillator potential by means of a Hartree-Fock calculation. Newton found that the oscillator wave functions are, in fact, close to being self-consistent. In addition, he found that the bound state eigen functions and eigen values of a "cut-off" oscillator well, (which is the physically more realistic case), differ negligibly from the corresponding states of an infinite oscillator well.

Further justification was added by Brueckner, Lockett and Rotenberg (BL61), who, in an investigation of the actual average potential seen by a nucleon in a light nucleus, by more fundamental techniques, found that the single particle orbitals they subsequently derived were very similar to those of the oscillator.

Although a still better single particle potential, (in the sense of being more realistic), has been found to be the Woods-Saxon potential, the much greater computational ease inherent with the use of oscillator functions, along with the above formal justification, has ruled in their favour[1].

It has also become more certain, since 1955, that some nuclei are best described by deformed, (in particular, spheroidal), single particle potentials, rather than spherically symmetric potentials. Although originally applied mainly to those regions of the nuclide chart where the nuclei show obvious deformation, more recent investigations have included light nuclei as well. Volkov (V64 and V65) and Volkov and Hughes (VH65) have performed extensive calculations for p-shell nuclei using the single particle wave functions

$$\Psi_s = C_s \exp\left(-a\,(x^2 + y^2)/2 - bz^2/2\right)$$

$$\Psi_o = C_o\, b_o z \exp\left(-a_o\,(x^2+y^2)/2 - b_o z^2/2\right)$$

$$\Psi_{\pm 1} = C_{\pm 1}\, a_1\,(x \pm iy) \exp\left(-a_1(x^2+y^2)/2 - b_1\, z^2/2\right)$$

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1 For light nuclei, Woods-Saxon and oscillator levels are very similar - see G. E. Brown - Unified Theory of Nuclear Models Chapter 3.

where each orbital has its own set of oscillator constants[2]. The "a" and "b" constants are related by a deformation-dependent factor. These calculations have shown that most 1p nuclei are, in fact, deformed and that the degree of deformation is a sensitive function of the two-nucleon interaction, in particular, of the amount of Majorana exchange included in the interaction.

These results have accentuated the importance of the deformed single particle potential and the necessity of extending these calculations to the 2s-1d shell. However, this extension is computationally difficult due partly to the fact that the wave functions used are not true harmonic oscillator functions for the $2s_o$ and $1d_o$ orbitals and so matrix elements must be worked out, laboriously, by hand in a Cartesian basis.

The present thesis describes a new approach in which the harmonic oscillator equation is solved in a cylindrical representation to provide single particle wave functions. These wave functions have the virtue that (a) they naturally preserve the cylindrical symmetry of the problem, (maintaining M as a good quantum number, where M is the projection of the total angular momentum, J, or the space-fixed z-axis), (b) they are expressible in terms of simple products of functions which form complete sets, thus permitting the simple derivation of general expressions for matrix elements as functions of the single-particle quantum numbers and oscillator constants, and

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2 The significance of having different oscillator constants, $a \neq a_o \neq a_1$, will be explained at a later point in the thesis.

(c), this derivation can be performed without a separation into centre of mass and relative coordinates so that one need not maintain the same oscillator constant for all single-particle orbitals.

These general expressions have been derived for a nuclear interaction with a Gaussian radial dependence and then used in an intermediate coupling calculation, with no configuration mixing, of relative binding energies in the 2s-1d shell. Since J is not a good quantum number, the term "intermediate coupling" is used in the sense that the calculation yields the result of such coupling in the limit of zero deformation. As described in (V65) this is done by the use of Slater determinants characterized by the total M value of the system.

The calculation shows the variation of the binding energies of possible configurations, for given A and Z, with deformation in a "Nilsson-like" manner.

Ideally, one would like to perform these calculations for the whole 2s-1d shell. However, certain obvious time limitations have permitted the extension of this work only to the first few nuclei of the shell.

CHAPTER 2: THE DERIVATION OF THE WAVE FUNCTIONS

In cylindrical coordinates ∇^2 has the form,

$$\nabla^2 \equiv \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2}$$

Thus, the wave equation for the three-dimensional harmonic oscillator is

$$\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial \Psi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \Psi}{\partial \varphi^2} + (\lambda - \alpha^2 \rho^2 - \alpha_z^2 z^2) \Psi = 0 \qquad (2\text{-}1)$$

where $\lambda = \frac{8\pi^2 m}{h^2} E, \quad \alpha = \frac{4\pi^2 m}{h} \nu_o$

and $\alpha_z = \frac{4\pi^2 m}{h} \nu_z$

In these definitions, E is the energy eigen value and ν_o and ν_z are the oscillator frequencies.

The wave functions we seek are the solutions of Equation (2-1) and can be obtained by the usual method of separation of variables, i.e., by setting $\Psi = P(\rho) \cdot \Phi(\varphi) \cdot Z(z)$

On substitution into (2-1) this yields the three separate equations,

$$\frac{d^2 Z}{dz^2} + (\lambda_z - \alpha_z^2 z^2) Z = 0 \qquad (2\text{-}2)$$

$$\frac{d^2\Phi}{d\varphi^2} + m^2\Phi = 0 \qquad (2\text{-}3)$$

and

$$\frac{1}{\rho}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \left(\lambda' - \alpha^2\rho^2 - \frac{m^2}{\rho^2}\right)P = 0 \qquad (2\text{-}4)$$

where $\lambda' + \lambda_z = \lambda$.

The solutions of (2-2) and (2-3) are well-known and are $Z_{n_z} = N_{n_z}\, e^{-\frac{\alpha_z z^2}{2}}\, H_{n_z}(\sqrt{\alpha_z}\, z)$ and $\Phi(\varphi) = \frac{1}{\sqrt{2\pi}}\, e^{im\varphi}$ respectively, where $H_n(x)$ is a Hermite polynomial.

The solution of (2-4) is not as well-known but works out quite easily, as is shown in Appendix A, to be

$$P(\rho) = e^{-\frac{\alpha}{2}\rho^2}\, (\sqrt{\alpha}\,\rho)^{|m|} \cdot L^{|m|}_{\frac{n}{2}}(\alpha\rho^2)$$

where $n = \frac{\lambda'}{2} - |m| - 1$ and $L^k_p(x)$ is the associated Laguerre polynomial defined by

$$^{3}L^k_p(x) = \sum_{s=0}^{p} \frac{(-1)^s \left[(p+k)!\right]^2 x^s}{(p-s)!\ (k+s)!\ s!}$$

Our wave function thus becomes

$$\Psi_{n,m,n_z} = N e^{im\varphi}\, e^{-\frac{\alpha}{2}\rho^2} (\sqrt{\alpha}\,\rho)^{|m|} L^{|m|}_{\frac{n}{2}}(\alpha\rho^2)\, e^{-\frac{\alpha_z z^2}{2}}\, H_{n_z}(\sqrt{\alpha_z}\, z) \qquad (2\text{-}5)$$

3 There exists an alternative definition for $L^k_p(z)$ which is $\sum_{n=0}^{p} \binom{p+k}{p-n} \frac{(-z)^n}{n!}$. Since this function is used in another context in Appendix B we adopt the convention of denoting it by $\mathcal{L}^k_p(z)$.

where the normalization constant N is given by

$$N = \frac{1}{\sqrt{2\pi}} \left(\frac{2\alpha\left(\frac{n}{2}\right)!}{\left[\left(|m| + \frac{n}{2}\right)!\right]^3} \right)^{1/2} \left(\frac{\alpha_z^{1/2}}{\pi^{1/2}\, 2^{n_z}\, n_z!} \right)^{1/2}$$

The quantum numbers, m, n and n_z are restricted as follows:

$$m = 0, \pm 1, \pm 2, \ldots$$

$$n = 0, 2, 4, 6, \ldots$$

$$n_z = 0, 1, 2, \ldots$$

In addition, the energy eigen values are given by

$$E_{m,n,n_z} = (|m| + n + 1)\, h\nu_o + \left(n_z + \frac{1}{2}\right) h\,\nu_z$$

The explicit "2s-1d" wave functions used in this work are:

$$\Psi_{2,0,0} = N_{2s}'\, e^{-\frac{\alpha_s}{2}\rho^2} (1 - \alpha_s \rho^2)\, e^{-\frac{b_s}{2} z^2} \quad -(2s_o') \qquad (2\text{-}6)$$

$$\Psi_{0,0,2} = N_{d_o}'\, e^{-\frac{\alpha_o}{2}\rho^2}\, e^{-\frac{b_o}{2} z^2} (4b_o z^2 - 2) \quad (1d_o') \qquad (2\text{-}7)$$

$$\Psi_{0,\pm 1,1} = N_{d\pm 1}\, e^{\pm i\varphi} (\sqrt{\alpha_{\pm 1}}\, \rho)\, e^{-\frac{\alpha_{\pm 1}}{2}\rho^2}\, e^{-\frac{b_{\pm 1}}{2} z^2} \cdot 2\, b_{\pm 1}\, z \quad (1d\pm 1) \qquad (2\text{-}8)$$

$$\Psi_{0,\pm 2,0} = 2 \cdot N_{d\pm 2}\, e^{\pm 2i\varphi} (\alpha_{\pm 2}\, \rho^2)\, e^{-\frac{\alpha_{\pm 2}}{2}\rho^2}\, e^{-\frac{b_{\pm 2}}{2} z^2} \quad (1d\pm 2) \qquad (2\text{-}9)$$

The symbols $1d_o'$ and $2s_o'$ indicate that these wave functions, at zero deformation, are not true d_o and s_o orbitals. However, they closely approximate the true functions and, if necessary, can be related to them by simple linear transformations. For example, the $1d_o$ orbital, in the spherical representation, is given by

$$\Psi_{1d_o} = \frac{1}{\sqrt{3}} \left(\sqrt{2} \; \Psi_{0,0,2} + \Psi_{2,0,0} \right) \qquad (2\text{-}10)$$

in the limit of zero deformation.

CHAPTER 3: CALCULATION OF MATRIX ELEMENTS

The interaction that concerns us most has the form

$$G = \sum_{i<j}' g(i,j)$$

where the g(i,j) have a Gaussian radial dependence

$$g_r(i,j) = e^{-\frac{k^2}{2}(r_i - r_j)^2}.$$

The matrix elements of this interaction which must be calculated can be written $\langle\Psi(N)/G/\Psi(M)\rangle$ where $\Psi(N)$ is a (Slater) determinantal wave function given explicitly by

$$\Psi(N) = (A!)^{\frac{1}{2}} \begin{vmatrix} \phi_{n_1}(1) & \phi_{n_2}(1) & \ldots & \phi_{n_A}(1) \\ \phi_{n_1}(2) & \phi_{n_2}(2) & \ldots & \phi_{n_A}(2) \\ \cdots & \cdots & \cdots & \cdots \\ \phi_{n_1}(A) & \ldots & & \phi_{n_A}(A) \end{vmatrix}$$

In our particular case $\phi_{n_i}(j)$ is the product of the single particle wave function (2-5) with a spin and an i-spin function, evaluated at the position of the jth particle with the quantum numbers (along with spin and i-spin) of the ith particle.

In the applications of this representation to actual nuclei a restriction to the case in which there is no configuration mixing has been imposed. This restriction considerably simplifies the present mathematics since we need consider only the diagonal elements $\langle\Psi(N)/G/\Psi(N)\rangle$ which are easily shown to be of the form (T64).

$$\langle\Psi(N)/G/\Psi(N)\rangle = \sum_{k>t} \langle\phi_{n_k}(1)\,\phi_{n_t}(2)\,|\,g\,(1,2)\,|\,\phi_{n_k}(1)\,\phi_{n_t}(2)\rangle$$

$$-\langle\phi_{n_k}(1)\,\phi_{n_t}(2)\,|\,g(1,2)\,|\,\phi_{n_t}(1)\,\phi_{n_k}(2)\rangle \qquad (3\text{-}1)$$

Explicit calculations are then required only for the simple direct and exchange elements shown in equation (3-1).

The spin-and i-spin-dependent parts of $g(i,j)$ are separable from the r-dependent part. In addition, the spin-and i-spin dependent parts of the matrix elements are easily worked out for all typical interactions. This leaves us then with just the two integrals

$$\langle\phi_{n_k}(1)\,\phi_{n_t}(2)\,|\,g_r(1,2)\,|\,\phi_{n_k}(1)\,\phi_{n_t}(2)\rangle = \iint\cdots\int \phi^{*(1)}_{n_1,n_{z_1},m_1}$$

$$\phi^{*(2)}_{n_2,n_{z_2},m_2}\; e^{-\frac{k^2}{2}\left[(\vec{\rho}_1-\vec{\rho}_2)^2-(z_1-z_2)^2\right]}\;\phi^{(1)}_{n_1,n_z,m_1}\;\phi^{(2)}_{n_2,n_{z_2},m_z}$$

$$\cdot\,\rho_1\,d\rho_1\,\rho_2\,d\rho_2\,d\phi_1\,d\phi_2\,dz_1\,dz_2 \qquad (3\text{-}2)$$

and

$$\langle \phi_{n_k}(1)\, \phi_{n_t}(2) / g_r(1,2) / \phi_{n_t}(1)\, \phi_{n_k}(2) \rangle =$$

$$\iint \cdots \int \phi^*_{n_1, n^{(1)}_{z_1}, m_1}\ \phi^*_{n_2, n^{(2)}_{z_2}, m_2}\ e^{-\frac{k^2}{2}(\vec{\rho}_1 - \vec{\rho}_2)^2 - \frac{k^2}{2}(z_1 - z_2)^2}\ \phi_{n_2, n^{(1)}_{z_2}, m_2}$$

$$\cdot\ \phi_{n_1, n^{(2)}_{z_1}, m_1}\ \rho_1\, d\rho_1\, \rho_2\, d\phi_1\, d\phi_2\, dz_1\, dz_2 \qquad (3\text{-}3)$$

to calculate.

These integrals are most easily worked out by separating them into products of a (ρ, ϕ)-integration and a z-integration and performing these integrations individually. This is worked out in detail in Appendices B and C. Thus, from equations (B-8), (B-16) and (B-26) we find that the solutions of (3-2) and (3-3) are

$$\langle \phi_{n_k}(1)\, \phi_{n_t}(2) \,|\, g_r(1,2) \,|\, \phi_{n_k}(1)\, \phi_{n_t}(2) \rangle$$

$$= (\sqrt{a})^{2|m_1|+2}\ (\sqrt{b})^{2|m_2|+2} \cdot \left(\frac{n_1}{2}\right)!\ \left(\frac{n_2}{2}\right)!\ \left(|m_1| + \frac{n_1}{2}\right)!$$

$$\cdot \left(|m_2| + \frac{n_2}{2}\right)!\quad 2 \cdot n_{z_1}!\ n_{z_2}!\ \left(\frac{a_z \cdot b_z}{\alpha}\right)^{\frac{1}{2}}$$

$$\sum_{t=0}^{\frac{1}{2}n_1} \sum_{s=0}^{\frac{1}{2}n_1} c_t\, d_s\, (-a)^{t+s}\, (r+t+s)!\, \left(a + \frac{k^2}{2}\right)^{-(|m_1|+t+s+1)}$$

$$\times \sum_{i=0}^{\frac{1}{2}n_2} \sum_{j=0}^{\frac{1}{2}n_2} \sum_{\ell=0}^{r+s+t} \frac{g_\ell\, e_i\, f_j\, (-b)^{i+j}\, (|m_2|+i+j+\ell)!}{\left(b + \frac{k^2}{2} - \frac{k^4}{2(2a+k^2)}\right)^{(|m_2|+i+j+\ell+1)}}$$

$$\times \sum_{s=0}^{\frac{1}{2}n_{z_1}} \sum_{r=0}^{\frac{1}{2}n_{z_1}} \gamma_s \, \delta_r \sum_{i=0}^{\min(n_{z_1}-2s,\, m_{z_1}-2r)} i! \binom{n_{z_1}-2s}{i} \binom{m_{z_1}-2r}{i}$$

$$\left(\frac{1}{e + k^2}\right)^{\frac{1}{2}(2n_{z_1}-2s-2r-2i+1)}$$

$$\times \sum_{t=0}^{\frac{1}{2}(2n_{z_1}-2s-2r-2i)} \sum_{\ell=0}^{\frac{1}{2} n_{z_2}} \sum_{j=0}^{\frac{1}{2} m_{z_2}} h_t \, \epsilon_\ell \, k_j \; 2^{-s-r-t-\ell-j} \times$$

$$\Gamma\left(\frac{2n_{z_1} - 2s - 2r - 2i - 2t - 2\ell + 2j + 1}{2}\right)$$

$$\Gamma\left(\frac{2n_{z_2} - 2n_{z_1} - 2\ell - 2j + 2s + 2r + 2i + 2t + 1}{2}\right)$$

$$\Gamma\left(\frac{2n_{z_1} - 2s - 2r - 2i - 2t - 2j + 2\ell + 1}{2}\right) \qquad (3\text{-}4)$$

and

$$\langle \phi_{n_k}(1)\, \phi_{n_t}(2) \,|\, g_r(1,2) \,|\, \phi_{n_t}(1)\, \phi_{n_k}(2) \rangle$$

$$= (k^2)^{(m_2-m_1)} \; 2^{(|m_1| + |m_2| + 2)} \; b^{|m_2| + 1} \; a^{|m_1| + 1} \left(\frac{n_1}{2}\right)! \; \left(\frac{n_2}{2}\right)!$$

$$\left(|m_1| + \frac{n_1}{2}\right)! \; \left(|m_2| + \frac{n_2}{2}\right)! \; \frac{2n_{z_1}!\, n_{z_2}!}{\sqrt{\alpha}} \, (a_z \cdot b_z)^{\frac{1}{2}}$$

$$\sum_{s=0}^{\frac{1}{2}n_1} \sum_{t=0}^{\frac{1}{2}n_2} CX_s \; DX_t \; (r+s+t)! \; 2^{s+t} \, (a+b+k^2)^{-\frac{1}{2}(|m_1| + |m_2| + m_2 - m_1 + 2s + 2t + 2)}$$

$$\sum_{p=0}^{\frac{1}{2}n_1} \sum_{q=0}^{\frac{1}{2}n_2} \sum_{i=0}^{r+s+t} \frac{CX_p \, DX_q \, E_i(\frac{1}{2}(m_2-m_1+|m_1|+|m_2|+2p+2q+2i))!\,2^{p+q+i}}{(a+b+k^2-k^4/(a+b+k^2))^{\frac{1}{2}(m_2-m_1+|m_2|+|m_1|+2p+2q+2i+2)}}$$

$$\sum_{s=0}^{\frac{1}{2}n_{z_1}} \sum_{r=0}^{\frac{1}{2}n_{z_2}} \gamma_s \, \delta_r \sum_{i=0}^{\min(n_{z_1}-2s,\, n_{z_2}-2r)} i! \binom{n_{z_1}-2s}{i}\binom{n_{z_2}-2r}{i}\left(\frac{1}{e+k^2}\right)^{\frac{1}{2}(n_{z_1}+n_{z_2}-2s-2r-2i+1)}$$

$$\sum_{t=0}^{\frac{1}{2}(n_{z_1}+n_{z_2}-2s-2r-2i)} \sum_{\ell=0}^{\frac{1}{2}n_{z_2}} \sum_{j=0}^{\frac{1}{2}n_{z_1}} h_t \, \epsilon_\ell \, k_j \; 2^{-s-r-t-\ell-j}$$

$$\times \Gamma\left(\frac{2n_{z_2}-2s-2r-2i-2t-2\ell+2j+1}{2}\right)$$

$$\times \Gamma\left(\frac{2n_{z_1}-2s-2r-2i-2t-2j+2\ell+1}{2}\right)$$

$$\times \Gamma\left(\frac{2s+2r+2i+2t-2\ell-2j+1}{2}\right) \qquad (3\text{-}5)$$

In these equations the oscillator constants (a, a_z) and (b, b_z) correspond to the quantum numbers (n_1, n_{z_1}, m_1) and (n_2, n_{z_2}, m_2), respectively. The other constants shown, (e.g. α, CX_s, γ_s, δ_r, etc.) are defined in Appendix B to which the reader is directed.

The large number of summations present in the equations are a result of the generality of the matrix elements, that is, of the fact that each orbital has been given a unique oscillator constant. In no way are they caused by any inherent difficulty involved in the problem.

Computer programs have been written to evaluate (3-4) and (3-5) for any given set of the variable parameters involved. These programs have already proved themselves to be tremendously useful since they reduce the usually exacting chore of matrix element calculation to a few simple computer operations.

CHAPTER 4: THE CALCULATION OF BINDING ENERGIES OF PARTICULAR CONFIGURATIONS AS A FUNCTION OF DEFORMATION

In every configuration in the s-d shell for which calculations are performed, a closed-shell O^{16} core which interacts with the single nucleons of the s-d shell has been used. In no case has the possibility of particle excitation out of the 1p-shell been considered. However, as in previous work, V64 and V65, all two particle interactions in and with the O^{16} core are included in the energy calculation.

As single nucleons are added to the s-d shell they are permuted about the available positions (a maximum of 24). Each unique configuration so obtained is then specified by A, Z, M and the single particle orbital occupancy and the binding energy is calculated as a function of deformation.

The calculation itself has the form of a limited type of Hartree-Fock calculation[4]. It involves taking the diagonal matrix elements of the Hamiltonian with respect to determinants with fixed M values. The diagonal matrix thus obtained is then minimized with respect to the single particle oscillator constants (or, effectively, with respect to the individual orbital sizes) and the nuclear deformation.

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4 A detailed analysis of this type of calculation may be found in V65.

Since the nuclear size is varied it is necessary to use a saturating effect force in order that the nuclei studied do not over-bind. The force that has, in fact, been used has a "soft" repulsive core and satisfies appropriate low energy scattering and binding energy criteria[5].

The fact that only diagonal elements are calculated means that configuration mixing is ignored and that the calculations are not directly comparable to ones of an intermediate coupling nature. However, this is not a serious drawback, since the study of interest here is that of deformation effects.

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5 See Chapter 5.

CHAPTER 5: THE EFFECTIVE NUCLEAR FORCE

The first two criteria to consider in a choice of a nuclear force are that the force be saturating and that the force be "realistic".

The general form of the Hamiltonian used is

$$H = \sum_{i=1}^{A} T_i - T_{CM} + \sum_{i>j=1}^{A} V(r_{ij}) \, (1-m+m\,P^x_{ij} + bP^\sigma_{ij} + hP^\tau_{ij}) + c \sum_{i=1}^{A} \ell_i \cdot s_i \qquad (5\text{-}1)$$

where the summations are taken over all particles in the nucleus. P^x_{ij}, P^σ_{ij} and P^τ_{ij} are the Majorana, Bartlett and Heisenberg exchange operators, respectively, and $T_{C.M.}$ is the centre of mass kinetic energy which must be subtracted out.

The radially dependent part of the two particle potential, $V(r_{ij})$, has the form

$$V(r_{ij}) = -V_a \exp\left(-\frac{k_r^2}{2} r_{ij}^2\right) + V_r \exp\left(-\frac{k_a^2}{2} r_{ij}^2\right) \qquad (5\text{-}2)$$

where V_a, V_r, k_a and k_r are parameters whose values are fixed by 1p-shell calculations performed for O^{16} by D. J. Hughes. These calculations also fixed the values of m, b, h and c used[6]. The criteria which these force parameters were made to satisfy are as follows: (i) the s-wave scattering length and the effective range must closely approximate the singlet and the triplet scattering lengths and effective ranges.

(ii) the binding energy and size of He^4 should be correctly given by the appropriate single-determinant equilibrium calculation.

(iii) the binding energy and size of O^{16} should be correctly given by the appropriate single-determinant equilibrium calculation.

Criterion (iii) is extremely important in determining the amount of Majorana exchange to be used. A change in m of 0.02 can cause a change in the O^{16} binding energy of 30 MeV and thus, once m is set for O^{16}, one would expect that it need not be changed again for at least the first half of the s-d shell.

It should also be pointed out that more emphasis was placed on the binding energy of O^{16} than on the size in the final choice of a force mixture.

The force finally chosen has a shape similar to the Kallio-Koltveit potential (KK64). It has a very "soft" core which is well-suited to the needs of this investigation since it will decrease, (to a small degree), the importance of configuration mixing.

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6 The computational program written for the energy calculations includes the possibility of varying m, b, h and c to obtain the best fits to experimental data, but in view of the approximation already made in ignoring configuration mixing, such variation would not be sufficiently meaningful to be worth the expense in research and computer time.

Pandya and Green (PG64) have shown that the core is very important in determining the (rotational) spectra of 2s-1d spectra and that the increasing "hardness" of the core uniformly lowers the levels with respect to the ground state. Of the various forces they tried, the one which best fits experimental data has a core somewhat "harder" than the one used here. However, although Volkov and Hughes have found similar effects in the 1p-shell, they have found in addition that cores "harder" than the one used here lower the spectra too much, (for an example of such a force see FORCE 1 of V65). Also, one must take into account that a long range attractive potential gives effects similar to a short range attractive potential with a repulsive core.

The explicit values of the parameters used are

$V_a = 97.54$ MeV,	$m = 0.75$,
$V_r = 103.95$ MeV,	$b = 0.200$,
$k_a = 0.9428\ \mathrm{fm}^{-1}$,	$h = 0.050$,
$k_r = 1.8856\ \mathrm{fm}^{-1}$,	$c = -4.00$

(The spin-orbit term is really a non-essential addition for the purposes of this study and hense c is frequently set equal to zero for purposes of simplification).

These parameters give an O^{16} binding energy of 127.4 MeV and a size parameter, (the oscillator constant in $e^{-\frac{1}{2}\left(\frac{r}{b}\right)^2}$), of 1.4 fm.

CHAPTER 6: THE DEPENDENCE OF THE WAVE FUNCTIONS AND MATRIX ELEMENTS ON DEFORMATION

The deformation ϵ is defined by the relation

$$\frac{A}{B} = (1 + \epsilon/3)/(1 - 2\epsilon/3) \qquad (6\text{-}1)$$

where A and B are the oscillator constants for the ρ-dependent and z-dependent parts of the wave function, respectively. This is the same deformation parameter as defined in Appendix A of N55. Values of $\epsilon > 0$ represents a prolate deformation while $\epsilon < 0$ represents an oblate deformation.

As mentioned in the Introduction, Volkov has found that the best results are obtained by describing each orbital with a unique set of oscillator constants.

This is theoretically justified by the fact that this provides a closer approximation to Woods-Saxon wave functions which are a more self-consistent choice.

At the same time, one imposes the restriction that the deformation, ϵ, be the same for each orbital, since the deformation represents a Hartree-Fock potential which should be similar for each orbital. Thus, in the case of the 1p-shell, one has $A/B = A_0/B_0 = A_1/B_1$.

In this investigation exactly the same procedure as the one used by Volkov is followed for the p-shell orbitals. This involves establishing the value of the parameter $\sigma = A_0/A = A_1/A$ and minimizing the energy with respect to A alone. Thus one obtains the value of A_0 for prolate deformations and of A_1 for oblate deformations. Once A_0 is determined for $\epsilon > 0$ and A_1 for $\epsilon < 0$, the corresponding values of A_1 and A_0 are obtained by setting the ratio of the $p_{\pm 1}$ kinetic energy to the p_0 kinetic energy equal to unity.

For the case of O^{16} it has been found that the best binding is obtained for $A \approx A_0 \approx A_1$. Thus, for the purposes of an initial investigation, this equality is maintained in the s-d shell calculations as well.

In the case of the s-d shell orbitals a somewhat different procedure is followed.

For the $2s_0'$ and $1d_0'$ orbitals it is necessary to use the same oscillator constants as for the $1s_0$ orbital in order to ensure the orthogonality and hence, the linear independence, of the wave functions. The alternative would be to use different oscillator constants and then renormalize the various Slater determinants affected which is in itself a non-trivial problem.

For the $1d_{\pm 1}$ and $1d_{\pm 2}$ orbitals new oscillator constants, C, D and E, F, respectively, were used. Once again, the restriction of having the same deformation for all orbitals is imposed so that $A/B = C/D = E/F$. In order to avoid the very time consuming task of having three independent energy minimizations with respect to the orbital sizes for each deformation, the ratios C/A and E/A were determined by the complete minimization process at zero deformation and then used for all other deformations. Thus, with the exception of the zero deformation calculation, only the minimization with respect to "A" is performed.

When different oscillator constants are used there is the added complication that one cannot use the method of Elliott and Skyrme (Elliott 1955) for subtracting out the centre of mass kinetic energy. Thus, the pertinent matrix elements have been worked out by hand and subtracted out explicitly in every case in which they occur.

The matrix elements involved in the energy calculation are the single particle kinetic energies, which are of the form

$$\langle \Psi_{n,m,n_z} | \frac{p^2}{2m} | \Psi_{n,m,n_z} \rangle = \frac{1}{2} \left[(|m| + n + 1) h \omega_o + (n_z + \tfrac{1}{2}) h \omega_z \right] \qquad (6\text{-}2)$$

and the interaction matrix elements which are given by equations (3-2) and (3-3) of Chapter 3. The relative importance of these matrix elements, with respect to deformation, is determined by the amount of Majorana exchange, m, in the force mixture. An investigation of the behaviour of the kinetic energies and the various matrix elements as a function of deformation has, therefore, been made in order to illustrate this.

This investigation is performed under the assumption of constant nuclear volume, $a^2 b = 0.064$, which is close to the O^{16} equilibrium size. The kinetic energies are plotted in Fig.1 and the most interesting interaction elements, (involving the $1d_o'$ state which makes prolate deformations more favourable and the $1d_{\pm 2}$ state which makes oblate deformations more favourable), are shown in Figs.2 through

In a similar investigation for the 1p-shell, Volkov, (V65), has shown that the direct matrix elements oppose the deformation favoured by the corresponding kinetic energies. The exchange elements, on the other hand, favour deformation and, although much smaller in magnitude than the corresponding direct elements, their energy gain is approximately the same as the corresponding energy loss of the latter. Thus, if the Majorana exchange parameter is small then, due to the predominance of the direct elements, deformation becomes unlikely and the nuclei tend to be badly overbound. As the value of m increases, so does the relative number of exchange matrix elements and the likelihood of deformation. For m slightly larger than 0.5 the opposing influences of the direct and exchange elements tend to balance and hence equilibrium deformations of nuclei are determined by the kinetic energies. Increasing m beyond this point gives a decrease in binding, but greater deformations and deformation energy gains.

CHAPTER 7: DETAILS OF THE ENERGY COMPUTATIONS

As mentioned in Chapter 6 a "complete" minimization is performed only for zero deformation. This is done by first calculating the (diagonal) Hamiltonian matrix, given the occupancy of the s-d orbitals in terms of whether the available 24 spaces are or are not occupied. The matrix is evaluated for the given force parameters to yield an energy value $\mathcal{E}_o$ (A, C, E) where A, C and E are the three independent oscillator constants defined in Chapter 6. This energy is then minimized in three independent calculations by applying a parabolic fit to each of

(a) $\mathcal{E}_o(A, C, E)$, $\mathcal{E}_o(A + \Delta A, C, E)$, $\mathcal{E}_o(A + 2\Delta A, C, E)$

to obtain the best value of A, say A_1

(b) $\mathcal{E}_o(A_1, C, E)$, $\mathcal{E}_o(A_1, C + \Delta C, E)$, $\mathcal{E}_o(A_1, C + 2\Delta C, E)$

to obtain the best value of C, say C_1, and

(c) $\mathcal{E}_o(A_1, C_1, E)$, $\mathcal{E}_o(A_1, C_1, E + \Delta E)$, $\mathcal{E}_o(A_1, C_1 + E + 2\Delta E)$

to obtain the best value of E, say E_1.

This gives the best fit value $\mathcal{E}_o(A_1, C_1, E_1)$ for zero deformation.

The consistency of this process has been tested in several cases by repeating each step, but starting with the best fit value, $\mathcal{E}_o(A_1, C_1, E_1)$, from the preceeding calculation. These tests have shown the calculation to be consistent to within at least 1 in 2000.

Although the tests were performed for the simple case of O^{17}, the results were considered sufficiently positive to ignore adding an automatic consistency check to the program, which would be quite time consuming.

Once the best fit value of $\mathcal{E}_o$ has been determined the ratios C_1/A_1 and E_1/A_1 are calculated and kept constant for all other values of deformation. Thus, only the single minimization (a) is performed for non-zero deformations.

With the energy calculated for nine values of deformation, such that $-0.8 \leq \epsilon \leq 0.8$ and including $\epsilon = 0$, one obtains an equilibrium energy curve from which the equilibrium value of ϵ can be determined.

The curves that have been calculated in this way are shown in Figs. 4-7 and described in the next chapter.

CHAPTER 8: EQUILIBRIUM ENERGY CURVES FOR O^{17}, O^{18}, F^{19} and Ne^{20}

The curves for O^{17} are divided into the two sets shown in Figs. 4a and 4b. The first set illustrates the case in which all orbitals have the same oscillator constant and in which the spin-orbit term has been omitted from the force mixture. One thus obtains the required degeneracy, due to orbital symmetry, of the dt1 and dt2 states at zero deformation. (The $1d_o$' state is slightly higher in energy due to its deviation from a true $1d_o$ state).

Since O^{17} has only one nucleon in the 2s-1d shell, these curves essentially show the single nucleon binding due to the field set up by, and interactions with, the core. One cannot generalize from these curves in order to predict what will happen in heavier 2s-1d nuclei, but they do give some understanding, in conjunction with the curves of other 2s-1d nuclei, of the dynamics of these nuclei.

The s-state is relatively higher than predicted by experiment but this is typical of harmonic oscillator potentials.*

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* The currect level ordering can be obtained with Woods-Saxon wavefunctions - G. E. Brown, ibid.

It is important to note that at this point, near the closed 1p-shell, deformation characteristics are mainly influenced by the O^{16} core. Only the $2s_o'$ and 1d±2 states have significant deviations from sphericity which is attributable to the kinetic energy deformation-dependence for these orbitals (see Fig.1). It would thus not be unreasonable to treat O^{17} as a spherical nucleus as has been done in the past with good agreement with experiment.

In Fig.4b the d±1 and d±2 oscillator constants have been varied independently and a spin-orbit term, with strength c = -4.00, has been added to the force mixture. One sees that the more symmetric d±1 states gain more energy from the more complete minimization than do the d±2 states. This is most probably due to the symmetry of the d±1 state, i.e. the lobes of the probability distribution for this state are distributed at 45° angles with respect to the z-axis and the x-y plane. As the size of the orbital is increased the nucleon's kinetic energy is decreased, but at the same time, the orbital's overlap with the core decreases which, in turn, decreases the energy of the nucleon and an equilibrium orbital size must eventually be reached. Clearly, a more symmetric orbital will maintain a better overlap with the core as its size is increased and so will gain more relative binding energy.

It should be noted, in view of the energy gains of the d±1 and d±2 states due to the more complete minimization that not allowing the $1d_o'$ orbital to have an oscillator constant which is independent of that of the s-states may be a rather drastic approximation. However, as will be demonstrated in the analysis of the curves for heavier nuclei, this can be partially corrected for by allowing variation of the $1p_0$ and $1p\pm1$ oscillator constants which are otherwise kept equal to the s-state constants.

The curves for O^{18} are shown in Fig.5a and Fig.5b. The first set, in Fig.5a, result from the force described in Chapter 5 but with no spin-orbit term. In this investigation only M=O configurations have been considered and of these, calculations were performed only for those expected to be important in configuration mixing considerations.

The configurations in the first set are underbound by about 10 MeV (which is less than 1 MeV per particle).

The configuration $[1d_0']^2$ appeared, at first, to be too high in energy relative to the others. In order to understand the relative binding of the different configurations, a systematic variation of the $1p_0$ and $1p_{\pm1}$ oscillator constants has been performed for each configuration. It has been found that, whereas configurations not involving the $1d_0'$ orbital have the greatest binding for $\sigma = 1.0$, (where σ is the parameter defined in Chapter 6), a value of σ somewhat greater than 1.0 is desirable for those configurations which do contain it. For O^{18} only the $[1d_0']^2$ configuration has a really significant energy gain resulting from the variation and this is for a value of $\sigma = 1.13$. The curve for this value of σ has been drawn with a dashed line in Fig.5a. As can be seen, the energy gain at equilibrium deformation is 2 MeV.

The set of curves, in Fig.5b, has been calculated for a Majorana parameter m=0.73 rather than m = 0.75. Only the case $\sigma = 1.13$ has been used for the $[1d_o']^2$ configuration in this set.

We see that the increase in binding resulting from the m value change is slightly more for the $[1d_o']^2$ and $[2s_o']^2$ configurations. However, this difference is probably not too significant.

If all M=0 configurations with configuration mixing are taken into account one would suspect from these graphs that O^{18} would be found to be a spherical nucleus. This would explain why reasonable agreement with experiment has been obtained for this nucleus using the Shell Model. However, the observation of anomalously large E-2 transition rates and of three 0^+ states below 6 MeV in O^{18} seems to indicate that deformed configurations may be important as well. (B64 and BG65).

The discussion of Ne^{20} will show that these phenomena are probably due to two-particle excitations from the 1p-orbitals to the $1d_o'$ orbital. Such excitations would lead to configurations with prolate deformations of the order $\epsilon = 0.2 - 0.4$.

The M=½ curves for F^{19} are shown in Fig.6 . Once again we have considered only those configurations expected to be important in a configuration mixing calculation. Also once again, the variation has been performed only for the prominent $1d_o'$ configuration giving the dashed curve in Fig.6.

Although the binding is again too low with m=0.75, no attempt has been made to correct this since experience has shown (see O^{18} and Ne^{20}) that no significant change in the shapes or relative spacings of the curves is obtained as a result of varying m.

These curves show the first definite prolate deformation obtained among the 2s-1d nuclei. The most important configuration is $[1d_0{}']^3$ which has an equilibrium deformation of $\epsilon = 0.25$ and a deformation energy gain of 4.0 MeV. The next lowest configuration, $[1d_{+1}]^2[1d_{-1}]$, has a minimum approximately 8.7 MeV above the $[1d_0{}']^3$ minimum. Since these configurations can only mix in the second order one can predict by analogy with results in the p-shell that the deformation energy gain which would be obtained in a complete calculation of the type performed by Volkov will be several MeV smaller. However, the shape of the M=½ curve near equilibrium deformation will be approximately that of the curve for the dominant configuration, i.e., the $[1d_0{}']^3$ configuration.

This very definite deformation is just what one would expect to find for F^{19} since good fits to the experimental level structure have been made using the collective, rotational, model (P57 and CD63).

Brown (B64) has pointed out the importance of the $\frac{1}{2}^-$ odd parity state in F^{19} which is only 110 keV above the ground state. To explain the existence of this state he has suggested the introduction of another deformed state by exciting a particle from the $\frac{1}{2}^-$ Nilsson level to put four particles in the $\frac{1}{2}^+$ level. Once again, the Ne^{20} graph offers a similar explanation by excitation of a $1p_{\pm 1}$ particle to completely fill the $1d_0{}'$ orbitals.

The last two Figs., 7a and 7b, show the more important M=0 configurations of Ne^{20}. The first set of curves, (Fig.7a), has been calculated for the force mixture of Chapter 5, but with no spin-orbit term. Once again, a σ-variation was performed for the important $1d_o'$-dependent states, the results of which are plotted with dashed lines.

The most important result obtained is the very pronounced deformation of the $[1d_o']^4$ configuration with an energy gain of 8 MeV. Appreciable mixing will occur only with the $[1d_o']^3$ $[1d_{-1}]$ configuration, which is also quite deformed so that essentially the same deformation characteristics will result from a complete calculation of the type performed by Volkov. As in the case of F^{19}, the complete calculation would produce a curve with a smaller deformation energy gain, but with a shape, at equilibrium deformation, very much like that of the curve for the dominant $[1d_o']^4$ configuration.

As already mentioned in the considerations of O^{18} and F^{19}, the prolate gain of the $[1d_o']^4$ configuration has repercussions throughout the first subshell, from O^{16} to Ne^{20}. In the case of F^{19}, there is an energy difference between the $[1d_o']^3$ state and the Ne^{20} $[1d_o']^4$ state of 16 MeV so that one-particle excitation from the p-shell is likely to be quite favourable. However, to obtain a binding of the $\frac{1}{2}^-$ level only 110 keV above the ground state it will probably be necessary to make allowance for an independent oscillator constant variation for the $1d_o'$ orbital.

In the case of O^{18} two-particle excitation to the $1d_o'$ orbital should be quite favourable as the energy difference between the Ne^{20} $[1d_o']^4$ state and the O^{18} $[1d_o']^2$ state is approximately 25 MeV whereas the binding energy per particle is only of the order of 6.0 to 7.0 MeV. To see which excitations are actually important it will be necessary to explicitly perform the calculations involved. These calculations are now being performed by D. J. Hughes. However, the graphs of this thesis suggest the qualitative functions to be expected.

For O^{16}, two particle and three-particle excitations have been suggested by Brown to explain definite rotational levels whose presence has recently been experimentally confirmed (C64). Once again, it will be interesting to see whether complete calculations can reproduce this phenomena. It would appear from this investigation that a four-particle excitation would be more favourable than a two-particle one, but there is insufficient evidence to explicitly stipulate that this is the case. However, it is interesting to note that Bassichis and Ripka (B65) have found, as a result of a limited Hartree-Fock calculation, that four particle-four hole states do give rise to the desired rotational band while two-particle-two hole states give rise to badly mixed rotational bands, that lie too high in energy.

The second set of curves, in Fig. 7b, show the four lowest states of Fig. 7a, recalculated for a Majorana parameter, m, equal to 0.74. This very small change in m gives a 10 MeV increase in binding but otherwise does not affect the curves.

It is important to note that only very small changes in the amount of Majorana exchange used in the force mixture is required to obtain a change in the binding energies of the order of 10 to 20 MeV.

This essentially confirms the original assumption that m could be kept at the value used to obtain the correct O^{16} binding as such changes cannot be considered significant in terms of relative gains and losses due to deformation.

CHAPTER 9: CONCLUSIONS

Harmonic oscillator wavefunctions in cylindrical coordinates have been found to form a representation especially suited for problems involving deformed nuclei. In applications to the 2s-1d shell it has been found that, while some formal difficulties, such as the independent variation of all oscillator constants, still require solution, several new areas have been opened for future investigation. Of these, two areas are of the most immediate interest. The first involves particle excitations from 1p-shell nuclei into the 2s-1d shell, such as in C^{12} and O^{16}, to attempt explanations of recent experimentally confirmed phenomena which cannot be predicted by conventional Shell Model calculations. The second involves the full extension of the calculations of Volkov and Hughes to the 2s-1d shell for which the present work has provided the necessary tools.

In the investigation of the 2s-1d shell it has been found that, except for possible excited states resulting from particle-hole states, O^{17} and O^{18} are essentially spherical nuclei. On the other hand, F^{19} and Ne^{20}, have strong prolate deformations resulting from the progressively dominant influence of the $1d_o'$ orbital. Although the calculations have not yet been extended beyond Ne^{20} it is expected that this prolateness will pass into pronounced oblate deformations as we proceed towards Mg^{24}. This prediction is based both on the studies of the 1p-shell and on the studies made of the interaction matrix elements and the kinetic energies.

It has been found that slight changes in the amount of Majorana exchange used in the force mixture is required to obtain good binding as we proceed from the closed shell at O^{16} to the closed sub-shell in Ne^{20}. Although not significant in this study, these slight changes probably will have much more importance when particle-hole excitations are studied. This is probably due to the absence of a tensor force in the force mixture. For closed shell nuclei the tensor force contributes nothing to the binding. However, away from the closed shell the Majorana admixture must be reduced to compensate for the tensor force contributions which are being ignored. This compensation will become really significant when particle excitations in O^{16} are considered since then maintaining the same amount of exchange for the excited state as for the ground state can cause a discrepancy of 10 to 20 MeV in the energy of the excited state.

APPENDIX A: THE SOLUTION OF THE RADIAL PART OF THE HARMONIC OSCILLATOR WAVE EQUATION

The equation which we wish to solve is

$$\frac{1}{\rho}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \left(\lambda' - \alpha^2\rho^2 - \frac{m^2}{\rho^2}\right) P = 0 \tag{A-1}$$

For $\rho \gg 0$, equation (A-1) becomes

$$\frac{d^2P}{d\rho^2} - \alpha^2\rho^2 \, P = 0$$

from which we immediately obtain, as an asymptotic solution of (A-1)

$$P \sim e^{\pm\frac{\alpha}{2}\rho^2}$$

We, therefore, make the substitution

$$P(\rho) = e^{-\frac{\alpha}{2}\rho^2} f(\rho)$$

which yields

$$f'' - 2\alpha\rho f' + \frac{1}{\rho} f' + (\lambda' - 2\alpha) f - \frac{m^2}{\rho^2} f = 0$$

Replacing $\sqrt{\alpha}\,\rho$ by ξ and $f(\rho)$ by $F(\xi)$, this becomes

$$\frac{d^2F}{d\xi^2} - 2\xi\frac{dF}{d\xi} + \frac{1}{\xi}\frac{dF}{d\xi} + \left(\frac{\lambda'}{\alpha} - 2 - \frac{m^2}{\xi^2}\right)F = 0 \qquad \text{(A-2)}$$

Writing (A-2) in the standard form,

$$\frac{d^2F}{d\xi^2} + p(\xi)\frac{dF}{d\xi} + q(\xi)F = 0,$$

we see that it possesses a regular point at $\xi = 0$ since $p(\xi) \sim \frac{1}{\xi}$ and $q(\xi) \sim \frac{1}{\xi^2}$. We are thus led to solve (A-2) by the Method of Froebenius, (B56), that is, by performing the substitution $F(\xi) = \xi^s \sum_{\nu=0}^{\infty} a_\nu \xi^\nu$.

Such a substitution leads to the indicial equation $(s^2 - m^2)\,a_0 = 0$ and hence we obtain $s = |m|$.

It is now convenient, rather than to continue the series solution, to define $G(\xi)$, such that $F(\xi) = \xi^{|m|}G(\xi)$, and to again substitute for F in equation (A-2). We now obtain

$$\frac{d^2G}{d\xi^2} + \left(\frac{1}{\xi}(2|m| + 1) - 2\xi\right)\frac{dG}{d\xi} + \left(\frac{\lambda'}{\alpha} - 2 - 2|m|\right)G(\xi) = 0 \qquad \text{(A-3)}$$

By performing yet another change in variables by setting $x = \xi^2$ and $g(x) = G(\xi)$, equation (A-3) becomes

$$x\frac{d^2g(x)}{dx^2} + \left((|m| + 1) - x\right)\frac{dg(x)}{dx} + \frac{n}{2}g(x) = 0 \qquad \text{(A-4)}$$

where $n = \frac{\lambda'}{2} - |m| - 1.$

In order that we may obtain a satisfactory wave function, the series solution of (A-4) must contain a finite number of terms. This can easily be shown to imply that n must be restricted to even integral values: 0, 2, 4, . . . If this restriction is made (A-4) has the form of the equation for the associated Laguerre polynomial (E54) and hence we can write $g(x) = L^{|m|}_{\frac{n}{2}}(x)$. The solution of (A-1) is then

$$P(\rho) = e^{-\frac{\alpha}{2}\rho^2} (\sqrt{\alpha}\,\rho)^{|m|} L^{|m|}_{\frac{n}{2}}(\alpha\rho^2)$$

The normalization for $P(\rho)$ is easily obtained from the properties of the Laguerre polynomials, i.e.

$$\int_0^\infty e^{-z} z^k L^k_p(z) L^k_q(z)\, dz = \frac{[(p+k)!]^3}{p!} \delta_{pq} \tag{A-5}$$

APPENDIX B: EXPLICIT CALCULATION OF THE DIRECT AND EXCHANGE MATRIX ELEMENTS OF A GAUSSIAN INTERACTION

The integrations which we wish to perform are described by equations (3-2) and (3-3) of Chapter 3. Both these integrals are handled in the same way and may in fact be treated as special cases of a single integral in which one has four different sets of quantum numbers and four different oscillator constants. This approach was in fact used for the $z_1 - z_2$ - integration but, for the sake of clarity, the direct and exchange elements were worked out separately for the integration over ρ_1, ϕ_1, ρ_2, ϕ_2. However, in the latter integration four different sets of quantum numbers were used for the direct element, thus enabling the reader to better visualize how the general integral could be performed. It is this part of the direct element which we will consider first.

Substituting from (2-5) and ignoring, for the present, the normalization factors, we have

$$M = \iiiint (\sqrt{\beta}\rho_2)^{|m_2| + |m_4|} L_{\frac{1}{2}n_2}^{|m_2|}(\beta\rho_2^2)\, L_{\frac{1}{2}n_4}^{m_4}(\beta\rho_2^2)\, (\sqrt{\alpha}\rho_1)^{|m_1| + |m_3|}$$

$$\times L_{\frac{1}{2}n_1}^{|m_1|}(\alpha\rho_1^2)\, L_{\frac{1}{2}n_3}^{|m_3|}(\alpha\rho_1^2)\, e^{-\beta\rho_2^2}\, e^{-\alpha\rho_1^2}\, e^{i(m_3-m_1)\phi_1}\, e^{i(m_4-m_2)\phi_2}$$

$$\times \exp\left(-\frac{k^2}{2}\rho_1^2 - \frac{k^2}{2}\rho_2^2 + k^2\rho_1\rho_2\cos(\phi_1-\phi_2)\right)\rho_1 d\rho_1\, \rho_2 d\rho_2\, d\phi_1\, d\phi_2 \qquad \text{(B-1)}$$

α and β are the oscillator constants for the wavefunctions of particles 1 and 2 respectively.

We can write

$$e^{i(m_3-m_1)\phi_1} \cdot e^{i(m_4-m_2)\phi_2}$$

$$= e^{i(m_3-m_1)(\phi_1-\phi_2)} \cdot e^{i(m_4-m_2+m_3-m_1)\phi_2}$$

and hence introduce a new variable of integration, $\chi = (\phi_1-\phi_2)$, We can now integrate separately over ϕ_2 and χ. The integration over ϕ_2 simply yields $2\pi\,\delta_{m_1+m_2-m_3-m_4,0}$ and the integration over χ is

$$\int_0^{2\pi} e^{i(m_3-m_1)\chi}\; e^{k^2\rho_1\rho_2\cos\chi}\, d\chi$$ which yields

$$2\pi\; e^{\frac{1}{2}i(m_3-m_1)\pi}\; J_{(m_3-m_1)}(-ik^2\rho_1\rho_2)\,^*$$

We thus have

$$M = (2\pi)^2\,\delta_{m_1+m_2-m_3-m_4,0}\iint e^{\frac{1}{2}i(m_3-m_1)\pi}\; J_{(m_3-m_1)}(-ik^2\rho_1\rho_2)$$

$$\times\,(\sqrt{\beta}\,\rho_2)^{|m_2|+|m_4|}\; L^{|m_2|}_{\frac{1}{2}n_2}(\beta\rho_2^2)\; L^{m_4}_{\frac{1}{2}n_4}(\beta\rho_2^2)\;(\sqrt{\alpha}\,\rho_1)^{|m_1|+|m_3|}$$

$$\times\, L^{|m_1|}_{\frac{1}{2}n_1}(\alpha\rho_1^2)\; L^{|m_3|}_{\frac{1}{2}n_3}(\alpha\rho_1^2)\;\exp\left(-\beta\rho_2^2-\alpha\rho_1^2-\frac{k^2}{2}(\rho_1^2+\rho_2^2)\right)$$

$$\rho_1\,d\rho_1\,\rho_2\,d\rho_2 \qquad \text{(B-2)}$$

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* Erdelyi et al - Higher Transcendental Functions Vol.2 p.20

Let us set $y = -i\rho_2$ and consider the integration over ρ_1. This has the form:

$$M\rho_1 = \int_0^\infty J_{(m_3-m_1)}(k^2 y\,\rho_1)\,(\alpha\rho_1)^{|m_1|+|m_3|}\,L_{\frac{1}{2}n_1}^{|m_1|}(\alpha\rho_1^2)$$

$$L_{\frac{1}{2}n_3}^{|m_3|}(\alpha\rho_1^2)\ \exp\left(-\alpha\rho_1^2 - \frac{k^2}{2}\rho_1^2\right)\rho_1\,d\rho_1 \qquad \text{(B-3)}$$

It is convenient at this point to let $x = \rho_1^2$ and substitute in (B-3) to obtain

$$M\rho_1 = \int_0^\infty \left(\frac{\sqrt{\alpha}}{2}\right)^{|m_1|+|m_3|} J_{(m_3-m_1)}(k^2 y x^{\frac{1}{2}})\ x^{\frac{1}{2}(|m_1|+|m_3|)}$$

$$L_{\frac{1}{2}n_1}^{|m_1|}(\alpha x)\ L_{\frac{1}{2}n_3}^{|m_3|}(\alpha x)\ e^{-(\alpha+\frac{k^2}{2})x}\,dx \qquad \text{(B-4)}$$

The best way to proceed is to now express the Laguerre polynomials as series, i.e.,

$$L_{\frac{1}{2}n_1}^{|m_1|}(\alpha x) = \sum_{t=0}^{\frac{1}{2}n_1} \frac{\left[(\frac{1}{2}n_1 + |m_1|)!\right]^2}{(\frac{1}{2}n_1-t)!\,(m_1+t)!}\ \frac{(-\alpha x)^t}{t!}$$

and

$$L_{\frac{1}{2}n_3}^{|m_3|}(\alpha x) = \sum_{s=0}^{\frac{1}{2}n_3} \frac{\left[(\frac{1}{2}n_3 + |m_3|)!\right]^2}{(\frac{1}{2}n_3-s)!\,(m_3+s)!}\ \frac{(-\alpha x)^s}{s!}$$

Therefore,

$$L_{\frac{1}{2}n_1}^{m_1}\cdot L_{\frac{1}{2}n_3}^{m_3} = \sum_{t=0}^{\frac{1}{2}n_1}\sum_{s=0}^{\frac{1}{2}n_3} \frac{\left[(\frac{1}{2}n_1+|m_1|)!\,(\frac{1}{2}n_3+|m_3|)!\right]^2(-\alpha x)^{t+s}}{(\frac{1}{2}n_1-t)!\,(m_1+t)!\,(\frac{1}{2}n_3-s)!\,(m_3+s)!\,t!\,s!}$$

$$= \left[(\tfrac{1}{2}n_1+|m_1|)!\,(\tfrac{1}{2}n_3+|m_3|)!\right]^2 \sum_{t=0}^{\frac{1}{2}n_1}\sum_{s=0}^{\frac{1}{2}n_3} c_t d_s(-\alpha x)^{t+s}$$

Thus, substituting into (B-4) we have,

$$M\rho_1 = \int_0^\infty \left(\frac{\sqrt{\alpha}}{2}\right)^{|m_1|+|m_3|} J_{(m_3-m_1)}(k^2yx^{1/2})\, x^{1/2(|m_1|+|m_3|)}$$

$$e^{-(\alpha+\frac{k^2}{2})x}\left[(1/2n_1+|m_1|)!\,(1/2n_3+|m_3|)!\right]^2 \sum_{t=0}^{1/2n_1}\sum_{s=0}^{1/2n_3} c_t d_s(-\alpha x)^{t+s}\,dx$$

Therefore $M\rho_1 = \left[(1/2n_1+|m_1|)!\,(1/2n_3+|m_3|)!\right]^2 \left(\frac{\sqrt{\alpha}}{2}\right)^{|m_1|+|m_3|}$

$$\sum_{t=0}^{1/2n_1}\sum_{s=0}^{1/2n_3} c_t d_s(-\alpha)^{t+s}(r+t+s)!\left(\frac{k^2y}{2}\right)^{(m_3-m_1)}$$

$$\left(\alpha+\frac{k^2}{2}\right)^{-(r+t+s)-(m_3-m_1)-1}\; e^{-\frac{k^4y^2}{(4\alpha+2k^2)}}$$

$$\mathcal{L}_{(r+s+t)}^{m_3-m_1}\left(\frac{k^4y^2}{4\alpha+2k^2}\right) \qquad \text{(B-5)}^*$$

where $r = 1/2(|m_1|+|m_3|-m_3+m_1)$.

We come now to the ρ_2-integration which is

$$M\rho_2 = \int_0^\infty \left(\frac{-ik^2\rho_2}{2}\right)^{(m_3-m_1)}(\sqrt{\beta}\rho_2)^{|m_2|+|m_4|}\mathcal{L}_{(r+s+t)}^{(m_3-m_1)}\left(\frac{-k^4\rho_2^2}{2(2\alpha+k^2)}\right)$$

$$\times L_{1/2n_2}^{|m_2|}(\beta\rho_2^2)\, L_{1/2n_4}^{|m_4|}(\beta\rho_2^2)\,\exp\left(-\left(\beta+\frac{k^2}{2}-\frac{k^4}{2(2\alpha+k^2)}\right)\rho_2^2\right)\rho_2\,d\rho_2$$

(B-6)

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* Erdelyi et al Tables of Integral Transforms Vol.1, p.185, No.33

Again, we make a substitution $x = \rho_2^2$ and so obtain,

$$L^{|m_2|}_{\frac{1}{2}n_2}(\beta x)\, L^{|m_4|}_{\frac{1}{2}n_4}(\beta x) = \left[(\tfrac{1}{2}n_2 + |m_2|)!\,(\tfrac{1}{2}n_4 + |m_4|)!\right]^2$$

$$\sum_{i=0}^{\frac{1}{2}n_2} \sum_{j=0}^{\frac{1}{2}n_4} e_i\, f_j\, (-\beta x)^{i+j}$$

where e_i and f_j are defined in the same way as c_t and d_s, and

$$\mathcal{L}^{(m_3-m_1)}_{(r+s+t)}\left(\frac{-k^4 x}{2(2\alpha+k^2)}\right) L^{|m_2|}_{\frac{1}{2}n_2}\; L^{|m_4|}_{\frac{1}{2}n_4} = \left[(\tfrac{1}{2}n_2+|m_2|)!\,(\tfrac{1}{2}n_4+|m_4|)!\right]^2$$

$$\sum_{i=0}^{\frac{1}{2}n_2} \sum_{j=0}^{\frac{1}{2}n_4} \sum_{\ell=0}^{r+s+t} \frac{(r+s+t+m_3-m_1)!\,\left[k^4/2(2\quad+k^2)\right]^{\ell} e_i f_j (-\beta)^{i+j} x^{i+j+\ell}}{(r+s+t-\ell)!\,(m_3-m_1+\ell)!\,\ell!}$$

Substituting this into (B-6) we obtain

$$M\rho_2 = \int_0^\infty \left(\frac{-ik^2}{2}\right)^{(m_3-m_1)} \left(\frac{\sqrt{\beta}}{2}\right)^{|m_2|+|m_4|} \exp\left(-\left(\beta + \frac{k^2}{2} - \frac{k^4}{2(2\alpha+k^2)}\right) x\right)$$

$$\left[(\tfrac{1}{2}n_2 + |m_2|)!\,(\tfrac{1}{2}n_4 + |m_4|)!\right]^2 \sum_{i=0}^{\frac{1}{2}n_2} \sum_{j=0}^{\frac{1}{2}n_4} \sum_{\ell=0}^{r+s+t} g_\ell\, e_i\, f_j (-\beta)^{i+j}$$

$$x^{\frac{1}{2}(2i+2j+2\ell+m_3-m_1+|m_2|+|m_4|)} \quad dx$$

$$= \left(\frac{-ik^2}{2}\right)^{m_3-m_1} \left(\frac{\sqrt{\beta}}{2}\right)^{|m_2|+|m_4|} \left[(\tfrac{1}{2}n_2+|m_2|)!\,(\tfrac{1}{2}n_4+|m_4|)!\right]^2$$

$$\sum_{i=0}^{\frac{1}{2}n_2} \sum_{j=0}^{\frac{1}{2}n_4} \sum_{\ell=0}^{r+s+t} \frac{g_\ell e_i f_j (-\beta)^{i+j} \quad (\frac{1}{2}(m_3-m_1+|m_2|+|m_4|+2i+2j+2\ell+2))}{\left(\beta + \frac{k^2}{2} - k^4/2(2\alpha+k^2)\right)^{\frac{1}{2}(m_3-m_1+|m_2|+|m_4|+2i+2j+2\ell+2)}}$$

(B-7)

where g_ℓ is defined similarly to e_i and f_j.

Combining (B-5) and (B-7) we then have that

$$M = (2\pi)^2 \delta_{m_1+m_2-m_3-m_4,0} \left(\frac{k^2}{2}\right)^{(m_3-m_1)} \left(\frac{\sqrt{\alpha}}{2}\right)^{|m_1|+|m_3|}$$

$$\times \left(\frac{\sqrt{\beta}}{2}\right)^{|m_2|+|m_4|} \left[(\tfrac{1}{2}n_1+|m_1|)!\,(\tfrac{1}{2}n_2+|m_2|)!\,(\tfrac{1}{2}n_3+|m_3|)!\,(\tfrac{1}{2}n_4+|m_4|)!\right]^2$$

$$\times \sum_{t=0}^{\frac{1}{2}n_1} \sum_{s=0}^{\frac{1}{2}n_3} c_t\, d_s\, (-\alpha)^{t+s}\, (r+t+s)!\, \left(\alpha+\frac{k^2}{2}\right)^{-\frac{1}{2}(|m_1|+|m_3|+m_3-m_1+2t+2s+2)}$$

$$\times \sum_{i=0}^{\frac{1}{2}n_2} \sum_{j=0}^{\frac{1}{2}n_4} \sum_{\ell=0}^{r+s+t} \frac{g_\ell e_i f_j (-\beta)^{i+j} (\frac{1}{2}(m_3-m_1+|m_2|+|m_4|+2i+2j+2\ell))!}{\left(\beta+\frac{k^2}{2}-k^4/2(2\alpha+k^2)\right)^{\frac{1}{2}(m_3-m_1+|m_2|+|m_4|+2i+2j+2\ell+2)}}$$

which is the solution of the integral in (B-1).

It is now an easy task to include the normalization and so obtain for the (ρ,ϕ) part of the direct matrix element:

$$\left(\frac{k^2}{2}\right)^{(m_3-m_1)} (\sqrt{\alpha})^{|m_1|+|m_3|+2} (\sqrt{\beta})^{|m_2|+|m_4|+2}$$

$$\times \sqrt{(\tfrac{1}{2}n_1)!\,(\tfrac{1}{2}n_2)!\,(\tfrac{1}{2}n_3)!\,(\tfrac{1}{2}n_4)!\,(|m_1|+\tfrac{1}{2}n_1)!\,(|m_2|+\tfrac{1}{2}n_2)!\,(|m_3|+\tfrac{1}{2}n_3)!\,(|m_4|+\tfrac{1}{2}n_4)!}$$

$$\times \sum_{t=0}^{\frac{1}{2}n_1} \sum_{s=0}^{\frac{1}{2}n_3} c_t\, d_s\, (-\alpha)^{t+s}\, (r+t+s)!\, \left(\alpha+\frac{k^2}{2}\right)^{-\frac{1}{2}(|m_1|+|m_3|+m_3-m_1+2t+2s+2)}$$

$$\sum_{i=0}^{\frac{1}{2}n_2} \sum_{j=0}^{\frac{1}{2}n_4} \sum_{\ell=0}^{r+s+t} \frac{g_\ell e_i f_j (-\beta)^{i+j} (\frac{1}{2}(m_3-m_1+|m_2|+|m_4|+2i+2j+2\ell))!}{\left(\beta+\frac{k^2}{2}-k^4/2(2\alpha+k^2)\right)^{\frac{1}{2}(m_3-m_1+|m_2|+|m_4|+2i+2j+2\ell+2)}}$$

(B-8)

The next step is to work out the $\rho_1, \phi_1, \rho_2, \phi_2$ integration of the exchange element which has the form:

$$MX = \iiiint (\sqrt{\beta}\rho_2)^{|m_2|} (\sqrt{\alpha}\rho_1)^{|m_1|} (\sqrt{\alpha}\rho_2)^{|m_1|} (\sqrt{\beta}\rho_1)^{|m_2|}$$

$$L^{|m_1|}_{\frac{1}{2}n_1}(\alpha\rho_1^2)\, L^{|m_2|}_{\frac{1}{2}n_2}(\beta\rho_2^2)\, L^{|m_2|}_{\frac{1}{2}n_2}(\beta\rho_1^2)\, L^{|m_1|}_{\frac{1}{2}n_1}(\alpha\rho_2^2)\, e^{-\frac{\alpha}{2}\rho_1^2}$$

$$e^{-\frac{\alpha}{2}\rho_2^2}\, e^{-\frac{\beta}{2}\rho_1^2}\, e^{-\frac{\beta}{2}\rho_2^2}\, e^{-im_1\phi_1-im_2\phi_2}\, e^{im_2\phi_1+im_1\phi_2}$$

$$\exp\left(-\frac{k^2}{2}\rho_1^2 - \frac{k^2}{2}\rho_2^2 + k^2\rho_1\rho_2\cos(\phi_1-\phi_2)\right)\rho_1 d\rho_1\, \rho_2 d\rho_2\, d\phi_1 d\phi_2$$

(B-9)

where α and β are the oscillator constants which correspond to the quantum numbers (n_1, m_1) and (n_2, m_2), respectively.

We can write $e^{i(m_2-m_1)\phi_1}\; e^{i(m_1-m_2)\phi_2} = e^{i(m_2-m_1)(\phi_1-\phi_2)}$ and once again set $(\phi_1 - \phi_2) = \chi$ and integrate over ϕ_2 and χ. The integration over ϕ_2 gives 2π and the integration over χ is

$$\int_0^{2\pi} e^{i(m_2-m_1)\chi}\; e^{k^2\rho_1\rho_2\cos\chi}\, d\chi = 2\pi\, e^{\frac{i}{2}(m_2-m_1)\pi}\; J_{(m_2-m_1)}(-ik^2\rho_1\rho_2)$$

as before.

Thus,

$$MX = (2\pi)^2\, e^{\frac{1}{2}i(m_2-m_1)\pi} \iint J_{(m_2-m_1)}(-ik^2\rho_1\rho_2)\, \alpha^{|m_1|}\, \beta^{|m_2|}$$

$$\times\, \rho_1^{|m_1|+|m_2|}\, \rho_2^{|m_1|+|m_2|}\, L^{|m_1|}_{\frac{1}{2}n_1}(\alpha\rho_1^2)\, L^{|m_2|}_{\frac{1}{2}n_2}(\beta\rho_1^2)\, L^{|m_2|}_{\frac{1}{2}n_2}(\beta\rho_2^2)\, L^{|m_1|}_{\frac{1}{2}n_1}(\alpha\rho_2^2)$$

$$\exp\left(-\tfrac{1}{2}(\alpha+\beta+k^2)(\rho_1^2+\rho_2^2)\right)\rho_1\, d\rho_1\, \rho_2\, d\rho_2 \qquad \text{(B-10)}$$

As in the case of the direct element we set $y = -i\rho_2$, $x = \rho_1^2$ and consider the integration over ρ_1 (x):

$$MX\rho_1 = \int_0^\infty J_{(m_2-m_1)}(k^2 y x^{1/2})\; x^{1/2(|m_1|+|m_2|)}\; L^{|m_1|}_{1/2 n_1}(\alpha x)$$

$$L^{|m_2|}_{1/2 n_2}(\beta x)\; e^{-1/2(\alpha+\beta+k^2)x}\; \frac{dx}{2} \qquad \text{(B-11)}$$

Now, $L^{|m_1|}_{1/2 n_1}(\alpha x)\; L^{|m_2|}_{1/2 n_2}(\alpha x) = \left[(1/2 n_2 + |m_2|)!\,(1/2 n_1 + |m_1|)!\right]^2$

$$\times \sum_{s=0}^{1/2 n_1} \sum_{t=0}^{1/2 n_2} \frac{(-\alpha)^s (-\beta)^t (x)^{s+t}}{(1/2 n_1 - s)!\,(|m_1|+s)!\,(1/2 n_2 - t)!\,(|m_2|+t)!\,s!\,t!}$$

and so (B-11) becomes

$$MX\rho_1 = \left[(1/2 n_1 + |m_1|)!\,(1/2 n_2 + |m_2|)!\right]^2 \sum_{s=0}^{1/2 n_1} \sum_{t=0}^{1/2 n_2} \frac{CX_s\, DX_t}{2}$$

$$\int_0^\infty J_{(m_2-m_1)}(k^2 y x^{1/2})\; e^{-1/2(\alpha+\beta+k^2)x}\; x^{1/2(|m_1|+|m_2|)}\; x^{s+t}\, dx$$

$$= \left[(1/2 n_1 + |m_1|)!\,(1/2 n_2 + |m_2|)!\right]^2 \sum_{s=0}^{1/2 n_1} \sum_{t=0}^{1/2 n_2} \frac{CX_s\, DX_t}{2}\,(r+s+t)!$$

$$\left(\frac{k^2 y}{2}\right)^{(m_2-m_1)} \left(1/2(\alpha+\beta+k^2)\right)^{-1/2(|m_1|+|m_2|+m_2-m_1+2s+2t+2)}$$

$$\exp\left(-k^4 y^2/2(\alpha+\beta+k^2)\right) \mathcal{L}^{(m_2-m_1)}_{(r+s+t)}\left(k^4 y^2/2(\alpha+\beta+k^2)\right) \qquad \text{(B-12)}$$

where $r = 1/2\,(|m_1| + |m_2| - m_2 + m_1)$.

We come now to the ρ_2-integration which is

$$MX\rho_2 = \int_0^{\infty} \left(\frac{-ik^2}{2}\right)^{(m_2-m_1)} \rho_2^{(m_2-m_1)} \rho_2^{|m_1| + |m_2|}$$

$$\mathcal{L}^{(m_2-m_1)}_{(r+s+t)}\left(-k^4 \rho_2^2/2(\alpha+\beta+k^2)\right) \quad L^{|m_2|}_{\frac{1}{2}n_2}(\beta\rho_2^2) \quad L^{|m_1|}_{\frac{1}{2}n_1}(\alpha\rho_2^2)$$

$$e^{-\frac{1}{2}(\alpha+\beta+k^2-k^4/(\alpha+\beta+k^2))\rho_2^2} \quad \rho_2 \, d\rho_2 \qquad \text{(B-13)}$$

Again following the methods used for the direct element, we have

$$MX\rho_2 = \left[(\tfrac{1}{2}n_1 + |m_1|)!\,(\tfrac{1}{2}n_2 + |m_2|)!\right]^2 \sum_{p=0}^{\frac{1}{2}n_1} \sum_{q=0}^{\frac{1}{2}n_2} \sum_{i=0}^{r+s+t}$$

$$\frac{CX_p\, DX_q\, E_i}{2} \int_0^{\infty} \left(-\frac{ik^2}{2}\right)^{(m_2-m_1)} x^{\frac{1}{2}(|m_1| + |m_2| + m_2 - m_1 + 2p + 2q + 2i)}$$

$$\exp\left(-\tfrac{1}{2}\left(\alpha+\beta+k^2 - \frac{k^4}{(\alpha+\beta+k^2)}\right)x\right) dx$$

where $E_i = \dfrac{(r+s+t+m_2-m_1)!\ \left(k^4/2(\alpha+\beta+k^2)\right)^i}{(r+s+t-i)!\ (m_2-m_1+i)!\ \ i!}$

We thus obtain

$$MX\rho_2 = \left[(\tfrac{1}{2}n_1 + |m_1|)!\,(\tfrac{1}{2}n_2 + |m_2|)!\right]^2 \sum_{p=0}^{\frac{1}{2}n_1} \sum_{q=0}^{\frac{1}{2}n_2} \sum_{i=0}^{r+s+t}$$

$$\left(-\frac{ik^2}{2}\right)^{(m_2-m_1)} (\tfrac{1}{2}) \frac{CX_p\, DX_q\, E_i\ \Gamma\left(\tfrac{1}{2}(m_2-m_1+|m_2|+|m_1|+2p+2q+2i+2)\right)}{\left(\frac{\alpha}{2}+\frac{\beta}{2}+\frac{k^2}{2}-k^4/2(\alpha+\beta+k^2)\right)^{\frac{1}{2}(m_2-m_1+|m_2|+|m_1|+2p+2q+2i+2)}}$$

(B-14)

Combining (B-12) and (B-14) we have the solution to (B-9). It now only remains to include the normalization and so obtain for the (ρ, ϕ) part of the exchange matrix element:

$$(k^2)^{(m_2-m_1)} \; 2^{(|m_1|+|m_2|+2)} \beta^{m_2+1} \alpha^{|m_1|+1} (\tfrac{1}{2}n_1)! \, (\tfrac{1}{2}n_2)!$$

$$(|m_1| + \tfrac{1}{2}n_1)! \, (|m_2| + \tfrac{1}{2}n_2)! \sum_{s=0}^{\frac{1}{2}n_1} \sum_{t=0}^{\frac{1}{2}n_2} CX_s \, DX_t \, (r+s+t)! \, 2^{s+t}$$

$$(\alpha+\beta+k^2)^{-\frac{1}{2}(|m_1|+|m_2|+m_2-m_1+2s+2t+2)} \sum_{p=0}^{\frac{1}{2}n_1} \sum_{q=0}^{\frac{1}{2}n_2} \sum_{i=0}^{r+s+t}$$

$$CX_p \, DX_q \, E_i \; \frac{(\tfrac{1}{2}(m_2 - m_1 + |m_1| + |m_2| + 2p + 2q + 2i))! \; 2^{p+q+i}}{(\alpha+\beta+k^2 - k^4/(\alpha+\beta+k^2))^{\frac{1}{2}(m_2-m_1+|m_2|+|m_1|+2p+2q+2i+2)}}$$

(B-16)

We now come to the z_1-z_2-integration, which, as mentioned before, shall be treated in the most general form, for which both direct and exchange elements will be special cases. This integral is

$$I = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{a}{2}z_1^2} \, e^{-\frac{b}{2}z_1^2} \, e^{-\frac{c}{2}z_2^2} \, e^{-\frac{d}{2}z_2^2} \, H_{n_1}(\sqrt{a}\,z_1)$$

$$H_{n_2}(\sqrt{c}\;z_2) \, e^{-\frac{k^2}{2}(z_1-z_2)^2} \, H_{m_1}(\sqrt{b}\;z_1) \, H_{m_2}(\sqrt{d}\;z_2) \, dz_1 \, dz_2$$

(B-17)

It is convenient to express $H_m(ax)$ in terms of a polynomial with just x as the argument. This may be done with the formula*

$$H_m(ax) = m! \sum_{r=0}^{\frac{1}{2}m} \frac{a^{m-2r}\,(a^2-1)^r}{r!\,(m-2r)!} H_{m-2r}(x)$$

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* W. N. Bailey, Jour. London Math. Soc. 23, 291, (1948)

where "$\tfrac{1}{2}m$" means either $\tfrac{1}{2}m$ or $\tfrac{1}{2}(m-1)$, whichever is an integer.

Thus, in our case we have

$$H_{m_1}(\sqrt{b}\; z_1) = m_1! \sum_{r=0}^{[\frac{1}{2}m_1]} \frac{(\sqrt{b})^{m_1-2r}\,(b-1)^r}{r!\;(m_1-2r)!}\; H_{m_1-2r}(z_1)$$

and

$$H_{n_1}(\sqrt{a}\; z_1) = n_1! \sum_{s=0}^{[\frac{1}{2}n_1]} \frac{(\sqrt{a})^{n_1-2s}\,(a-1)^s}{s!\;(n_1-2s)!}\; H_{n_1-2s}(z_1)$$

so that, $H_{n_1}(\sqrt{a}\; z_1)\; H_{m_1}(\sqrt{b}\; z_1) = n_1!\; m_1! \sum_{s=0}^{[\frac{1}{2}n_1]} \sum_{r=0}^{[\frac{1}{2}m_1]}$

$$\frac{(\sqrt{a})^{n_1-2s}\,(a-1)^s}{s!\;(n_1-2s)!}\quad \frac{(\sqrt{b})^{m_1-2r}\,(b-1)^r}{r!\;(m_1-2r)!}\; H_{n_2-2s}(z_1)\; H_{m_1-2r}(z_1)$$

$$= n_1!\; m_1! \sum_{s=0}^{[\frac{1}{2}n_1]} \sum_{r=0}^{[\frac{1}{2}m_1]} \gamma_s\, \delta_r\; H_{n_1-2s}(z_1)\; H_{m_1-2r}(z_1)$$

where γ_s and δ_r are constants with obvious definitions.

Equation (B-17) may now be written

$$I = \int_{-\infty}^{\infty} e^{-\frac{1}{2}(c+d)z_2^2}\; H_{n_2}(\sqrt{c}\; z_2)\; H_{m_2}(\sqrt{d}\; z_2)\; dz_2$$

$$\int_{-\infty}^{\infty} e^{-\frac{1}{2}(a+b)z_1^2 - \frac{k^2}{2}(z_1^2 - 2z_1z_2 + z_2^2)}\; n_1!\; m_1! \sum_{s=0}^{[\frac{1}{2}n_1]} \sum_{r=0}^{[\frac{1}{2}m_1]} \gamma_s\, \delta_r$$

$$H_{n_1-2s}(z_1)\; H_{m_1-2r}(z_1)\quad dz_1 \qquad \text{(B-18)}$$

The z_1-integral is

$$I_1 = e^{-\frac{1}{2}(ek^2/e+k^2)\, z_2^2}\; n_1!\, m_1! \sum_{s=0}^{\lfloor \frac{1}{2}n_1 \rfloor} \sum_{r=0}^{\lfloor \frac{1}{2}m_1 \rfloor} \gamma_s\, \delta_r$$

$$\int_{-\infty}^{\infty} H_{n_1-2s}(z_1)\; H_{m_1-2r}(z_1)\, \exp\left(-\tfrac{1}{2}\left(\left(\sqrt{e+k^2}\; z_1 - k^2/\sqrt{e+k^2}\; z_2\right)\right)^2\right) dz_1$$

where $e = a + b$.

We now let $x = \sqrt{e+k^2}\; z_1$ and $y = \dfrac{k^2}{\sqrt{e+k^2}}\; z_2$ and so obtain

$$I_1 = e^{-\frac{1}{2}(ek^2/e+k^2)z_2^2}\; n_1!\, m_1! \sum_{s=0}^{\lfloor \frac{1}{2}n_1 \rfloor} \sum_{r=0}^{\lfloor \frac{1}{2}m_1 \rfloor} \gamma_s\; \delta_r \int_{-\infty}^{\infty} H_{n_1-2s}(x/\sqrt{e+k^2})$$

$$H_{m_1-2r}\,(x/\sqrt{e+k^2})\quad e^{-\frac{1}{2}(x-y)^2}\quad \frac{dx}{\sqrt{e+k^2}} \qquad \text{(B-19)}$$

We now introduce $He_n(y)$ such that,

$$H_n(\alpha x) = 2^{\frac{1}{2}n}\; He_n\,(2^{\frac{1}{2}}\alpha x)$$

and substitute into (B-19). Integrating, we then obtain*

$$I_1 = e^{-\frac{1}{2}(ek^2/e+k^2)z_2^2}\; \frac{(2\pi)^{\frac{1}{2}}\, n_1!\, m_1!}{e + k^2} \sum_{s=0}^{\lfloor \frac{1}{2}n_1 \rfloor} \sum_{r=0}^{\lfloor \frac{1}{2}m_1 \rfloor} \gamma_s\, \delta_r$$

$$\sum_{i=0}^{\min(n_1-2s,\, m_1-2r)} i!\; \binom{n_1-2s}{i} \binom{m_1-2r}{i} \left(\frac{e + k^2 - 2}{e + k^2}\right)^{\frac{1}{2}(n_1+m_1-2s-2r-2i)}$$

$$2^i\; H_{n_1+m_1-2s-2r-2i}\left(k^2\, z_2/\sqrt{e+k^2}\;\sqrt{e + k^2 - 2}\right) \qquad \text{(B-20)}$$

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* Erdelyi et al. Integral Transforms Vol.2 p.290 No.17

We turn now to the z_2-integral which is

$$I_2 = \int_{-\infty}^{\infty} e^{-\frac{1}{2}(c+d)\, z_2^{\,2}}\; e^{-\frac{1}{2}(ek^2/e+k^2)\, z_2^{\,2}}\; H_{n_2}(\sqrt{c}\, z_2)$$

$$H_{m_2}(\sqrt{d}\, z_2)\; H_{n_1+m_1-2s-2r-2i}(k^2\, z_2/\sqrt{e+k^2}\;\sqrt{e+k^2-2})\, dz_2$$

(B-21)

We let $\alpha = (c+d) + \dfrac{ek^2}{e+k^2}$

and $\beta = \dfrac{k^4}{e+k^2}$ so that (B-21) becomes

$$I_2 = \int_{-\infty}^{\infty} e^{-\frac{1}{2}\alpha z_2^{\,2}}\; H_{n_2}(\sqrt{c}z_2)\; H_{m_2}(\sqrt{d}\;z_2)\; H_{n_1+m_1-2s-2r-2i}(\sqrt{\beta}\, z_2/\sqrt{e+k^2-2})\, dz_2$$

(B-22)

We make the further substitution,

$2x^2 = \frac{1}{2}\alpha z_2^2$ and so obtain

$$I_2 = \int_{-\infty}^{\infty} e^{-2x^2}\; H_{n_2}(2\sqrt{\tfrac{c}{\alpha}}\;x)\; H_{m_2}(2\sqrt{\tfrac{d}{\alpha}}\;x)\; H_{n_1+m_1-2s-2r-2i}(2\sqrt{\beta}\,x/\sqrt{\alpha}\sqrt{e+k^2-2})$$

$$\frac{2}{\sqrt{\alpha}}\; dx \qquad \text{(B-23)}$$

$$\text{Now, } H_{n_2}(2\sqrt{\tfrac{c}{\alpha}}\,x) = \sum_{\ell=0}^{\frac{1}{2}n_2} \frac{n_2!\,(2\sqrt{\frac{c}{\alpha}})^{n_2-2\ell}\,(4\frac{c}{\alpha}-1)^{\ell}}{\ell!\,(n_2-2\ell)!}\, H_{n_2-2\ell}(x)$$

$$= n_2! \sum_{\ell=0}^{\frac{1}{2}n_2} \epsilon_\ell\, H_{n_2-2\ell}(x)$$

Similarly, $H_{m_2}(2\sqrt{\frac{d}{\alpha}}\,x)$ may be written

$$m_2! \sum_{j=0}^{\frac{1}{2}m_2} k_j\, H_{m_2-2j}(x)$$ where k_j is the appropriate

function of m_2, d and α, and,

$$H_{n_1+m_1-2s-2r-2i}\left(\frac{2\sqrt{\beta}\;x}{\sqrt{\alpha}\sqrt{e+k^2-2}}\right) = \sum_{t=0}^{\frac{1}{2}(n_1+m_1-2s-2r-2i)} \frac{(n_1+m_1-2s-2r-2i)!}{t!\,(n_1+m_1-2s-2r-2i-2t)!}$$

$$\left(2\sqrt{\frac{\beta}{\alpha}}\right)^{n_1+m_1-2s-2r-2i-2t} \left(\sqrt{e+k^2-2}\right)^{-n_1-m_1+2s+2r+2i+2t}$$

$$\left(\frac{4\beta}{\alpha(e+k^2-2)} - 1\right)^t H_{n_1+m_1-2s-2r-2i-2t}(x)$$

$$= \sum_{t=0}^{\frac{1}{2}(n_1+m_1-2s-2r-2i)} (e+k^2-2)^{-\frac{1}{2}(n_1+m_1-2s-2i+2r)}\; h_t\; H_{n_1+m_1-2s-2r-2i-2t}(x)$$

Substituting into (B-23) we obtain

$$I_2 = \sum_{t=0}^{\frac{1}{2}(n_1+m_1-2s-2r-2i)} \sum_{\ell=0}^{\frac{1}{2}m_2} \sum_{j=0}^{\frac{1}{2}m_2} h_t\, \epsilon_\ell\, k_j \frac{2}{\sqrt{\alpha}} (e+k^2-2)^{-\frac{1}{2}(n_1+m_1-2s-2r-2i)}$$

$$n_2!\; m_2! \int_{-\infty}^{\infty} e^{-2x^2}\, H_{n_2-2\ell}(x)\; H_{m_2-2j}(x)\; H_{n_1+m_1-2r-2s-2i-2t}(x)\, dx$$

$$= \frac{2}{\sqrt{\alpha}}\; m_2!\; m_2! \sum_{t=0}^{\frac{1}{2}(n_1+m_1-2s-2r-2i)} \sum_{\ell=0}^{\frac{1}{2}n_2} \sum_{j=0}^{\frac{1}{2}m_2} h_t \epsilon_\ell\, k_j\, (e+k^2-2)^{-\frac{1}{2}(n_1+m_1-2s-2r-2i}$$

$$\frac{2}{\pi}^{\frac{1}{2}(m_1+n_1-2s-2r-2i-2t+n_2-2\ell+m_2-2j-1)}$$

$$\times \Gamma\left(\frac{m_1+n_1-2s-2r-2i-2t+n_2-2\ell-m_2+2j+1}{2}\right)$$

$$\Gamma\left(\frac{m_1+n_1-2s-2r-2i-2t+m_2-2j-n_2+2\ell+1}{2}\right) \qquad \text{(B-24)}^{*}$$

$$\Gamma\left(\frac{n_2-2\ell+m_2-2j-m_1-n_1+2s+2r+2i+2t+1}{2}\right)$$

Thus, combining (B-20) and (B-24) and including the normalization of the wavefunctions, we obtain for the z-integration of the generalized matrix element

$$I = \frac{2\ (n_1!\ n_2!\ m_1!\ m_2!)^{1/2}\ (abcd)^{1/4}}{\sqrt{\alpha}} \sum_{s=0}^{\frac{1}{2}n_1} \sum_{r=0}^{\frac{1}{2}m_1} \gamma_s\ \delta_r$$

$$\sum_{i=0}^{\min(n_1-2s,\,m_1-2r)} i!\ \binom{n_1-2s}{i} \binom{m_1-2r}{i} \left(\frac{1}{e+k^2}\right)^{\frac{1}{2}(n_1+m_1-2s-2r-2i+1)}$$

$$\sum_{t=0}^{\frac{1}{2}(n_1+m_1-2s-2r-2i)} \sum_{\ell=0}^{\frac{1}{2}n_2} \sum_{j=0}^{\frac{1}{2}m_2} h_t\, \epsilon_\ell\, k_j\ 2^{-s-r-t-\ell-j} \times$$

$$\times \Gamma'\left(\frac{m_1+n_1-2s-2r-2i-2t+n_2-2\ell-m_2+2j+1}{2}\right)$$

$$\times \Gamma'\left(\frac{m_1+n_1+m_2-n_2-2s-2r-2i-2t-2j+2\ell+1}{2}\right) \qquad \text{(B-26)}$$

$$\times \Gamma'\left(\frac{n_2+m_2-m_1-n_1-2\ell-2j+2s+2r+2i+2t+1}{2}\right)$$

---

* Titchmarsh, Jour. London Math. Soc. 23, 15, (1948)

Note that in (B-26) $(\Gamma(\frac{1}{2}))^3$ has been removed by cancellation with the normalization and hence we have written Γ' in place of Γ.

We thus have in (B-26), (B-16) and (B-8) all the calculations necessary for the diagonal Slater determinant matrix elements. To satisfy the requirements of non-diagonal elements as well would merely involve the use of four different oscillator constants, instead of only two, in the derivation of (B-8).

It is of interest to note that were we to use a Cartesian basis rather than a cylindrical one we would need to use only equation (B-26) three times, once each for the x-, y-, and z-integrations respectively. Such a basis is, of course, unsuited to a problem such as the one considered in this thesis, because of the inherent cylindrical symmetry.

It should also be noted that when the oscillator constants are all equal there is a much more simple and elegant solution to the z_1-z_2-part of the matrix elements. This solution is shown in Appendix C.

APPENDIX C: THE z_1-z_2-PART OF THE MATRIX ELEMENTS FOR THE CASE OF EQUAL OSCILLATOR CONSTANTS

We are faced with an integral of the form

$$I = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-az_1^2} e^{-az_2^2} H_{n_1}(\sqrt{a}\, z_1) H_{n_2}(\sqrt{a}\, z_2)$$

$$e^{-\frac{k^2}{2}(z_1 - z_2)^2} H_{m_1}(\sqrt{a}\, z_1) H_{m_2}(\sqrt{a}\, z_2)\, dz_1\, dz_2.$$

We first set $H_n(y) = 2^{\frac{1}{2}n} He_n(2^{\frac{1}{2}} y)$ and so obtain,

$$I = \int_{-\infty}^{\infty} e^{-az_2^2 + k^4 z_2^2/2(2a+k^2) - \frac{k^2}{2} z_2^2} 2^{\frac{1}{2}(n_2+m_2)}$$

$$He_{n_2}(\sqrt{2a}\, z_2) He_{m_2}(\sqrt{2a}\, z_2)\, dz_2 \int_{-\infty}^{\infty} e^{-\frac{1}{2}\left(\sqrt{2a+k^2}\, z_1 - \frac{k^2}{\sqrt{2a+k^2}} z_2\right)^2}$$

$$2^{\frac{1}{2}(n_1+m_1)} He_{n_1}(\sqrt{2a}\, z_1) He_{m_1}(\sqrt{2a}\, z_1)\, dz_1 \qquad \text{(C-1)}$$

Let $x = \sqrt{2a + k^2}\, z_1$ and $y = \frac{k^2}{\sqrt{2a+k^2}} z_2$ and

substitute into (C-1) to obtain

$$I = \int_{-\infty}^{\infty} e^{-az_2^2 + k^4 z_2^2/2(2a+k^2) - \frac{k^2}{2} z_2^2} 2^{\frac{1}{2}(n_2+m_2)} He_{n_2}(\sqrt{2a}\, z_2)$$

$$He_{m_2}(\sqrt{2a}\, z_2)\, dz_2 \int_{-\infty}^{\infty} e^{-\frac{1}{2}(x-y)^2} 2^{\frac{1}{2}(n_1+m_1)} He_{n_1}\left(\sqrt{\frac{2a}{2a+k^2}}\, x\right)$$

$$He_{m_1}\left(\sqrt{\frac{2a}{2a+k^2}}\, x\right) \frac{dx}{\sqrt{2a+k^2}} \qquad \text{(C-2)}$$

But, the x-integration yields

$$\frac{2^{\frac{1}{2}(n_1+m_1)}}{\sqrt{2a+k^2}} \quad (2\pi)^{\frac{1}{2}} \sum_{\ell=0}^{\min(n_1,m_1)} \ell! \binom{n_1}{\ell} \binom{m_1}{\ell} \left(\frac{k^2}{2a+k^2}\right)^{\frac{1}{2}(m_1+n_1-2\ell)}$$

$$\times \, He_{m_1+n_1-2\ell}\left(\frac{\sqrt{2a}}{k} \, y\right) \quad * \qquad (C\text{-}3)$$

We thus must now consider the integral

$$\int_{-\infty}^{\infty} e^{-w^2} \; 2^{-\frac{1}{2}(m_1+n_1-2\ell)} \; H_{n_2}\left(\sqrt{\frac{2a^2+ak^2}{2a^2+2ak^2}} \, w\right) H_{m_2}\left(\sqrt{\frac{2a^2+ak^2}{2a^2+2ak^2}} \, w\right)$$

$$H_{m_1+n_1-2\ell}\left(\frac{kw}{\sqrt{2a+2k^2}}\right) \sqrt{\frac{2a+k^2}{2(a^2+ak^2)}} \; dw \qquad (C\text{-}4)$$

where we have set $w = \sqrt{\frac{2(a^2+ak^2)}{k^4}} \; y$ and used the fact that $He_n(y) = 2^{-\frac{1}{2}n} \; H_n(2^{-\frac{1}{2}}y)$.

(C-4) may be integrated to obtain **

$$(-1)^{r-m_1-n_1+2\ell} \; 2^{2r} \, \Gamma(r+\tfrac{1}{2}) \left(\frac{k}{\sqrt{2a+2k^2}}\right)^{n_2+m_2}$$

$$\times \left(\sqrt{\frac{2a^2+ak^2}{2a^2+2ak^2}}\right)^{m_1+n_1-2\ell} \; 2^{-\frac{1}{2}(m_1+n_1-2\ell)} \sqrt{\frac{2a+k^2}{2(a^2+ak^2)}}$$

$$\times \, F\left(\begin{matrix}-n_2, -m_2; \\ \tfrac{1}{2}-r\end{matrix} \; \frac{a+k^2}{2k^2}\right) \qquad (C\text{-}5)$$

---

* Erdelyi et al - Tables of Integral Transforms, Vol.2, p.291

** W. N. Bailey - Jour. London Math. Soc. 23, 295, (1948) where $2r = m_2 + n_2 + m_1 + n_1 - 2\ell$ and $F\left({a,\, b; \atop c}\; z\right) = \sum_{n=0} \frac{(a)_n\,(b)_n}{n!\;(c)_n}\, z^n$ - the hypergeometric series.

It should be noted that the integral is zero if $(n_2 + m_2 + m_1 + n_1 - 2\ell)$ is odd so that r is always an integer.

Rearranging (C-5) and, with (C-3), substituting into (C-2) we obtain

$$I = \frac{2^{\frac{1}{2}(n_1+m_1+n_2+m_2)}}{\sqrt{a^2+ak^2}}\,(\pi)^{\frac{1}{2}} \sum_{\ell=0}^{\min(m_1,n_1)} \ell!\,\binom{n_1}{\ell}\binom{m_1}{\ell}$$

$$\times \left(\frac{k^2}{2a+k^2}\right)^{\frac{1}{2}(m_1+n_1-2\ell)} (-1)^{\frac{1}{2}(n_2+m_2-n_1-m_1+2\ell)}$$

$$\times\, \Gamma(r+\tfrac{1}{2}) \left(\frac{k}{\sqrt{a+k^2}}\right)^{n_2+m_2} \times \left(\sqrt{\frac{2a^2+ak^2}{a^2+ak^2}}\right)^{m_1+n_1-2\ell}$$

$$\times\, F\left({-n_2,\, -m_2; \atop \frac{1}{2}-r}\; \frac{a+k^2}{2k^2}\right) \qquad \text{(C-6)}$$

In deriving (C-6) we have once again used unnormalized wavefunctions. However, the normalization may be added in a straightforward way as demonstrated in Appendix B.

CAPTIONS FOR FIGURES

Figure 1: The kinetic energies' deformation-dependence is plotted for a constant nuclear volume, $a^2b = 0.064$. KEDS is the kinetic energy of the $2s_o'$ state and KEDO, KED1 and KED2 are the kinetic energies of the d_o', $d_{\pm1}$ and $d_{\pm2}$ states respectively.

Figures 2 and 3: The deformation-dependence of typical interaction matrix elements is plotted for a constant nuclear volume, $a^2b = 0.064$. The elements labelled VADO and VAD2 are direct elements between $1s_o$, $1p_{\pm1}$ wave functions and $1d_o'$ and $1d_{\pm2}$ wave functions respectively. A equals s for the $1s_o$ state, 0 for the $1p_o$ state and 1 for the $1p_{\pm1}$ state. The corresponding exchange elements are labelled with the same name followed by an X.

Figures 4 to 7: The binding energy is plotted as a function of deformation for various configurations in the first subshell of the 2s-1d shell. The nucleus, configuration and value of the Majorana exchange parameter used are indicated on the diagrams in each case.

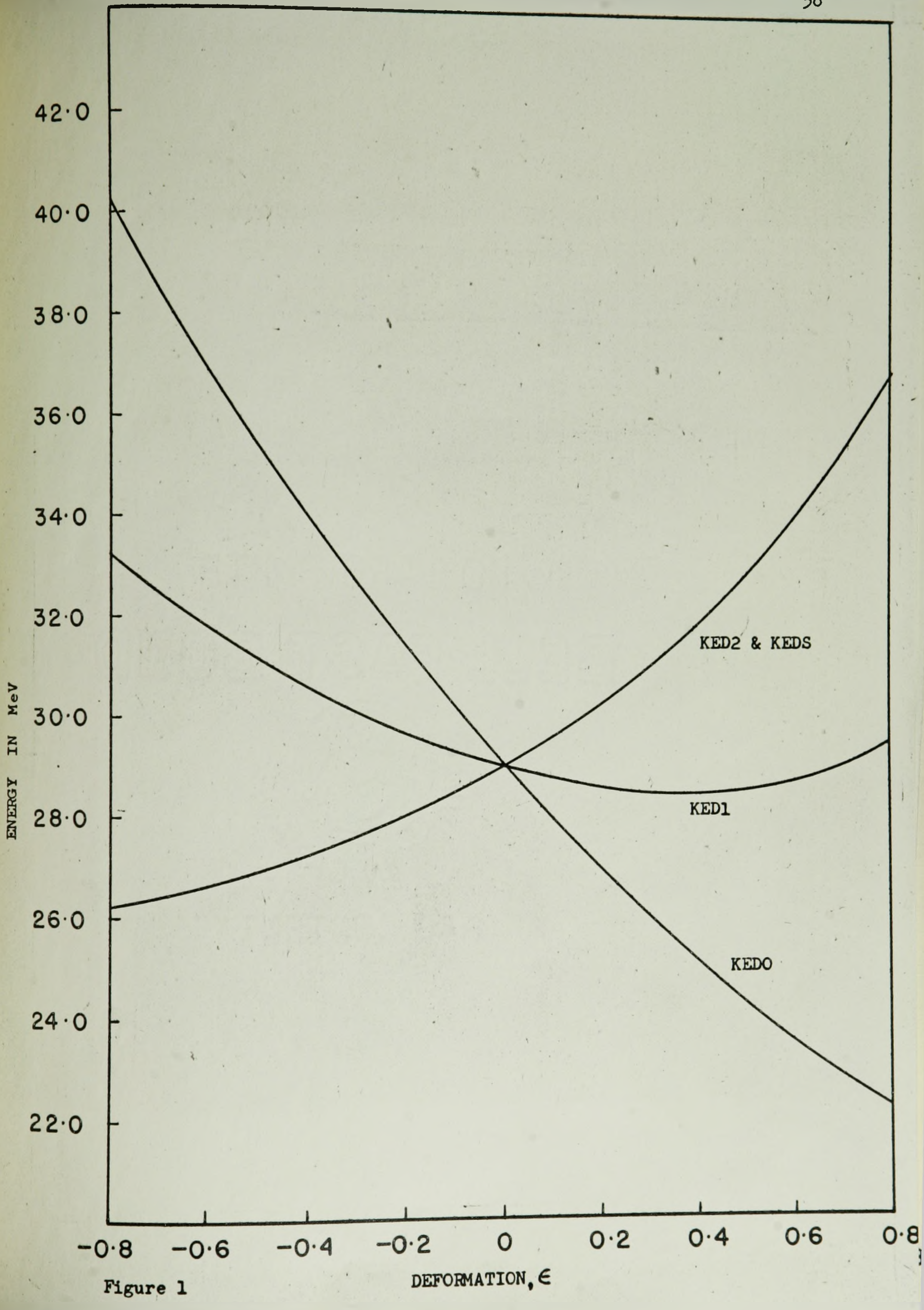

42·0
40·0
38·0
36·0
34·0
32·0
30·0
28·0
26·0
24·0
22·0
ENERGY IN MeV
KED2 & KEDS
KED1
KEDO
−0·8
−0·6
−0·4
−0·2
0
0·2
0·4
0·6
0·8
DEFORMATION, ∈

Figure 1

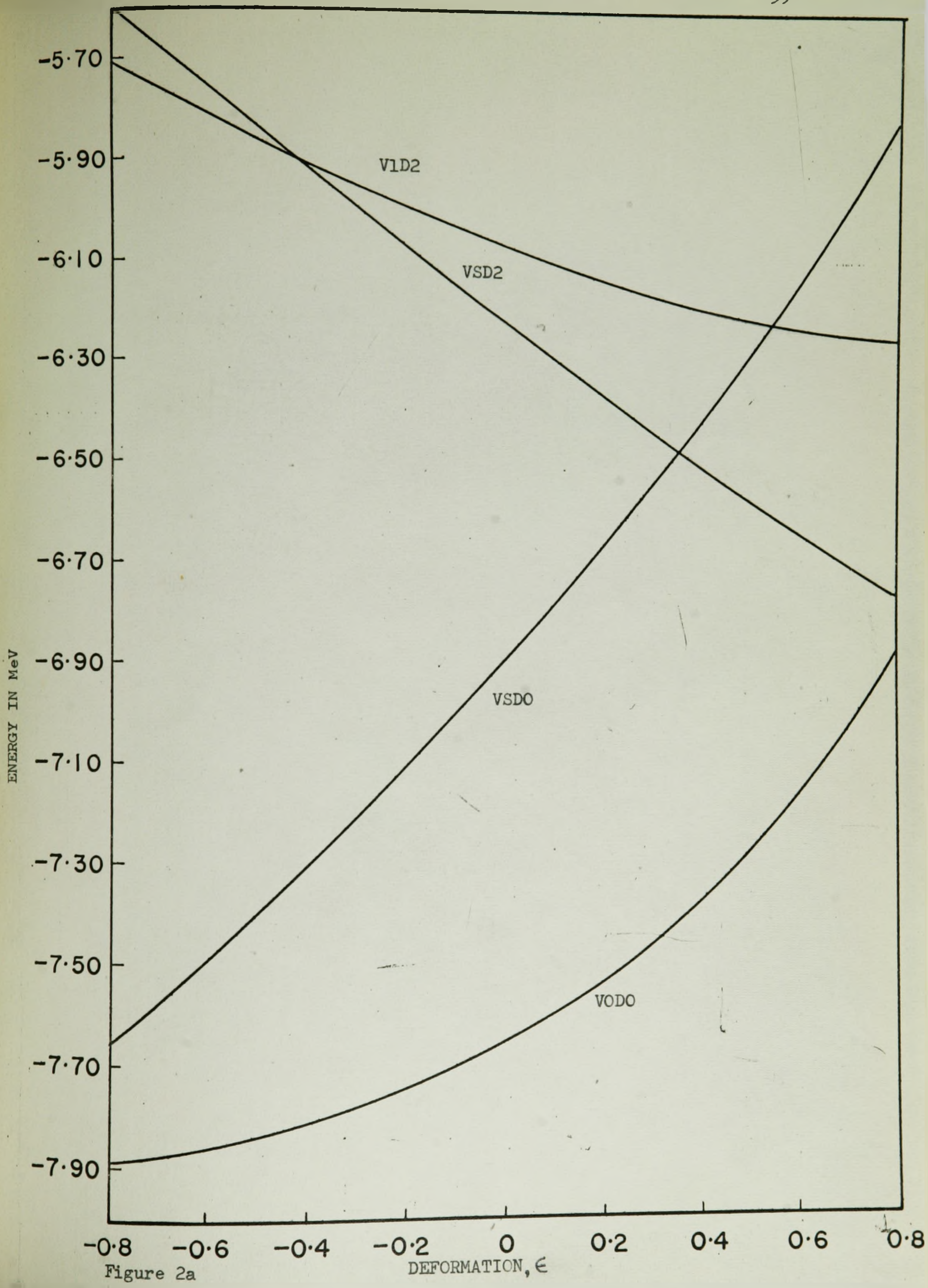

ENERGY IN MeV
-5·70
-5·90
-6·10
-6·30
-6·50
-6·70
-6·90
-7·10
-7·30
-7·50
-7·70
-7·90
V1D2
VSD2
VSDO
VODO
-0·8
-0·6
-0·4
-0·2
0
0·2
0·4
0·6
0·8
DEFORMATION, ∈

Figure 2a

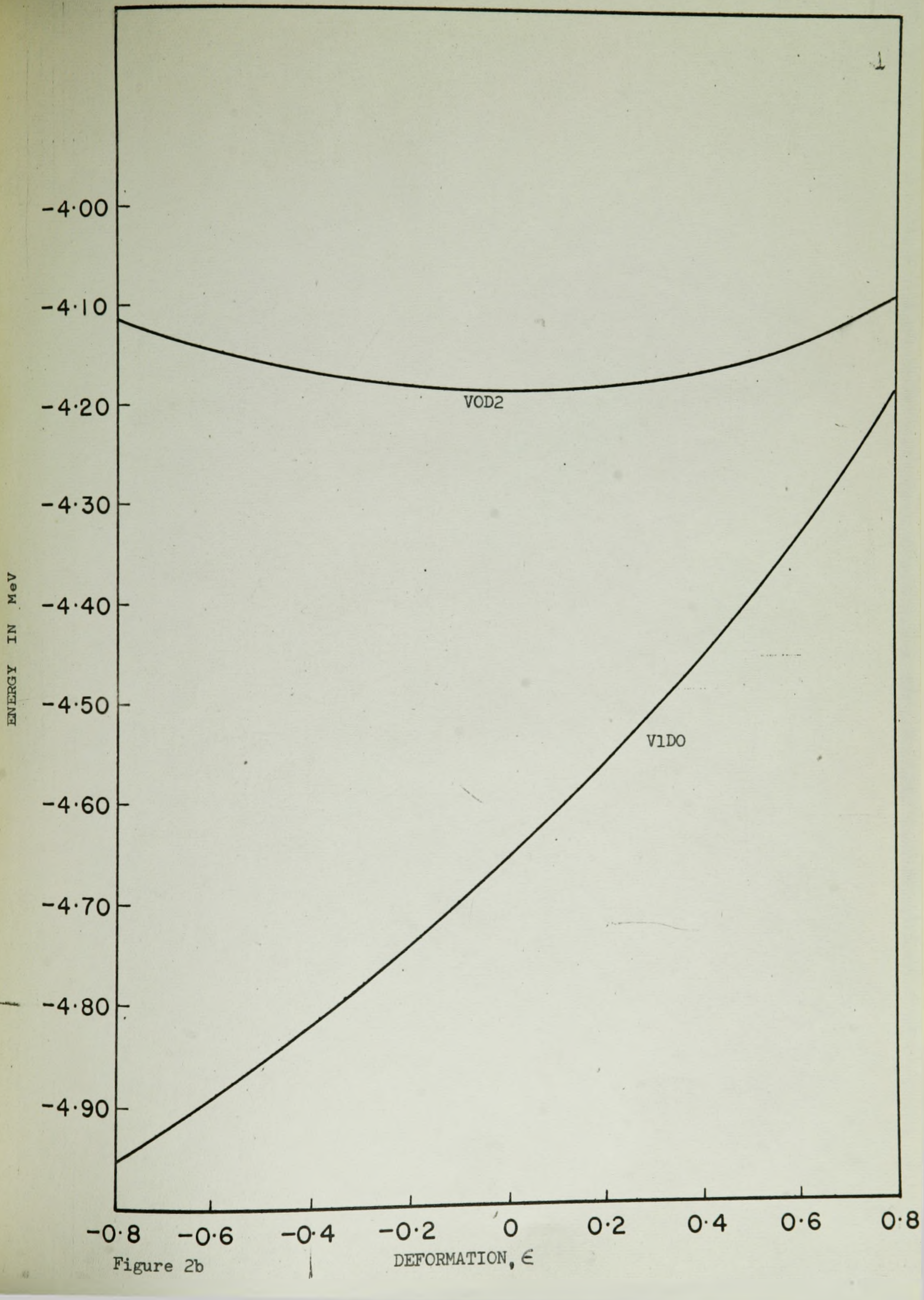
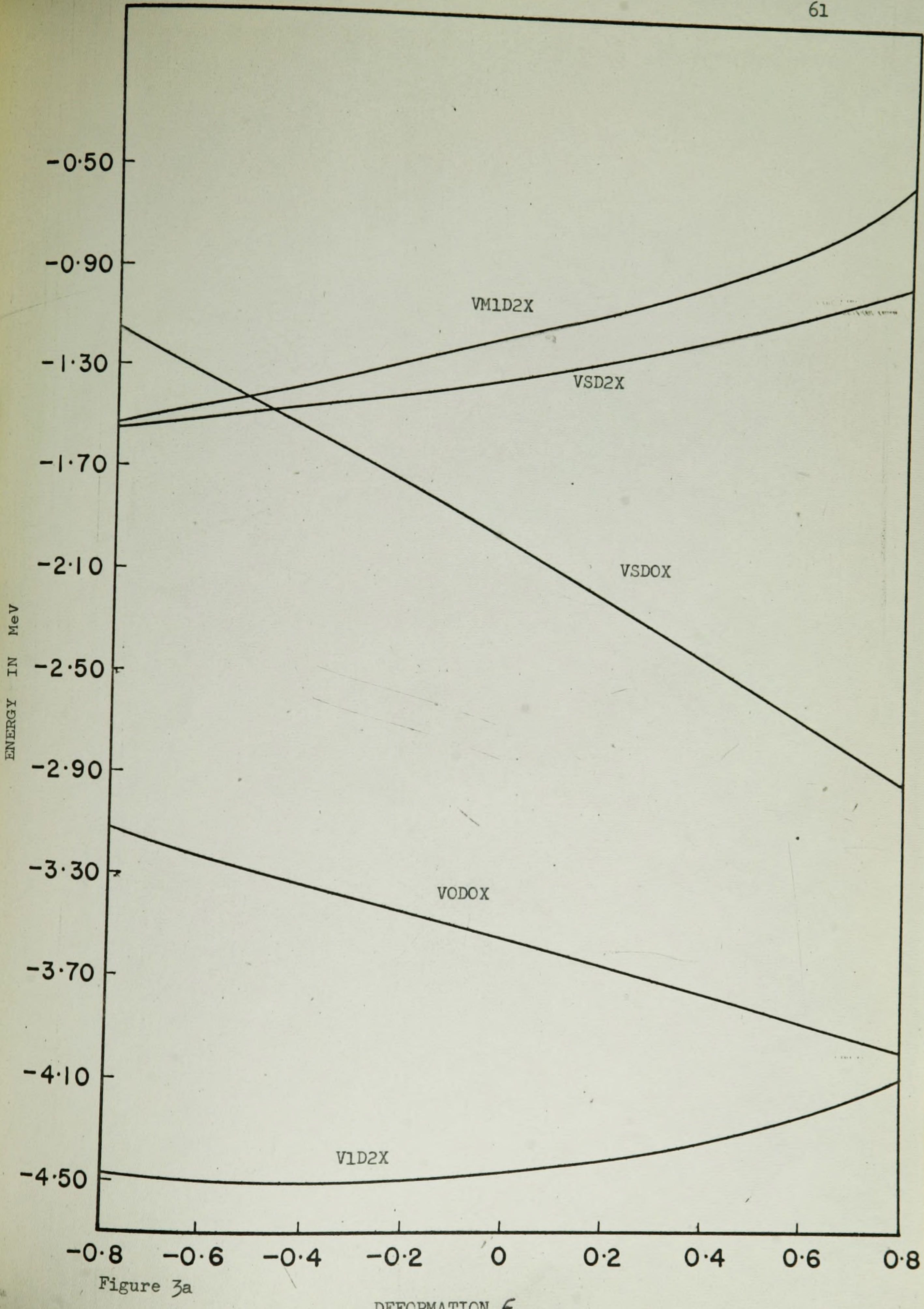

-4·00
-4·10
-4·20
-4·30
-4·40
-4·50
-4·60
-4·70
-4·80
-4·90
ENERGY IN MeV
VOD2
V1DO
-0·8
-0·6
-0·4
-0·2
0
0·2
0·4
0·6
0·8
DEFORMATION, ∈

Figure 2b



-0·50
-0·90
-1·30
-1·70
-2·10
-2·50
-2·90
-3·30
-3·70
-4·10
-4·50
ENERGY IN MeV
VM1D2X
VSD2X
VSDOX
VODOX
V1D2X
-0·8
-0·6
-0·4
-0·2
0
0·2
0·4
0·6
0·8
DEFORMATION, ϵ

Figure 3a

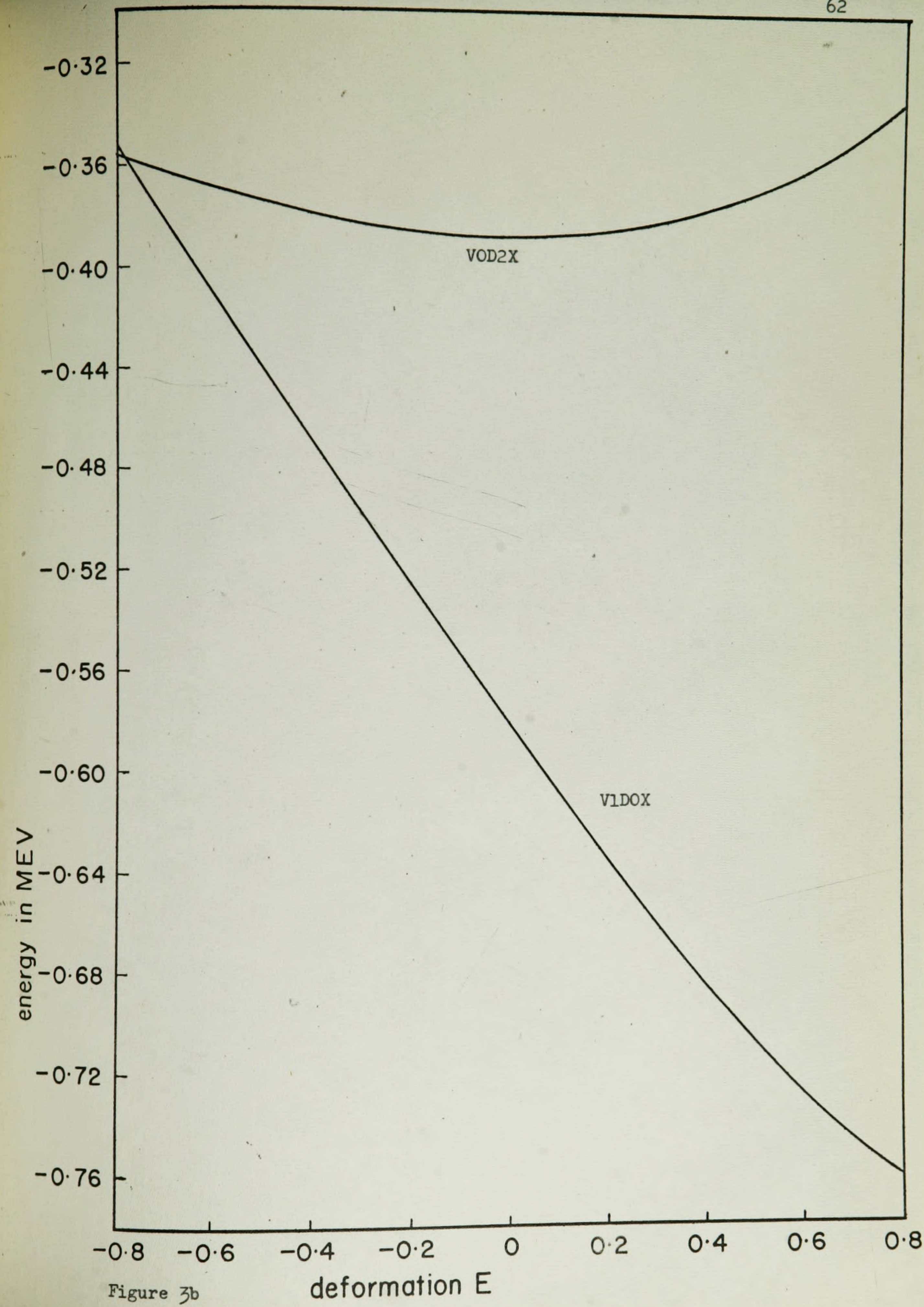

-0·32
-0·36
-0·40
-0·44
-0·48
-0·52
-0·56
-0·60
-0·64
-0·68
-0·72
-0·76
energy in MEV
VOD2X
V1DOX
-0·8
-0·6
-0·4
-0·2
0
0·2
0·4
0·6
0·8
deformation E

Figure 3b

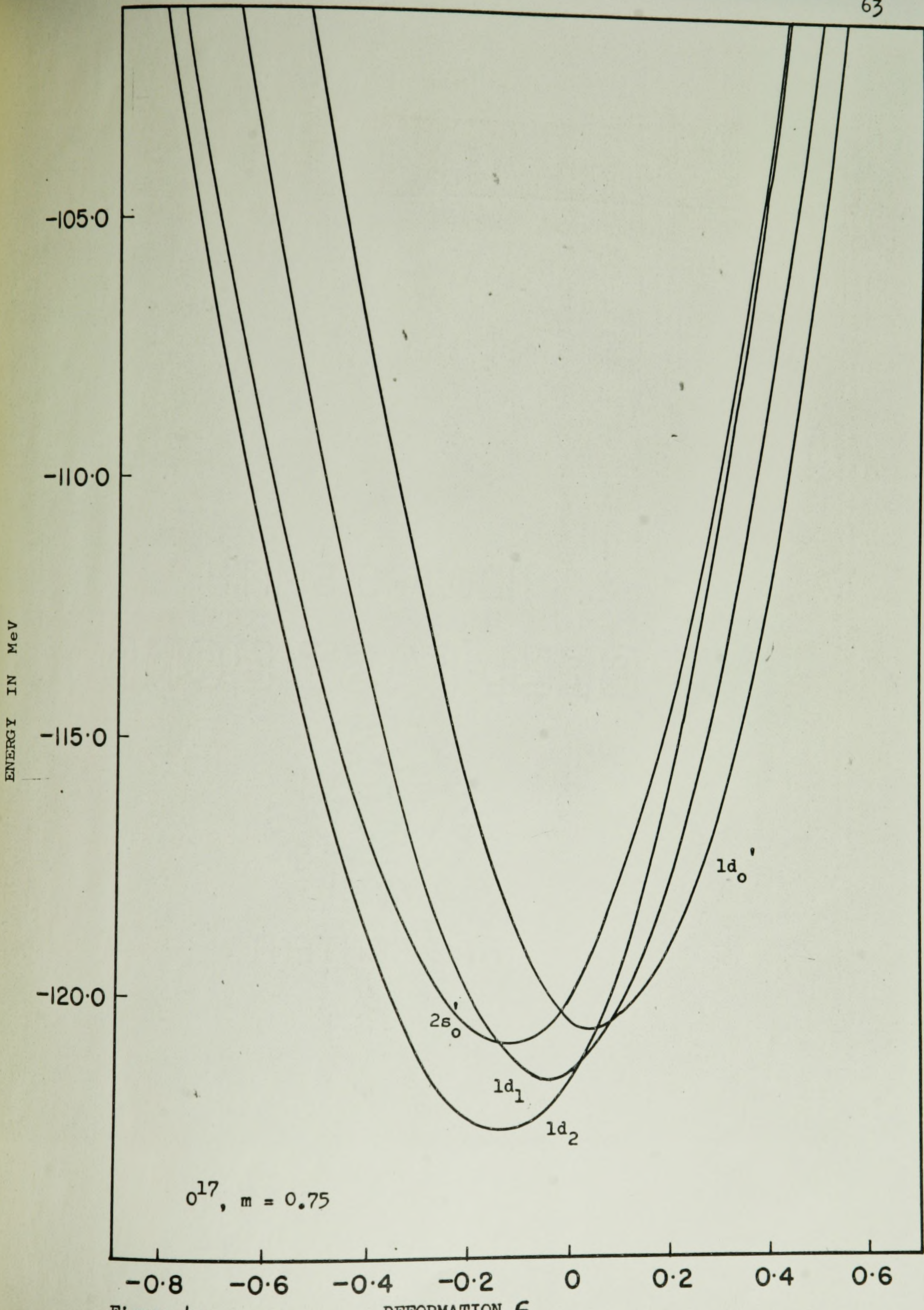

ENERGY IN MeV
-105·0
-110·0
-115·0
-120·0
1d$_0$'
2s$_0$'
1d$_1$
1d$_2$
O^{17}, m = 0.75
−0·8
−0·6
−0·4
−0·2
0
0·2
0·4
0·6
DEFORMATION, ∈

Figure 4a

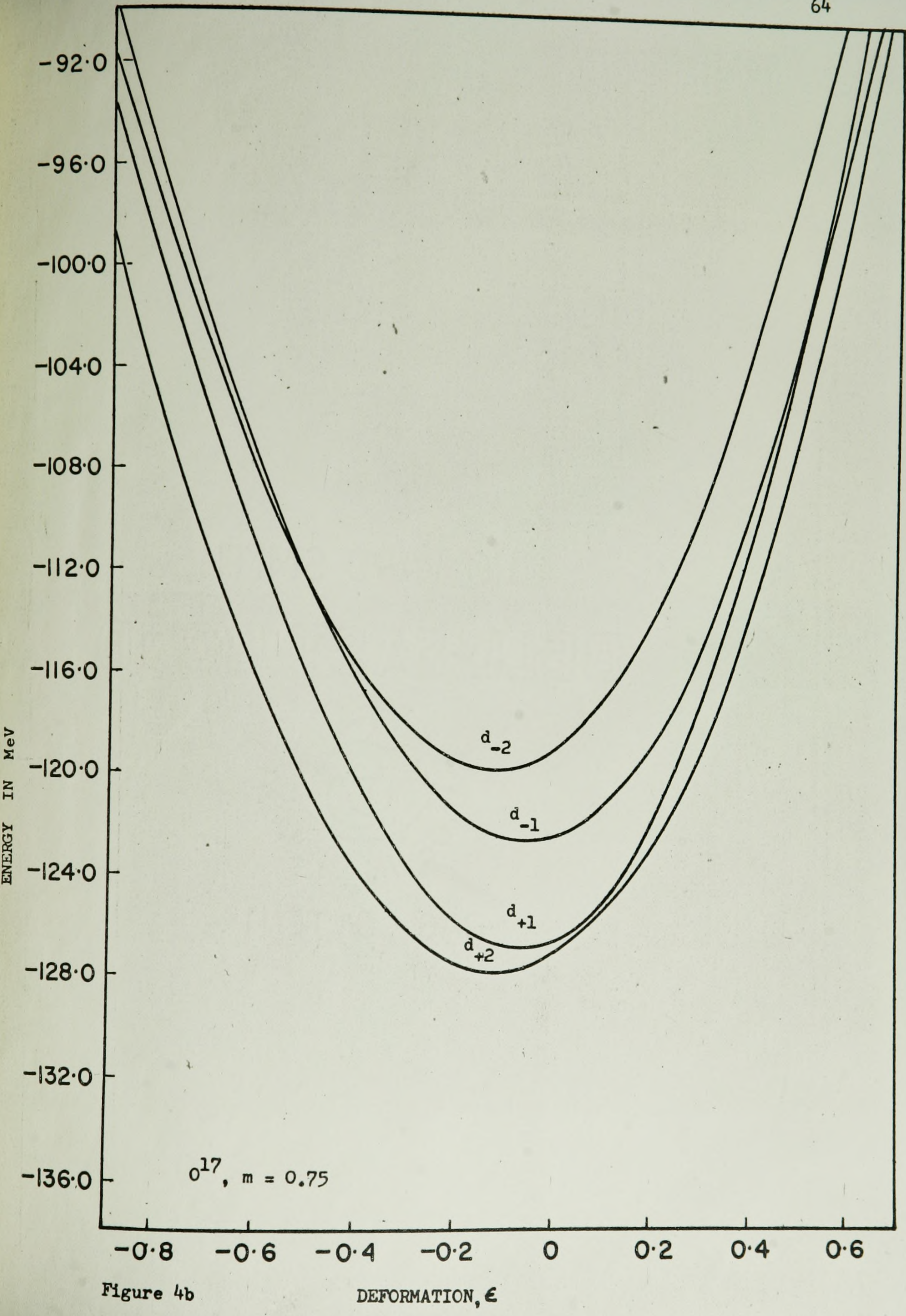
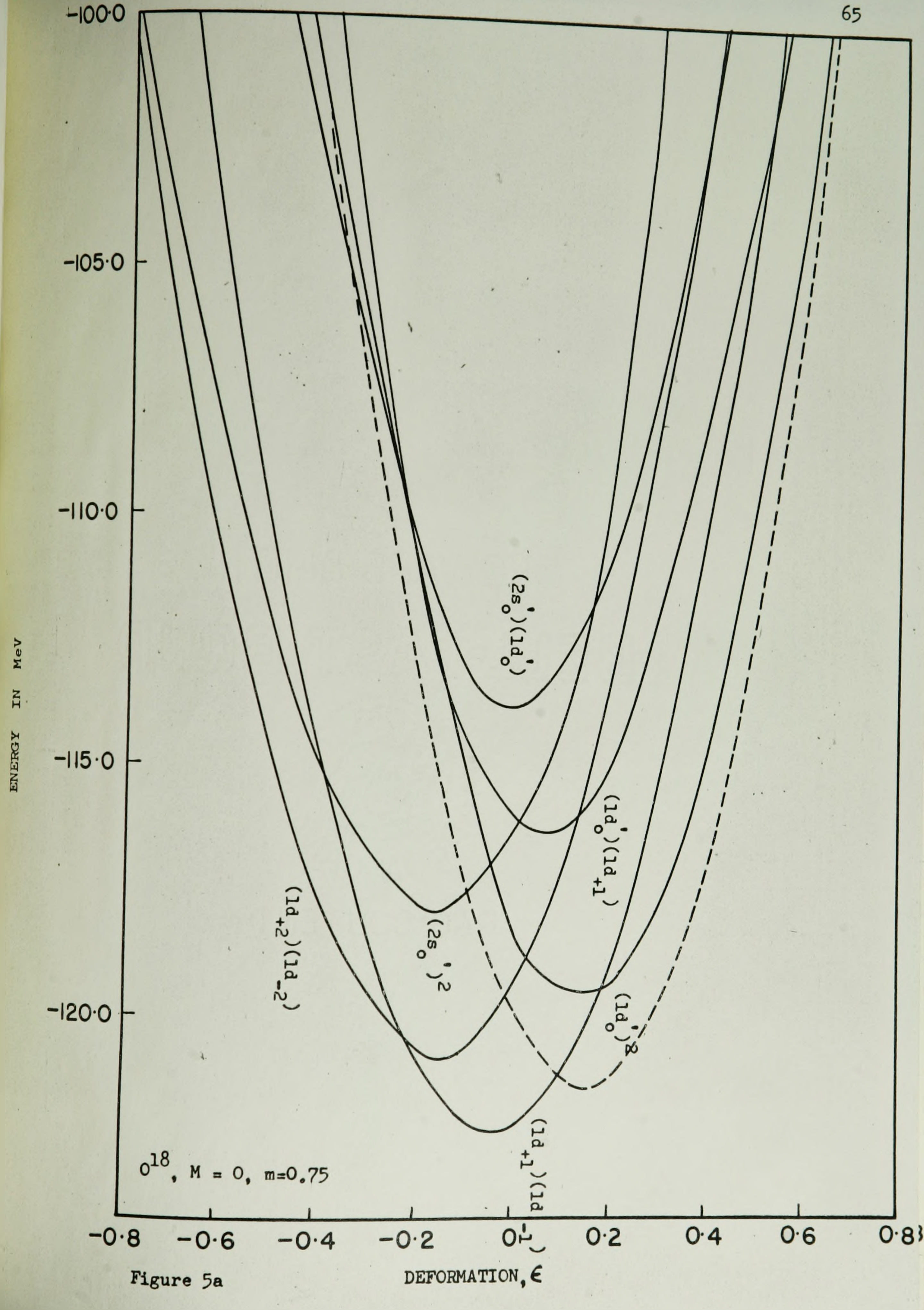

-92·0
-96·0
-100·0
-104·0
-108·0
-112·0
-116·0
-120·0
-124·0
-128·0
-132·0
-136·0
ENERGY IN MeV
d_{-2}
d_{-1}
d_{+1}
d_{+2}
O^{17}, m = 0.75
−0·8
−0·6
−0·4
−0·2
0
0·2
0·4
0·6
DEFORMATION, ϵ

Figure 4b



-100.0
-105.0
-110.0
-115.0
-120.0
ENERGY IN MeV
$(2s_o')(1d_o')$
$(1d_o')(1d_{+1})$
$(2s_o')^2$
$(1d_{+2})(1d_{-2})$
$(1d_o')^2$
$(1d_{+1})(1d_{-1})$
O^{18}, M = 0, m=0.75
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
DEFORMATION, ϵ

Figure 5a

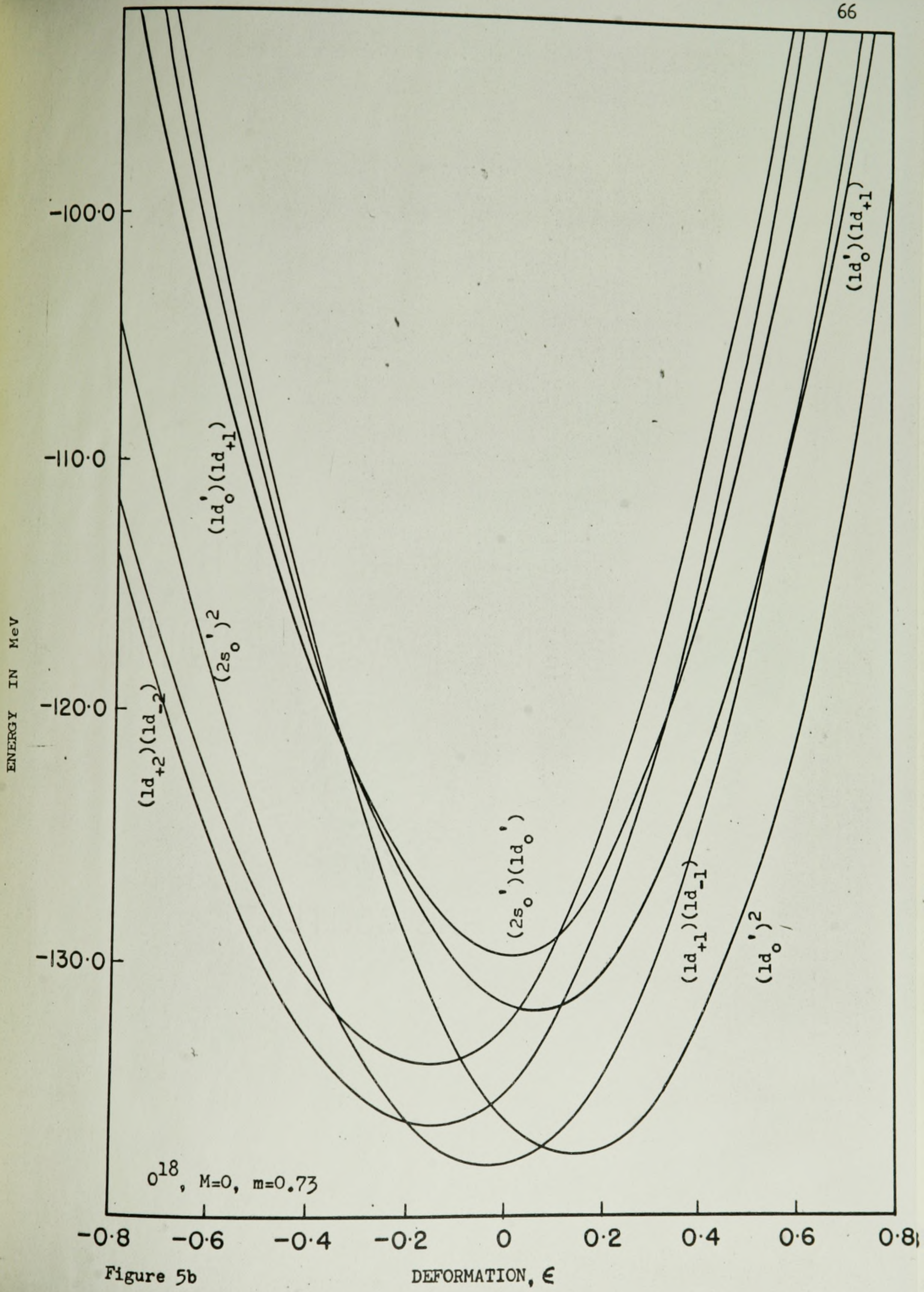

-100·0
-110·0
-120·0
-130·0
ENERGY IN MeV
$(1d_o')(1d_{+1})$
$(2s_o')^2$
$(1d_{+2})(1d_{-2})$
$(2s_o')(1d_o')$
$(1d_{+1})(1d_{-1})$
$(1d_o')^2$
$(1d_o')(1d_{+1})$
O^{18}, M=0, m=0.73
-0·8
-0·6
-0·4
-0·2
0
0·2
0·4
0·6
0·8
DEFORMATION, ϵ

Figure 5b

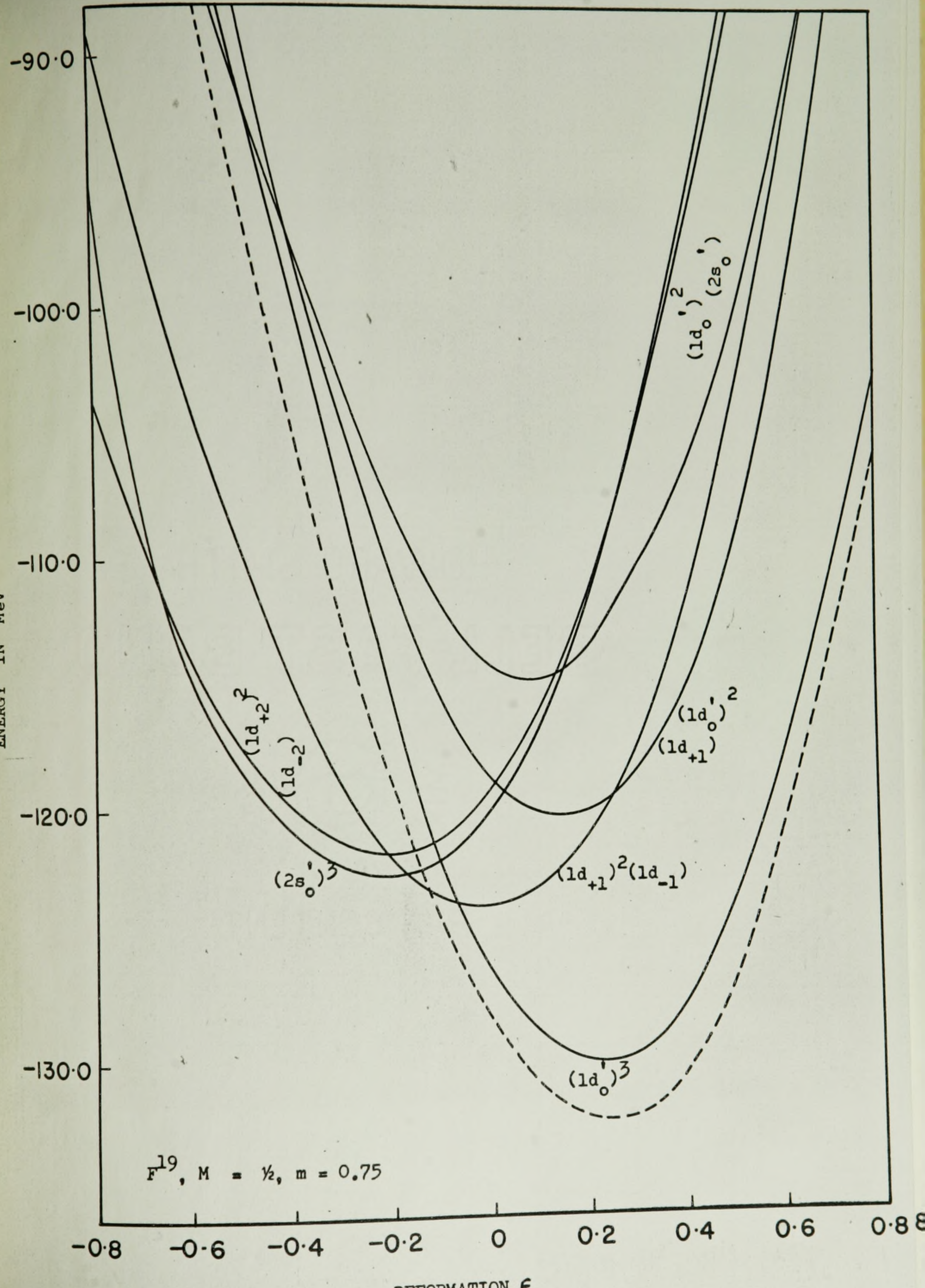

-90·0
-100·0
-110·0
-120·0
-130·0
ENERGY IN MeV
$(1d_o')^2(2s_o')$
$(1d_o')^2(1d_{+1})$
$(1d_{+2})^2(1d_{-2})$
$(2s_o')^3$
$(1d_{+1})^2(1d_{-1})$
$(1d_o')^3$
F^{19}, M = ½, m = 0.75
-0·8
-0·6
-0·4
-0·2
0
0·2
0·4
0·6
0·8
DEFORMATION, ε

Figure 6

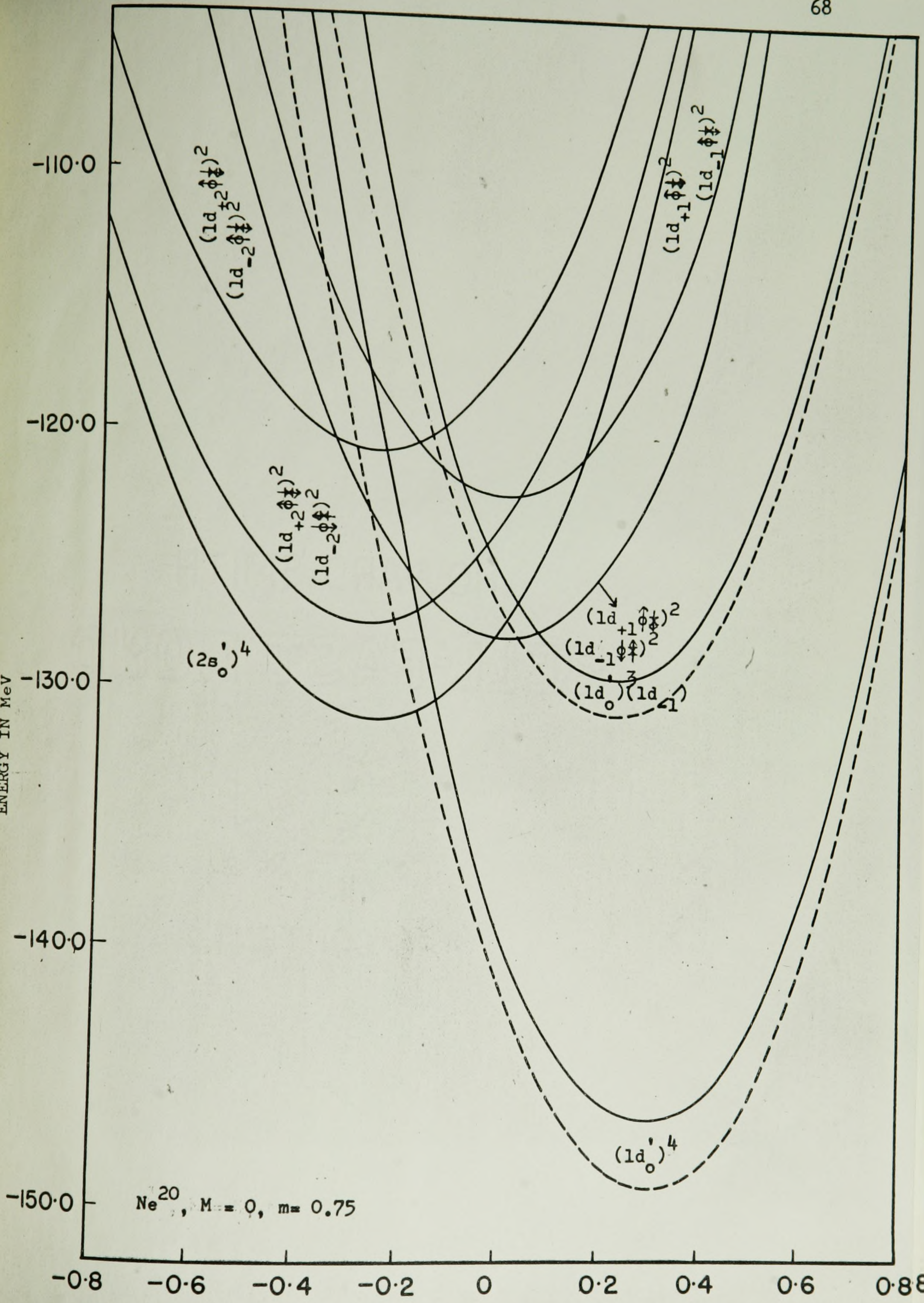
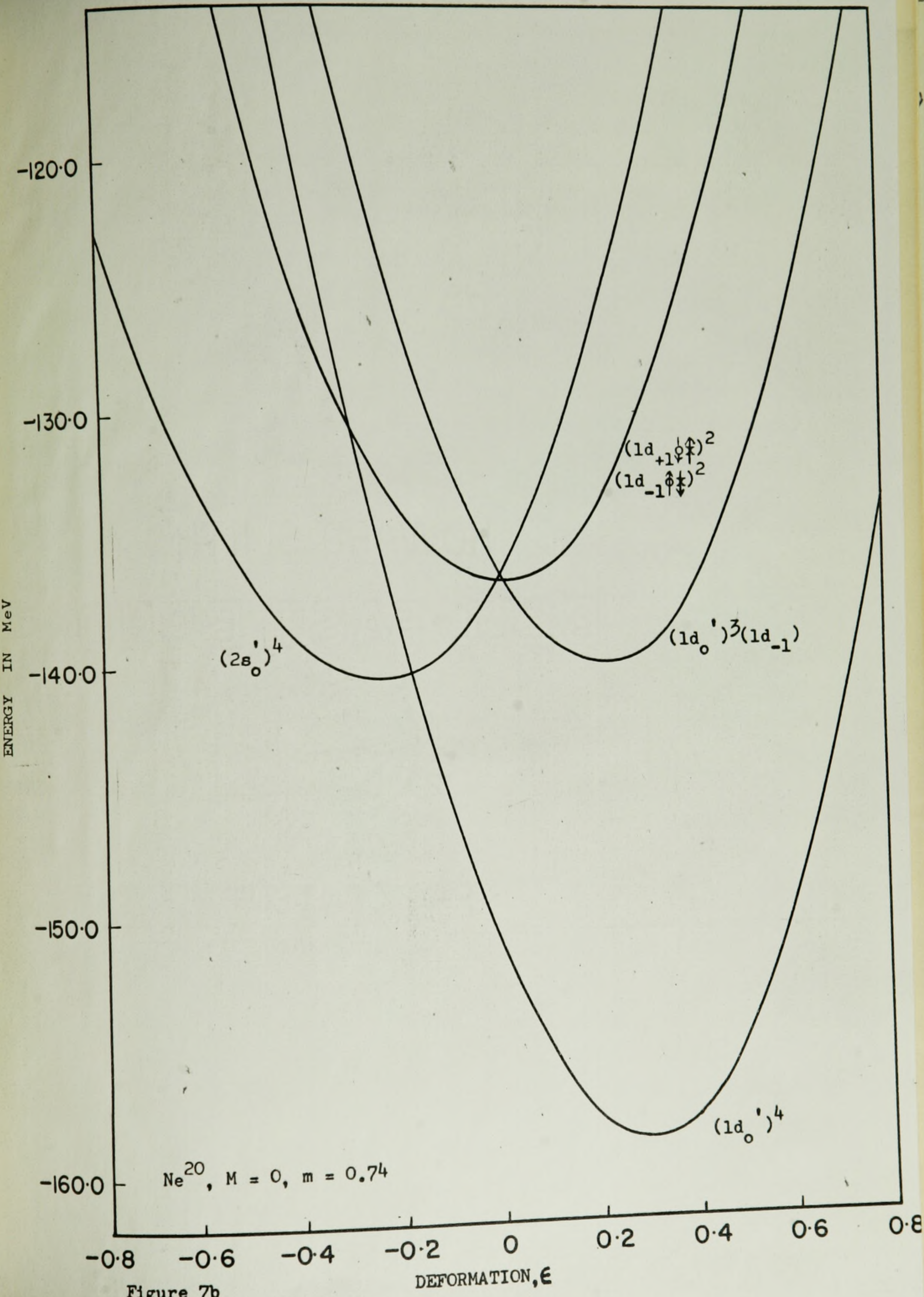

ENERGY IN MeV
-110·0
-120·0
-130·0
-140·0
-150·0
-0·8
-0·6
-0·4
-0·2
0
0·2
0·4
0·6
0·8
DEFORMATION, ϵ
Ne^{20}, M = 0, m = 0.75
(2s$_o'$)^4
(1d$_o'$)^4
(1d$_o$)(1d$_{-1}$)^3

Figure 7a



-120·0
-130·0
-140·0
-150·0
-160·0
ENERGY IN MeV
-0·8
-0·6
-0·4
-0·2
0
0·2
0·4
0·6
0·8
DEFORMATION, ϵ
$(1d_{+1}\downarrow\uparrow)^2$
$(1d_{-1}\uparrow\downarrow)^2$
$(1d_o')^3(1d_{-1})$
$(2s_o')^4$
$(1d_o')^4$
Ne^{20}, M = 0, m = 0.74

Figure 7b

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