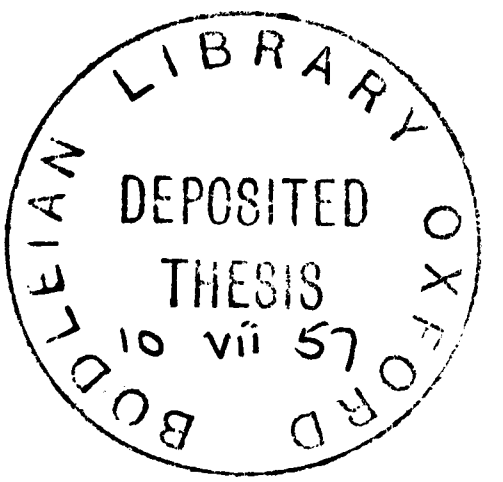
SOME PROBLEMS IN THE THEORY OF NUCLEAR STRUCTURE

being a study of

WEAK COLLECTIVE EFFECTS IN THE NUCLEAR SHELL MODEL



by

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PREFACE

The research described in this dissertation was carried out in Oxford during the years 1954 to 1957 under the supervision of Dr. R. J. Elin-Stoyle. A resume of the work has been accepted for publication in the Proceedings of the Physical Society, Section A, and is due to appear shortly.

I should like to express my sincere thanks to Dr. R. J. Elin-Stoyle for his extremely helpful and enthusiastic supervision throughout this work. It is a pleasure to acknowledge also the help and interest of Dr. D. M. Brink, Mr. C. A. Caine, Dr. J. P. Elliott, Miss M. J. Kearsley, Dr. E. B. Paul, Miss A. A. Ross, and Dr. G. R. Satchler in various phases of this work.

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May, 1957. R. D. Amado

ABSTRACT

Eigen-states generated by considering particles moving independently in a spherically symmetric potential well are, according to the shell model of Mayer and Jensen, good approximations for calculating the ground state and low energy properties of nuclei, particularly near closed shells. But even for nuclei differing by only one particle from a closed shell, weak collective effects have been found that can only be explained by calling into play most or all of the particles in the closed shell core. Hitherto, effects of this type have generally been interpreted in terms of weak collective coupling between the odd particle and the surface of the core.

In Chapter 1 the shell model of Mayer and Jensen and the collective model of Bohr and Mottelson are briefly discussed and an alternative approach, more nearly in the spirit of the shell model, is proposed for the explanation of the weak collective effects in which the residual two-body interaction between the odd particle and the core is used as a perturbation to mix in excited core configurations.

The formalism for this type of configuration mixing is developed in Chapter 2 for collective contributions to the expectation value of the electric quadrupole operator. These will come from admixtures of excitations of the core to 2+ states differing from the zero order state by only one particle. For an L-S closed shell these will result from excitations of a particle to a state two shells away in the oscillator sense and from higher excitations. For a j-j closed shell there may also be contributions from excitations to the other member of the spin-orbit doublet. In either case, by virtue of the energy stability of the closed shell core, the threshold for these excitations will be high. In some cases, as for example O^{17} with harmonic oscillator wave functions, stringent selection rules will operate to give non-vanishing contributions from only a few excitations, and in this case the configuration mixing sum can be evaluated exactly.

In other cases, however, the number of possible excitations is very large and a complete evaluation of the sum is prohibitive, but progress can still be made by replacing the energy denominators in the configuration mixing sum by a mean energy, and doing closure. If we assume that the combined effect of the large energy denominator, the selection of states by the quadrupole operator, and the potential coupling, all contribute to cutting off the actual con-

figuration mixing sum quickly, then the mean excitation energy will be fairly independent of the odd particle states, and can be assigned as a property of the core. If one can do this, one obtains a one-parameter fit of the weak collective quadrupole effects in a given nucleus or for a given closed shell core. Situations in which the closure assumption, that is the assumption that the mean excitation energy is a property of the core, independent of the odd particle state, is justified are discussed and the formalism for reducing the matrix elements in the closure calculation to a sum over particle states in the core is presented in Chapter 2.

In O^{17} the low lying positive parity levels and the ground state magnetic moment are very well understood on the pure single particle model. But the decay of the $2s_{1/2}$ first excited state to the ground state is E2 with a lifetime of the order of a single proton lifetime. Furthermore the $d_{5/2}$ ground state is usually taken to have a very small negative quadrupole moment. Recent work, however, indicates that a good deal of doubt still exists about the value of the moment. Both of these electric effects are forbidden by a pure single particle model for an odd neutron. In Appendix 1 the effect of centre of mass recoil is considered and it is shown that even when large departures from proper internal states are considered, the recoil contribution to the ground

state quadrupole moment is extremely small.

Chapter 3 is devoted to a discussion of these weak collective effects from the point of view of configuration mixing. Firstly the closure formalism is applied using an interaction with a Gaussian radial dependence and a Rosenfeld exchange mixture. The wave functions are taken as determinants of harmonic oscillator single particle eigen-functions. The matrix elements are then evaluated by expanding the interaction in spherical harmonics. A discussion of the evaluation of radial integrals is presented in Appendices 2, 3 and 4. We find that the mean excitation energy needed to fit the old value for the ground state moment is about 7 times larger than the one needed to fit the E2. This result is independent of the exchange mixture and very insensitive to the range of the force. In fact since for oxygen the range of the force is of the order of the nuclear radius, reasonable variations in the form of the force or of the wave functions have almost no effect on the relative values of the calculated collective effects.

If one neglects spin-orbit splittings, the closure assumption is exact for O^{17}, since for harmonic oscillator functions the selection rules on matrix elements of the quadrupole operator only allow excitations from the core of 1s to 1d, 1p to 2p, and 1p to 1f, all of which have an energy of twice the oscillator splitting.

A detailed calculation without closure of the separate contribution of each of the excitations in j-j coupling using the same interaction and wave functions as in the closure calculation is presented. We find that the 1p to 2p excitations contribute very little, and that the $1p_{3/2}$ to $1f_{7/2}$ gives the largest contribution, but in general the calculation yields no great surprises. One still finds that no reasonable values of the parameters will remove the factor of seven between the fitting of the E2 and of the ground state moment. Using semi-empirical values for the excitation energies, one finds that one can fit the transition probability quite well, but this still leaves the ground state quadrupole moment a factor of seven too large.

The failure of other attempts to fit these two collective effects is also discussed and a brief discussion of the possibility of obtaining agreement with experiment by using a zero order state with an equilibrium deformation is presented.

In Chapter 4 configuration mixing with closure is applied to the weak collective effects in the region of the lead doubly closed shell. To evaluate the matrix elements we use a nuclear density distribution which reproduces the main features of the nuclear charge density obtained from the high energy electron scattering experiments. (In Appendix 5 we discuss the terms

neglected in doing this.) For the odd particle we use eigenstates in an infinite potential well. The interaction is treated in a range expansion going to one term beyond zero range and its exchange dependence is taken as a Rosenfeld mixture. The matrix elements are evaluated in a straightforward manner, the radial integrals being done graphically. A fit of experiment can be made treating the mean excitation energy and the density edge thickness as parameters.

The formalism is applied to two E2 transitions in Pb^{207}, an E2 transition in Pb^{206}, and the collective part of the ground state quadrupole moment of Bi^{209}. In Pb^{206} a wave function is used that allows for configuration mixing between the two neutron holes. One finds that for a value of the edge thickness consistent with the electron scattering data, and only for such an edge thickness, the mean excitation energies for the two transitions in Pb^{207} and for the ground state moment of Bi^{209} all agree very well. For Pb^{206} the mean excitation energy consistent with the data is somewhat smaller, but this can be accounted for in terms of the terms discussed in Appendix 5, as well as in terms of an expected "softness" of Pb^{206} due to the fact that it differs from a closed shell by two rather than only one particle.

A discussion of the corroboration of the closure assumption is given. Finally the weak surface coupling formalism is compared with the configuration mixing approach with closure, and it is seen that the latter contains the former, but also contains more, essentially through the relaxation of the requirement of incompressibility of the core.

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CHAPTER I

THE SHELL MODEL

1.1 Introduction

The difficulty of giving an exact solution of the many-body problem and the extreme singularity of the interaction between nucleons make the exact solution of any but the simplest nuclear problems essentially impossible at present. In view of the large amount of experimental data acquired in recent years, useful models of the nucleus are at a premium. Particularly for low energy and ground state properties, the data has become sufficiently precise to warrant detailed calculations, and hence our requirements from models have become very exacting.

Perhaps the most fruitful of models introduced in recent years is the shell model of Mayer and Jensen (1955).

In this model, constructed in analogy with the shell model for the atom, nucleons are considered to move independently in a spherically symmetric potential well with a large spin-orbit coupling. In the nucleus this potential must be assumed to arise from some sort of averaging of the interaction between nucleons. That any such average can be effectively taken is ostensibly very surprising in view of the very short range and great strength of nuclear forces. But the nuclear shell model has proved extremely rewarding, particularly for giving many of the ground state and low energy properties of nuclei, and has gained strong pragmatic justification. Recently the work of Brueckner et al.[†] has indicated the way to a sound theoretical justification as well. This is not the place for a survey of this work, but one point that emerges is particularly interesting.

The theory makes quite clear the model aspect of the shell model. The distinction between model, fact, and theory has not always been entirely clear in physics, and in nuclear physics there is a certain tendency to call any theory a model (Rosenfeld, 1956). A model is not just an approximation to the complete theory, but is rather a simplified account, emphasizing certain

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[†] An analysis of this work and a summary of references can be found in the paper by Bethe (1956).

aspects of the system and purposely omitting certain others. Thus, for example, the optical model, or cloudy crystal ball model, (Feshbach, Porter and Weisskopf, 1954), contains no information about the resonance levels in nuclear reactions since it is constructed specifically to occlude such information. A model need not represent a picture of the "actual system" - not even a simplified picture of it. So long as the model is useful it is a good model, and in as much as a model is useful we must be able eventually to find a justification for it in the complete theory. The fact that a useful model need not picture the "actual system" is brought out by the work of Brueckner. He points out that an expansion of the proper nuclear wave function, that is the eigen-function of the actual nuclear Hamiltonian, in terms of independent particle model eigen-functions would be very complicated indeed, and would be very poorly approximated by keeping only a few terms in the expansion. Thus we are let out of the embarrassing position of having to claim that the nucleus is, even roughly, an independent particle system. The Brueckner theory tells us that without making this extravagant claim we can still use the independent particle model wave functions to get reasonable values for many of the nuclear properties. Just which properties the theory allows us, so to speak, model observables, is not yet clear; but

if pragmatism is to be our guide, then the list of model observables will be a large one.

The Brueckner theory, at least in its present state, is not a complete panacea. Eigen-functions generated by a static spherically symmetric potential - particularly an infinite one - are very far from those generated in the sophisticated, self-consistent formalism of Brueckner. It is true that these shell model wave functions do not give a good account of nuclear energetics, as the Brueckner model functions are designed to do, but the simple functions give a surprisingly good account of many of the dynamic properties of nuclei. Why this should be so is still far from completely clear.

I.2 The Independent Particle Model

In the shell model as first postulated by Mayer and Jensen, it was assumed that the internucleon interaction was such that an even number of neutrons or protons in a given level coupled to spin zero while an odd number coupled to the spin j of that level. This assumption is the natural reverse of Hund's rule for atomic spectra and follows from the fact that the interactions between particles in the nucleus are short range and attractive rather than long range and repulsive as is the case in atoms. This as-

sumption is particularly successful in accounting for the spins and parities of the ground states of even-even nuclei (all 0+) and of odd-A nuclei. It is tempting to regard the properties of the odd-A nuclei at zero or low excitation energies as due, loosely speaking, to the last odd nucleon; the remaining nucleons being assumed to form an inert spin zero core. This single particle model, although a considerable oversimplification, forms a convenient reference model; but clearly a less restrictive assumption must be made if the model is to be a very fruitful one.

In the individual particle model the single particle assumption is relaxed and nuclear ground state properties are interpreted in terms of all the particles outside closed shells. This is done by treating the internucleon interaction as a perturbation between all of these particles, and thus splitting the highly degenerate zero order shell model states of equivalent particles. In general the ground state spins and parities obtained in this way will still follow the reversed Hund rules discussed above, but for nuclei differing by many particles from a closed shell the ground state configuration will be quite different from the extreme single particle model prediction. The application of this perturbation procedure is a problem of some magnitude, even for only a few particles, but fortunately the

labour can be reduced considerably in many cases by introducing a system of classification of nuclear states according to various symmetry properties.[+]

The procedure can be improved and complicated still further by not simply considering one zero order shell model level, but a group of close levels. The perturbation can be applied to all the various configurations of particles among the different levels as well as in the same level, and the resulting energy matrix diagonalised. This procedure is known as configuration mixing, and it should give information not only about the ground state properties of nuclei, but also about the properties of the low lying levels of the same parity. Clearly the computational complexity of such a procedure increases markedly as one moves away from closed shells, and except for the light nuclei, the procedure has been applied only near closed shells. Where the procedure has been carried out, it has given a remarkably close account of the experimental data - energy levels, static moments, transition probabilities, etc. (Lane, 1956). Limited calculations in which any number of particles outside closed shells have been considered have also been done for ground state magnetic dipole moments (Arima and Horie, 1954), ground state electric quadrupole moments

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[+] A brief survey of these classification systems is given by Blin-Stoyle (1956). A more complete account of this and other aspects of the shell model and a complete list of references can be found in the lecture notes by Lane, (1956).

(Horie and Arima, 1955), and comparative half-lives in beta decay (Blin-Stoyle and Caine, 1957 and Caine 1957). The calculations for magnetic moments and log ft values give quite good agreement with experiment, even in regions where we might expect the spherically symmetric shell model to be a bad zero order approximation. This is perhaps related to the operators $\underline{\ell}$ and $\underline{\sigma}$ involved. They greatly restrict the number of states that can contribute in first order mixing, and it is for this reason that the calculation is feasible. Only states involving excitations to the other member of a spin-orbit doublet will contribute. The calculations for quadrupole moments is not nearly so good far from closed shells, but this can be understood in terms of the collective model (see below).

It is perhaps surprising that ordinary perturbation theory can be so successfully applied using the extremely strong and singular nuclear two-body interaction V as a perturbation,* but Swiatecki (1956b) has shown that the ratio of second to first order perturbation terms with V treated as a perturbation is quite small for infinite nuclear matter. For large but finite nuclei the perturbation procedure thus seems reasonable. In small nuclei the justification remains pragmatic.

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* Strictly speaking one uses V minus the shell model generating potential as the perturbation, as we shall see later.

I.3 Collective Effects

Near closed shells we expect that the equilibrium shape of the nucleus is spherical and that the model generating potential well should thus be taken as spherical. On the other hand, in regions far from closed shells the nucleus finds it energetically more favourable to take up a nonspherical shape. There can then be collective oscillations and large collective contributions to ground state moments, particularly quadrupole moments. A theory of these collective effects has been developed by Bohr and Mottelson (1953) which gives an excellent account of the collective aspects of nuclei in the region of large deformations. For large deformations the energy associated with the collective modes is small compared with the single particle excitation energies, and thus the particles may be considered as strongly coupled to a distorted core. The motion of the core can then be treated in a quantum mechanical, quasi-hydrodynamical fashion.

Collective effects are not limited to nuclei far from closed shells. Even for nuclei differing by only one particle from a closed shell there are small collective effects. Near closed shells the energy of excitation of the core is large compared with the particle energies, and the particles may be considered as weakly coupled to the core. In the Bohr-Mottel-

son formalism this coupling gives rise to surface waves on the core and the collective properties are interpreted in terms of these waves. (c.f. 4.4 for a detailed account of this formalism). This explanation of the weak collective effects near closed shells has not been particularly successful, as we shall see. The subject of this thesis is the treatment of these effects within the framework of the shell model.

In ordinary configuration mixing the two body interaction mixes different zero order shell model configurations of particles outside closed shells. Similarly the interaction of an odd particle with the closed shell core will mix in excited configurations of the core, even for a nucleus with only one particle outside the closed shell. Because of the great stability of the closed shell, the admixtures of these excited states will be small. But because there are many possible core excited states, even very small admixtures can give fairly large collective contributions, particularly for electric moment operators like the quadrupole operator. From this configuration mixing point of view, then, collective effects are due to mixtures of excited states of the core caused by interaction with the odd particle.

CHAPTER 2

THE FORMALISM OF CONFIGURATION MIXING

2.1 Configuration Mixing

In configuration mixing the difference between the nuclear two body[+] interaction, V, and the independent particle model generating potential, U, is treated as a perturbation. This perturbation, the so-called residual interaction, mixes higher configurations into the zero order state. It is in the spirit of the model to assume that the effect of the residual interaction will be small near the doubly closed shells, and therefore one need only go to first order in the perturbation series. If we consider a nucleus with a doubly closed shell plus or minus one particle, standard perturbation theory gives for the wave function in first order

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[+] Only two body forces are considered throughout this work.

$$|\rangle_J = |0J\rangle + \sum_{ik}{}' \frac{|ik\rangle\langle ik|V-U|0J\rangle}{E_{0J} - E_{ik}} \qquad (1)$$

where $|0J\rangle$ is the zero order model state and the $|ik\rangle$ are the excited states, and where i and k represent a schematic separation of core and odd particle quantum numbers respectively. E_{ik} and E_{oJ} are the eigen-energies of the model in the usual way. The prime on the sum excludes the term oJ = ik.

The perturbed wave function (1) can be used to calculate the matrix elements of some nuclear operator to first order, and in this work we shall be interested in the nuclear electric quadrupole operator, Q. The matrix element of Q between two states J and J' is

$$\underset{J'}{\langle}|Q|\rangle_J = \langle 0J'|Q|0J\rangle + \sum_{ik}{}' \frac{\langle 0J'|Q|ik\rangle\langle ik|V-U|0J\rangle}{E_{0J} - E_{ik}} + \sum_{ik}{}' \frac{\langle 0J'|V-U|ik\rangle\langle ik|Q|0J\rangle}{E_{0J'} - E_{ik}} \qquad (2)$$

Since U is a scalar one-body operator it will only have non-vanishing matrix elements between excited states of the same angular symmetry as the zero order state and differing from the zero order state in the radial function of one particle only. Thus excited core states i coupled in by U will still be

spherically symmetric. These will not be coupled by the quadrupole operator to the zero order state, since Q transforms under rotation as the spherical harmonic Y_{2m}. For the case in which the odd particle is a neutron, then, U and the prime on the sum may be omitted since the zero order expectation value of Q is zero. We are interested in admixtures due to V of core states i corresponding to excitations of only one proton, since Q is a one-body operator, and having angular momentum 2 and positive parity. In the odd neutron case (2) can be re-written

$$ {}_{J'}\langle |Q| \rangle_{J} = -\sum_{i} \frac{\langle oJ'|Q|iJ'\rangle\langle iJ'|V|oJ\rangle}{E_i + \Delta_{JJ'}} - \sum_{i} \frac{\langle oJ'|V|iJ\rangle\langle iJ|Q|oJ\rangle}{E_i - \Delta_{JJ'}} \qquad (3) $$

where E_i is the core excitation energy needed to form the 2^+ state i, and $\Delta_{JJ'}$ is the difference in energy between the odd particle states J and J'. The selection of excited states depends on V, since it is a symmetric operator, if the initial zero order state is anti-symmetric, then only anti-symmetric states will be coupled into the sum.

It should be noted that since the model generating potential U generally refers to some fixed external origin, the model wave functions will have three extra internal degrees of freedom that do not correspond to internal degrees of freedom

for the actual nucleus. Thus the model states will in general have a part that is spurious and must be eliminated. This problem has been studied in some detail by Elliott and Skyrme (1955, 1956), and as they point out, if operators are chosen so that they depend only on relative coordinates, they will not couple proper and spurious parts. Since V is such an operator, if the zero order states are proper states of the internal motion, then only the proper parts of the excited states will be mixed in.

For an L-S closed shell* the excitations i in (3) will occur from excitations of a proton to a state two shells away in the oscillator sense and from higher excitations. Only every other oscillator shell will contribute since the oscillator shells alternate in parity and we are interested in excitations of positive parity. For a j-j closed shell there may also be contributions from excitations to the other member of the spin-orbit doublet. In either case by virtue of the energy stability of the closed shell configuration, $E_i >> \Delta_{jj'}$, even for the lowest E_i, and thus we can neglect $\Delta_{jj'}$. If the number of states that can contribute to the sums in (3) is small, as happens in O^{17} with harmonic oscillator wave functions

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* In an L-S closed shell each occupied orbit $j = l \pm 1/2$ is completely filled, whereas if the shell is closed only in the j-j sense, then an orbit $j = l + 1/2$ is full and its spin-orbit partner $j = l - 1/2$ is empty.

because of selection rules on matrix elements of Q, then one can evaluate the sums in detail term by term. However if the number of terms contributing is large, some approximation must be found.

2.2 Closure

One can always treat the sums in (3) by replacing the energy denominators by some mean excitation energies, $\bar{E}$ and $\bar{E}'$ and then doing closure over the excitations. This gives for (3)

$$\sum_{J'} \langle 1 | Q | 1 \rangle_J = -\frac{1}{\bar{E}} \langle 0J' | Q V | 0J \rangle$$

$$-\frac{1}{\bar{E}'} \langle 0J' | V Q | 0J \rangle \qquad (4)$$

This expression can be treated as a definition of the mean excitation energies, and has the advantage of averaging the information about the excited configurations into the mean energies so that one need not specify any but the zero order configuration. The closure expression (4) is particularly useful if one can assume that the mean excitation energy is a property that can be assigned to the core, independent of the odd particle state. If this can be done then (4) can be used to give a one parameter fit for the weak collective quadrupole

effects in a given nucleus or for a given closed shell core.

Since we are interested in obtaining just such a fit of the weak quadrupole effects near closed shells, it is of interest to see in what cases the closure assumption, that is the assumption that the mean excitation energy is independent of the single particle states for a given core, will be valid. Clearly the assumption will be trivially true if all the excited core states contributing to the sum have the same excitation energy. It will still remain a good approximation if the major contribution to the sum comes from a spread of excitations small compared with the mean excitation energy. This condition is likely to be satisfied fairly often. Since E_i in (3) is an energy for the break-up of the core, it will have a large threshold, as we have seen. It is reasonable to assume that after threshold the combined effect of the energy denominator, of the small potential coupling between the highly excited states and the closed shell state, and the selection rules on the operator Q, all contribute to making the sum converge rapidly and in an energy interval small compared with the threshold, in which case $\bar{E}$ will be of the order of the threshold energy independent of the odd particle state.

For the closure assumption to be valid however, it is not necessary that the important contribution to the sum come from a

small energy range. The closure expression (4) defines $\bar{E}$ as the harmonic mean* of E_i over the configuration mixing sum. And hence the closure assumption is valid so long as the odd particle state does not affect the harmonic mean of E_i. Thus for example if the relative contribution of each excitation is always the same, and the only effect of the odd particle state is to provide a scale for the contributions, then the assumption will be true. In Chapter 4 we shall discuss situations in which this may be almost the case and hence for which the closure assumption is a good approximation.

In the case in which the odd particle is a proton, two important changes must be made in the closure formulation. Firstly it is no longer justifiable to drop U in the perturbation sum, and secondly allowance must be made for the non-vanishing of the zero order matrix elements of Q_ν. In the case of an odd proton the closure expression just gives the collective contribution, there being also a single particle contribution from the first term in (2). The closure expression (4) can be corrected for the odd proton case by replacing V in (4) by V-U and by subtracting the zero order term from the closure sum, that is by sub-

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* In the usual way, the harmonic mean, $\bar{x}$, of x_i over some distribution $g(x_i)$ is defined by

$$\frac{1}{\bar{x}} = \frac{\sum_i \frac{g(x_i)}{x_i}}{\sum_i g(x_i)}$$

treating the term

$$-\langle oJ'|Q|oJ\rangle\left(\frac{1}{E}\langle oJ|V-U|oJ\rangle - \frac{1}{E'}\langle oJ'|V-U|oJ'\rangle\right) \quad (5)$$

from (4).

If the zero order solutions are self-consistent, the effect of using V-U in the configuration mixing sum rather than V will be to forbid those excitations in which only the radial part of the odd particle state is changed. It is clear that if U for the odd particle is an average of V over the core, then excitations in which only the odd particle radial function is changed will be coupled in as strongly by V as by U, and hence not at all by V-U.

The value of the mean excitation energy in any case will depend on the operator Q. Thus in our case $\bar{E}$ represents some sort of average over the excitation energies of the 2+ states of the core, and we expect the major contribution from these to come from excitations of the order of twice the oscillator splitting. Actually the value of the mean excitation energy consistent with experiment comes out to be roughly twice this value for a heavy nucleus, a fact which is in accordance with the idea of the nucleon mass being replaced by an effective mass of one half the free value for large nuclei. This increase in $\bar{E}$, due essentially to the velocity dependence of U, increases

the validity of the perturbation expansion (Swiatecki, 1956a).[+]

It will be noticed that (4) could be obtained from a wave function of the form

$$|\rangle_J = \left(1 - \frac{V}{\bar{E}}\right)|0J\rangle \qquad (6)$$

Such wave functions have often been used (Lennard-Jones, 1930, and Feingold, 1956) as trial wave functions to get energies, in which case $\bar{E}$ is usually treated as a variational parameter. But by emphasising the closure approach we see more clearly that the mean excitation energy is an average over the spectrum of states picked out by V and Q, and that the value of $\bar{E}$ one gets from minimising the value of some energy operator might well be quite different from the value of $\bar{E}$ for an electric quadrupole operator which depends only on the distribution of 2+ states in the

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[+] A rough estimate of the validity of a perturbation expansion is given by the amount that admixtures contribute to the normalisation of the perturbed wave function. If this is small compared with unity, then we can neglect the re-normalisation due to the perturbation, and assume that the perturbation expansion is reasonably valid. Since in the usual way, we do not consider diagonal matrix elements of the perturbation V-U in first order, the contribution of the perturbation to the normalisation will be second order, and in terms of the closure formalism will be given by $\dfrac{\langle 0J|(V-U)^2|0J\rangle}{(\bar{E})^2}$

We wish this to be small compared with unity, and clearly an increase in $\bar{E}$ will help this to be so. We shall assume that the contribution of the perturbation to the normalisation can always be neglected.

core. Physically the wave function (6) can be thought of as representing a polarisation of the core by the odd particle due to the interaction V. If one treats V as a delta function one sees that, to the zero order wave function, one is adding a function in the core with the density distribution of the odd particle. The amount added depends on $V/\overline{E}$ and so $\overline{E}$ can be thought of as a measure of the "stiffness" of the core, as might be expected. That this effect should occur in analogy to the distortion of the core in non-penetrating atomic orbits has often been pointed out (e.g. Bohr and Mottelson, 1953). The formulation of the effects has, however, been largely from a different point of view, (Rainwater, 1950, Feenberg and Hammack, 1951, Bohr and Mottelson, 1953). We shall return in Chapter 4 to a discussion of the relation of this formulation with the one using configuration mixing and closure.

2.3 Calculation with the Closure Wave Function

The closure expression (4) can be used to calculate the weak quadrupole effects in the odd neutron nucleus O^{17} and the results compared with the calculation using the exact summation (3). Since, as we shall see, all of the states contributing to the sum have the same energy neglecting spin-orbit splittings (3) and (4) will give just the same result with a mean excitation

energy corresponding to this energy. By evaluating (3) one is able to see in detail how each excited state contributes to the sum, whereas the closure expression (4), is a more convenient one for investigating the effect of varying parameters. In the case of O^{17} where the range of the force is of the order of the nuclear radius, the matrix elements are evaluated by expanding the two body potential V in spherical harmonics and treating the nuclear states as anti-symmetric products of single particle states, that is as determinantal functions. A three dimensional isotropic harmonic oscillator is used to generate the single particle model eigen-functions, and the interaction V is taken to have a Gaussian radial dependence. The calculations and results are presented in the next Chapter.

There are three nuclear species near the lead closed shell that exhibit known weak collective electric quadrupole effects; Pb^{207} with one hole* in the neutron closed shell, and a closed shell of 82 protons, Pb^{206} with two neutron holes, and Bi^{209} with one proton outside the 82 closed shell and a closed shell of 126 neutrons. In the region of lead the interaction can be treated in a range expansion since the range of the force is small compared with the nuclear radius, and the sum over particle states

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* Throughout this work it is assumed that holes can be treated as particles in the usual way. A good account of the formalism for doing this is given by Brink and Satchler (1956).

in the core can be replaced by a density distribution. This greatly simplifies the calculation since much is known about the charge density in the heavy nuclei, (Hofstadter, 1956) whereas very little is known about the single particle states deep down in the well. The odd particle states are taken as eigen-states in an infinite square well, this being a better approximation than the harmonic oscillator for the heavy nuclei.

O^{17} and most of the nuclei we shall be interested in in the region of lead are odd neutron nuclei and hence we can use the closure expression (4). In order to evaluate the matrix elements in (4) it is convenient to transform the matrix elements between nuclear wave functions into a sum over matrix element between single particle states. We need only look in detail at one of the terms in (4) the other being just the same with V and Q interchanged and $\bar{E}$ replaced by $\bar{E}'$. Thus we wish to expand

$$\frac{1}{2}\frac{1}{\bar{E}}\langle 0J'|\sum_{k\,\text{protons}} Q_k \sum_{i\neq j} V_{ij}|0J\rangle \qquad (7)$$

It is clear from symmetry arguments that one of the indices of V_{ij} must be on the odd neutron state, ν_J, and the other on some core proton. If the index of Q refers to this same proton we get a two-body matrix element, and if not a three-body one. Treating the proton part of the nuclear state as a determinant of

single particle proton states, $\phi_i(r)$, where i refers to the quantum numbers necessary to specify the state, (7) can be expanded in the usual way (Condon and Shortley, 1935, p.169 et seq.), giving

$$\frac{1}{E}\sum_i \langle \phi_i \nu_J, 1 | Q_1 V_{12} | \phi_i \nu_J \rangle + \frac{1}{E}\sum_{ij}\Big(\langle \phi_i \nu_J, 1 | V_{12} | \phi_i \nu_J \rangle \langle \phi_j | Q | \phi_j \rangle - \langle \phi_i \nu_J, 1 | V_{12} | \phi_j \nu_J \rangle \langle \phi_j | Q | \phi_i \rangle\Big) \tag{8}$$

where we use the convention that 1 refers to the coordinates of the first particle state in either bra or ket, 2 to the second, etc. Making use of the fact that for a closed shell

$$\sum_j \langle \phi_j | Q | \phi_j \rangle$$

(8) can be simplified to

$$\frac{1}{E}\sum_i \langle \phi_i \nu_J, 1 | Q_1 V_{12} | \phi_i \nu_J \rangle - \frac{1}{E}\sum_{ij} \langle \phi_i \nu_J, 1 | V_{12} | \phi_j \nu_J \rangle \langle \phi_j | Q | \phi_i \rangle \tag{9}$$

For the odd proton nucleus Bi^{209} we must use V-U in (4) and take into account (5). But for single particle eigenstates generated by an infinite square well, U = constant in the range of definition of the particle wave functions, and

thus the term in U from (4) will just cancel with the one in (5) and we can simply neglect U. We shall be interested in the ground state quadrupole moment of Bi^{207} and hence in the diagonal expectation value of Q. Making use of the fact that for diagonal matrix elements, QV = VQ, the collective contribution can be written

$$-\frac{1}{E}\sum_{\substack{i\neq j\\ k_{protons}}}\left(\langle 0J|V_{ij}Q_k|0J\rangle - \langle 0J|V_{ij}|0J\rangle\langle 0J|Q_k|0J\rangle\right) \tag{10}$$

Clearly any part of the first term for which both i and j refer to neutron core states will be cancelled by a corresponding part of the second term. In fact the only non-vanishing parts of (10) involving the neutrons will be those terms between the core neutrons and the odd proton. These terms correspond to excitations involving a change in the radial part of the odd particle state only, and since these would not occur if the model had been properly self-consistent, we wish to exclude them here. Thus we can leave out the neutron core altogether and consider only the protons.

It is more difficult to exclude the terms arising from excitations of the odd proton through interaction with the core protons, but leaving them in does not really introduce much error. Excitations involving a change in the radial part of the odd

particle function only occur in alternate shells in the oscillator sense, as do the excitations for states from the core. Each excitation, whether of the odd proton or of a core proton, gives a contribution of the same order of magnitude, and hence the contribution from excitations of the odd particle will be smaller by a factor of $1/(Z-1)$ compared with the contribution from the $Z-1$ particles in the core. Thus we introduce negligible error by taking i, j, and k in (10) over all the proton states. As before there will be a part of the first sum in which either i or j equals k and we get a two-body term and there will be a part for which all three are different, giving a three-body term. Treating the proton part of the wave function as a determinant of the single particle states, ϕ_i, and expanding as before, we get for (10)

$$-\frac{2}{E}\sum_{ij}\left(\langle\phi_i\phi_j|V_{12}Q_2|\phi_i\phi_j\rangle-\langle\phi_i\phi_j|V_{12}Q_2|\phi_j\phi_i\rangle\right)$$

$$-\frac{1}{3!}\frac{1}{E}\sum_{ijk}\langle\sum_p(-1)^p P(\phi_i\phi_j\phi_k)|V_{12}Q_3|\sum_p(-1)^p P(\phi_i\phi_j\phi_k)\rangle \tag{11}$$

$$+\frac{1}{E}\sum_{ijk}\langle\phi_k|Q|\phi_k\rangle\left(\langle\phi_i\phi_j|V_{12}|\phi_i\phi_j\rangle-\langle\phi_i\phi_j|V_{12}|\phi_j\phi_i\rangle\right)$$

where once again 1 refers to the coordinates of the first ϕ in either bra or ket, 2 to the second, etc., and where P is the

usual permutation operator - the sum over P making the states anti-symmetric. Upon expanding the three-body term, one finds that certain terms cancel with the last two terms in (11), and that other terms combine giving for (11)

$$-\frac{2}{E}\sum_{ij}\Big(\langle\phi_i\phi_j|V_{12}\,Q_2|\phi_i\phi_j\rangle - \langle\phi_i\phi_j|V_{12}Q_2|\phi_j\phi_i\rangle\Big)$$

$$-\frac{2}{E}\sum_{ijk}\Big(\langle\phi_i\phi_j|V_{12}|\phi_k\phi_i\rangle\langle\phi_k|Q|\phi_j\rangle - \langle\phi_i\phi_j|V_{12}|\phi_i\phi_k\rangle\langle\phi_k|Q|\phi_j\rangle\Big) \qquad (12)$$

It is clear from symmetry considerations that the matrix elements will vanish unless one of the ϕ's refers to the odd particle state, which we designate as ϕ_o. If there are no states in the core of the same symmetry as ϕ_o then since V is a scalar, if ϕ_k refers to the odd particle in either of the three body terms, so must ϕ_j, and vice versa. Putting these conditions in, one finally gets for (12)

$$
\begin{aligned}
&-\frac{2}{E}\sum_{i}\Big(\langle\phi_i\phi_o|\,V_{12}(Q_1+Q_2)\,|\phi_i\phi_o\rangle \\
&\qquad\qquad -\langle\phi_i\phi_o|\,V_{12}(Q_1+Q_2)\,|\phi_o\phi_i\rangle\Big) \\
&+\frac{2}{E}\sum_{ij}\langle\phi_i|Q|\phi_j\rangle\Big(\langle\phi_o\phi_j|\,V_{12}\,|\phi_o\phi_i\rangle \\
&\qquad\qquad -\langle\phi_o\phi_j|\,V_{12}\,|\phi_i\phi_o\rangle\Big) \\
&+\frac{2}{E}\langle\phi_o|Q|\phi_o\rangle\sum_{i}\Big(\langle\phi_i\phi_o|\,V_{12}\,|\phi_i\phi_o\rangle \\
&\qquad\qquad -\langle\phi_i\phi_o|\,V_{12}\,|\phi_o\phi_i\rangle\Big)
\end{aligned}
\tag{13}
$$

where the sums now extend only over core states.

CHAPTER 3

OXYGEN 17

3.1 Single Particle Behaviour

On the shell model, O^{17} has one neutron outside the extremely stable O^{16} (Z=8, N=8) doubly closed shell. One is therefore not surprised to find that the low lying positive parity levels (Ajzenberg and Lauritsen, 1955) as well as the ground state magnetic dipole moment (Blin-Stoyle, 1956) are very well accounted for on the extreme single particle model. However two electric quadrupole effects are known that cannot be explained by this simple model. The first excited state, .872 Mev above the ground state and assigned the single particle configuration $2s_{1/2}$, decays to the ground state by E2 radiation with a life time of $2.5 \pm 1 \times 10^{-10}$ sec. (Ajzenberg and

Lauritsen, 1955), corresponding to a reduced matrix element[+] for the decay of $2.6 \times 10^{-26} cm^2$ (Satchler, 1954). The ground state, which on the single particle model has the odd neutron in a $1d_{5/2}$ state, has a small static electric quadrupole moment. Geschwind, Gunther-Mohr, and Townes (1951) have measured the nuclear quadrupole hyperfine structure resulting from O^{17} in the rotational microwave spectrum of the molecule $O^{17}CS$. They find a quadrupole coupling constant, eqQ, of -1.2 ± 0.2 Mc, and estimating q from the electronic structure of the molecule, they give the ground state quadrupole moment as $Q = -0.005 \pm 0.002$ barns. Recent work indicates that a good deal of doubt still exists about the ground state moment, largely because of uncertainties in calculating the electronic structure factor, q, and the moment may actually be very much larger than the one given

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[+] The matrix element between angular momentum eigen-vectors $|JM\rangle$ (total angular momentum J and z-component M) and $|jm\rangle$ of some tensor operator $T(\lambda\mu)$, that is some operator that transforms under rotations like the angular momentum eigen-vector $|\lambda\mu\rangle$, can be factored by making use of the Wigner-Eckart theorem into a reduced matrix element, (or double-bar matrix element) which is independent of rotations, and a vector addition, or Wigner coefficient, (e.g. Edmonds, 1955). We use the following convention for doing this

$$\langle JM \mid T(\lambda\mu) \mid jm \rangle = \langle J \| T(\lambda) \| j \rangle C^{J\lambda j}_{M\mu m}$$

where $C^{J\lambda j}_{M\mu m}$ is the usual vector addition coefficient (Condon and Shortley, 1935, p.73) for the vector addition $\underline{J} = \underline{\lambda} + \underline{j}$ and the corresponding scalar addition $M = \mu + m$. Phases of the Wigner coefficients and of the spherical harmonics are chosen as in Condon and Shortley.

by Geschwind et al. (Stevenson, 1957). No new results are as yet available for the quadrupole moment, however, and thus when referring without comment to the quadrupole moment of O^{17} we shall mean the value of Geschwind et al.*

Attempts have been made to explain these weak collective effects in O^{17} on the basis of the so-called recoil effect which arises from the motion of the charged core about the common centre of mass of the core and the odd particle. In particular this has been tried for the ground state quadrupole moment since it is of the order of the "classical" recoil, i.e. Z/A^2 times the contribution for a single proton in the $1d_{5/2}$ state. However as has been suggested by Elliott and Skyrme (1955, 1956), there is no recoil moment if proper states are used, that is if states are used in which the superfluous degrees of freedom introduced by the artificial external potential well have been removed. A discussion of this for the electric quadrupole and magnetic dipole moments is given in Appendix 1, and as we see there the vanishing comes about essentially because of anti-symmetry. Elliott and Skyrme show that harmonic oscillator shell model states for one particle in the lowest state outside a doubly closed shell are proper states, and thus there is no recoil contribution to these moments. In Appendix 1 we discuss the effect of deviations from the harmonic oscillator in O^{17}, and in the extreme case in which

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* See Addendum p. 67a

radial integrals are calculated with eigen-states in an infinite square well rather than a harmonic oscillator well, one finds a recoil contribution to the ground state quadrupole moment of the order of or less than 0.1 of the classical recoil with the exact magnitude and sign uncertain and dependent on how one relates the square well to the harmonic oscillator well. Thus even if large deviations from the harmonic oscillator are considered, the recoil contribution seems too small to account for the ground state moment and the harmonic oscillator is usually considered to be a good model for a nucleus as light as O^{17}. We must therefore look for some other mechanism to explain the collective effects.

3.2 Evaluation in the Closure Formalism

One can investigate the weak collective effects in O^{17} in terms of the configuration mixing formalism outlined in Chapter 2. For the protons in the stable O^{16} core, we take the standard configuration, $(1s)^2(1p)^6$. The single particle states are taken as eigen-states in a three dimensional isotropic harmonic oscillator potential. Under these assumptions very strong selection rules are imposed on the matrix elements of Q (Shaffer, 1944), and the only excitations i that will contribute to the sum in (3) are the proton excitations 1s to 1d, 1p to 2p,

and 1p to 1f. Neglecting the spin-orbit splitting, all of these excitations have the same energy, i.e. twice the harmonic oscillator splitting. Since $\Delta_{JJ'}$ is certainly negligible compared with this energy, the closure expression (4) is a very good approximation in O^{17} with $\bar{E} = \bar{E}' =$ twice the oscillator splitting.

We wish to evaluate expressions of the form (9). For states in the core, the single particle wave functions can be written

$$\phi_i = \mathcal{R}_{N\ell}(r)\, Y_{\ell m}(\theta\varphi)\, \chi_{m_s} \qquad (14)$$

where χ_{m_s} is the spin function, and $Y_{\ell m}$ is the usual spherical harmonic. There is no need to couple up the states in some particular coupling scheme, since we are considering determinantal wave functions for L-S closed shells. For harmonic oscillator eigen-states the radial function is (Talmi, 1952)

$$\mathcal{R}_{N\ell}(r) = N_{N\ell}\, e^{-\frac{\rho^2}{2}}\, \rho^{\ell}\, \mathcal{L}_{N\ell}(\rho) \qquad (15)$$

where $N_{N\ell}$ is a normalising constant, $\mathcal{L}_{N\ell}$ is the associated Laguerre polynomial, and $\rho = \frac{r}{b}$ with $b = \left(\frac{\hbar}{Mk}\right)^{\frac{1}{2}}$ if the generating potential U is given by $U = \frac{1}{2} M k^2 r^2$

For the odd neutron the single particle function is

$$\nu_{JM} = R_{n\ell} \mathcal{Y}_{J\ell M} = R_{n\ell} \sum_{m} C^{J}_{M\, m\, M-m}\, Y_{\ell m}\, \chi_{M-m} \tag{16}$$

Defining the quadrupole operator as

$$Q_M(r_i) = r_i^2\, Y_{2M}(\theta_i, \phi_i) \tag{17}$$

we get for the ground state quadrupole moment of O^{17}

$$\langle Q \rangle = -\frac{8}{E}\sqrt{\frac{\pi}{5}} \left(\sum_i \langle \phi_i \nu_{\frac{5}{2}\frac{5}{2}} \mid Q_0(r_i)\, V_{12} \mid \phi_i \nu_{\frac{5}{2}\frac{5}{2}} \rangle \right.$$

$$\left. - \sum_{ij} \langle \phi_i \nu_{\frac{5}{2}\frac{5}{2}} \mid V \mid \phi_j \nu_{\frac{5}{2}\frac{5}{2}} \rangle \langle \phi_j \mid Q_0 \mid \phi_i \rangle \right) \tag{18}$$

Similarly the reduced matrix element for the E2 transition can be written

$$\langle \tfrac{1}{2} \| E2 \| \tfrac{5}{2} \rangle = -\begin{pmatrix} \frac{1}{2} & 2 & \frac{5}{2} \\ m_s & M & m_d \end{pmatrix}^{-1} \frac{1}{E} \times$$

$$\left[\sum_i \langle \phi_i \nu_{\frac{1}{2} m_s} \mid Q_M(r_i)\, V_{12} + V_{12}\, Q_M(r_i) \mid \phi_i \nu_{\frac{5}{2} m_d} \rangle \right. \tag{19}$$

$$\left. - 2 \sum_{ij} \langle \phi_i \nu_{\frac{1}{2} m_s} \mid V \mid \phi_j \nu_{\frac{5}{2} m_d} \rangle \langle \phi_j \mid Q \mid \phi_i \rangle \right]$$

For the interaction V_{12} we take

$$V(r_{12}) = -B\left(\gamma + \epsilon P_M + \beta P_B + \delta P_B P_M\right) f(r_{12}) \qquad (20)$$

where the P's are the exchange operators, P_M space exchange and P_B spin exchange, as defined by Blatt and Weisskopf (1952, p.136). B is the strength of the interaction and the constants $\gamma, \epsilon, \beta, \delta$ are defined so that $\gamma + \epsilon + \beta + \delta = 1$. $f(r_{12})$ is the radial dependence of the interaction. One can easily verify that the effect of the spin exchange operator, P_B, in the matrix elements in (18) and (19) is to reduce by one the number of spin sums that are free. Since each of these sums contributes a factor of two to the matrix element, we can simply replace P_B by a factor of one half. Thus the interaction in (20) can be re-written

$$V(r_{12}) = -B\left[\gamma + \frac{\beta}{2} + \left(\epsilon + \frac{\delta}{2}\right) P_M\right] f(r_{12}) \qquad (21)$$

and the expression for the quadrupole moment, or $\langle \| E2 \| \rangle$, splits up into a direct and a space exchange part. One can write

$$\langle Q \rangle = \left(\gamma + \frac{\beta}{2}\right) \langle Q \rangle_{direct} + \left(\epsilon + \frac{\delta}{2}\right) \langle Q \rangle_{exchange} \qquad (22)$$

for the quadrupole moment and there is clearly a similar expression for the M2.

In order to calculate the matrix elements it is convenient to expand $f(r_{12})$ into spherical harmonics.

$$f(r_{12}) = \sum_{k=0}^{\infty} (2k+1)\, f_k(r_1, r_2)\, P_k(\cos\theta_{12})$$

$$= 4\pi \sum_{k=0}^{\infty} f_k(r_1, r_2) \sum_m Y_{km}(\theta_1, \phi_1)\, Y^*_{km}(\theta_2, \phi_2) \qquad (23)$$

where $P_k(\cos\theta_{12})$ is the usual Legendre polynomial of order k, and where use has been made of the addition theorem for the spherical harmonics (Bethe, 1933). One can now combine (14), (16), (17), and (23) into the expression for the quadrupole moment (18) or the E2 (19) written as in (22). The resulting matrix elements split up in the usual way into an angular part and a radial part. For example the first term in (18) gives for the direct part in the case of the 1p protons

$$-\frac{64}{E}\pi\sqrt{\frac{\pi}{5}} \sum_{k m \mu} \langle R_{1p}^{(1)}\, Y_{1m}^{(1)}\, R_{1d}^{(2)}\, Y_{22}^{(2)} | \times$$

$$(r_1^2 Y_{20}^{(1)}\, f_k^{(12)}\, Y_{k\mu}^{(1)}\, Y_{k\mu}^{*(2)}) | R_{1p}^{(1)} Y_{1m}^{(1)} R_{1d}^{(2)} Y_{22}^{(2)} \rangle$$

$$= -\frac{64}{E}\pi\sqrt{\frac{\pi}{5}} \sum_k \langle R_{1p}^{(1)} R_{1d}^{(2)} | r_1^2 f_k^{(12)} | R_{1p}^{(1)} R_{1d}^{(2)} \rangle \times$$

$$\sum_{m\mu} \langle Y_{1m} | Y_{20}\, Y_{k\mu} | Y_{1m} \rangle \langle Y_{22} | Y^*_{k\mu} | Y_{22} \rangle \qquad (24)$$

The angular matrix elements can be evaluated in the standard way making repeated use of the expression (Blatt and Weisskopf, 1952, p.793)

$$Y_{lm}(\theta,\varphi)\, Y_{l'm'}(\theta,\varphi) = \sum_{L} \left[\frac{(2l+1)(2l'+1)}{4\pi(2L+1)}\right]^{\frac{1}{2}} C^{L\,l\,l'}_{0\,0\,0}\, C^{L\quad l\quad l'}_{m+m'\;m\;m'}\, Y_{L\,m+m'}(\theta\varphi) \quad (25)$$

and using the methods of Racah (1942). From evaluating the angular parts one gets strong selection rules on k. In the particular case treated in (24), for example, only k = 2 contributes. The evaluation of the angular parts is lengthy but straightforward and gives finally for the quadrupole moment

$$\langle Q\rangle_{direct} = -\frac{32\,B}{7\,E}\left[\frac{1}{2}\mathcal{R}_2(s\,d\,s\,d) + \frac{3}{2}\mathcal{R}_2(p\,d\,p\,d) - \frac{3}{5}\mathcal{R}'_2(p\,d\,p\,d)\right] \quad (26)$$

and

$$\langle Q\rangle_{exchange} = -\frac{16\,B}{35\,E}\left[6\mathcal{R}_1(p\,d\,d\,p) + 5\mathcal{R}_2(s\,d\,d\,s) + 9\mathcal{R}_3(p\,d\,d\,p) - \frac{21}{5}\mathcal{R}'_1(p\,d\,d\,p) - \frac{9}{5}\mathcal{R}'_3(p\,d\,d\,p)\right] \quad (27)$$

where the R's are the radial integrals

$$\mathcal{R}_k(l_1 l_2 l_3 l_4) = \langle R_{l_1}^{(1)} R_{l_2}^{(2)} | r_1^2 | f_k^{(12)} | R_{l_3}^{(1)} R_{l_4}^{(2)} \rangle$$

$$\mathcal{R}_k'(l_1 l_2 l_3 l_4) = \langle R_{1p} | r^2 | R_{1p} \rangle \times$$

$$\langle R_{l_1}^{(1)} R_{l_2}^{(2)} | f_k^{(12)} | R_{l_3}^{(1)} R_{l_4}^{(2)} \rangle \quad (28)$$

where s p d refer to the 1s, 1p, and 1d states respectively.

Similarly for the E2 reduced matrix element, one gets

$$\langle \| E2 \| \rangle_{direct} = \frac{8B}{E}\sqrt{\frac{3}{4\pi}}\left[\frac{1}{2}\mathcal{R}_2(s\,2s\,s\,d) + \frac{3}{2}\mathcal{R}_2(p\,2s\,p\,d) - \frac{3}{5}\mathcal{R}_2'(p\,2s\,p\,d)\right] \quad (29)$$

and

$$\langle \| E2 \| \rangle_{exchange} = \frac{15}{E}\sqrt{\frac{3}{\pi}}\left[\mathcal{R}_0(s\,2s\,d\,s) + 3\mathcal{R}_1(p\,2s\,p\,d) + \frac{6}{5}\mathcal{R}_1(2s\,p\,p\,d) + \mathcal{R}_2(2s\,s\,s\,d) + \frac{9}{5}\mathcal{R}_2(2s\,p\,p\,d) - \frac{12}{5}\mathcal{R}_1'(p\,2s\,d\,p)\right] \quad (30)$$

where 2s refers to the odd neutron 2s radial function.

For ease of calculation we take $f(r_{12})$ to have a Gaussian form

$$f(r_{12}) = e^{-\left(\frac{r_{12}}{a}\right)^2} \tag{31}$$

The method for evaluating the f_k's in this case and for doing the radial integrals has been given by Swiatecki (1951). A generalization of his procedure for the integrals of interest in this calculation is given in Appendix 2. Putting in the radial integrals, one gets

$$\langle Q \rangle_{direct} = -\frac{8 B b^2 \alpha^{3/2}}{E (\alpha+2)^{7/2}} (6\alpha^2 + 11\alpha + 7) \tag{32}$$

and

$$\langle Q \rangle_{exchange} = -\frac{8 B b^2 \alpha^{3/2}}{E (\alpha+2)^{7/2}} (\alpha^3 + 3\alpha^2 + 10\alpha + 7) \tag{33}$$

where $\alpha = \left(\frac{a}{b}\right)^2$. Similarly for the E2 we have

$$\langle \| E2 \| \rangle_{direct} = \frac{B b^2 \alpha^{3/2}}{E (\alpha+2)^{7/2}} \sqrt{\frac{15}{2\pi}} (24\alpha^2 + 26\alpha + 19) \tag{34}$$

and

$$\langle 11E211\rangle_{exchange} = \frac{B b^2 \alpha^3 \ell}{2\bar{E}(\alpha+2)^{\frac{11}{2}}} \sqrt{\frac{15}{2\pi}} (11\alpha^3 + 15\alpha^2 + 68\alpha + 38) \quad (35)$$

Swiatecki (1951) gives a value for b by relating the point at which the shell model density distribution falls to one fourth its maximum value to the nuclear radius, defined by $1.4 \times A^{1/3} \times 10^{-13}$cm. For O^{17} this gives $b = 1.6 \times 10^{-13}$ cm. Taking $a = 1.9 \times 10^{-13}$cm. (Rosenfeld, 1948, p.153) gives $\alpha = 1.4$. Putting this into (32) and (33) one finds

$$\langle Q \rangle_{direct} = -1.2 \frac{B}{E} \times 10^{-26} \text{ cm}^2$$

$$\frac{\langle Q \rangle_{exchange}}{\langle Q \rangle_{direct}} = 0.9 \quad (36)$$

Hence for reasonable values of the parameters, the direct and exchange contributions are essentially the same. One can write therefore

$$\langle Q \rangle = -1.2 \frac{B}{E} \left(\gamma + \frac{\beta}{2} + \epsilon + \frac{\delta}{2} \right) \times 10^{-26} \text{ cm}^2 \quad (37)$$

Using a Rosenfeld mixture (Rosenfeld, 1948, p.234) for which $\gamma = -.13$, $\epsilon = .93$, $\beta = .46$, and $\delta = -.26$, this gives

$$\langle Q \rangle = -1.0 \frac{B}{E} \times 10^{-26} \text{ cm}^2 \tag{38}$$

A similar evaluation for the reduced matrix element gives

$$\langle 11E211 \rangle_{direct} = 0.85 \frac{B}{E} \times 10^{-26} \text{ cm}^2$$

$$\frac{\langle 11E211 \rangle_{exchange}}{\langle 11E211 \rangle_{direct}} = 1 \tag{39}$$

Once again the exchange and direct contributions are the same and one gets for a Rosenfeld mixture

$$\langle 11E211 \rangle = 0.79 \frac{B}{E} \times 10^{-26} \text{ cm}^2 \tag{40}$$

A comparison of (38) with the experimental value for the quadrupole moment of $-0.005 \times 10^{-24} \text{cm}^2$ requires that $B/E = 0.5$. Comparison of (40) with the experimental value of $2.6 \times 10^{-26} \text{cm}^2$ requires $B/E = 3.3$. This is a most unsatisfactory state of affairs.

3.3 Variations of Assumptions within the Closure Calculation

It is interesting that both for the quadrupole moment and the E2, the direct and exchange parts are essentially the same.

We can investigate how this result changes in varying the range of the force, that is in varying α. The ratio in (36) is unity for $\alpha = 0$, goes through a broad minimum of 0.9 around $\alpha = 1.4$ and then increases very slowly with increasing α only reaching unity again for $\alpha = 3.5$ and 1.5 for $\alpha = 7$. For the $E2$ the ratio in (39) is even less sensitive to variation of α. Thus the insensitivity of the results to the exchange character of the force holds for all reasonable values of the range of the force. The ratio

$$\frac{\langle |E2|^2 \rangle}{\langle Q \rangle} \tag{41}$$

is also very insensitive to the range of the force. It is 0.64 for $\alpha = 0$, increases slowly to 0.78 for $\alpha = 1.4$ and goes on increasing slowly, reaching only 1.0 for $\alpha = 7$. In a sense it is very gratifying that the results are insensitive to variations in the exchange character or range of the force, but on the other hand this means that that avenue to improving agreement with experiment is closed.

The insensitivity of the ratio (41) to the range of the force, particularly down to zero range, means that any attempt to reduce the result for the quadrupole moment by introducing a zero range repulsive core, will cause a corresponding reduction in the $E2$. This can be seen since if the results are essentially independent of the range, then the introduction of a zero range repulsive core

only has the effect of changing the overall interaction strength, B. It seems then that repulsive cores, in perturbation theory, will not account for the discrepancy between theory and experiment.

The tensor force cannot be called upon in first order to explain the discrepancy since with an L-S closed shell the tensor force gives no first order contribution. Feingold (1957) suggests that second order may be important for any perturbation if the contribution of that perturbation to the nuclear binding energy is comparable with the excitation energy of the states one is mixing in. But this is not the case here since the contribution of the tensor force to the binding energy is probably not comparable with the spacing of the 2+ states in the O^{16} core.

For reasons of simplicity, the calculations thus far have been done with a Gaussian radial dependence for the force, but they can also be done with a Yukawa dependence for $f(r_{12})$. Evaluation of the radial integrals becomes very much more complicated in this case, and therefore we have only investigated the direct parts of the quadrupole moment and of the M2. Most of the radial integrals are then given by Swiatecki (1951), and computation of the remaining one is treated in Appendix 3. Putting the radial integrals into (26) and using $\alpha = 0.66$ for Yukawa interaction, we get

$$\langle Q \rangle_{direct} = -0.3 \frac{B}{E} \times 10^{-26} \text{ cm}^2 \qquad (42)$$

This is an encouraging result, being a factor of three smaller than the result for a Gaussian interaction, but evaluating (29) with a Yukawa interaction gives

$$\langle \| E2 \| \rangle_{direct} = 0.49 \frac{B}{E} \times 10^{-26} \text{ cm}^2 \qquad (43)$$

This too is smaller than before, and we find that the ratio of the $B/\bar{E}$ needed to fit the E2 and the one needed to fit the quadrupole moment is improved only by a factor of 2. The fact that both (42) and (43) are smaller than the corresponding results for the Gaussian interaction reflects the well known fact emerging from effective range theory (e.g. Blatt and Weisskopf, 1952, p. 55) that one needs a larger B for the Yukawa interaction than for the Gaussian interaction to provide the same effective interaction. It is also effective range theory that gives $\alpha = 0.66$ for the Yukawa case rather than $\alpha = 1.4$. In order to investigate the effect of range variation we have tried putting $\alpha = 1.4$ in the Yukawa results. This changes the ratio of $\langle \| E2 \| \rangle_{direct}$ to $\langle Q \rangle_{direct}$ from - 1.5 as in (42) and (43) to - 0.6. This is not a very big change for such a large variation in range, and further it is in the wrong direction.

There is of course no proof that the exchange parts for the Yukawa interaction will not be very different from the direct parts,

unlike the Gaussian case. Explicit evaluation of the exchange radial integrals for the Yukawa interaction would be extremely tedious, particularly because of the odd Legendre polynomial components of $f(r_{12})$ that come in. It is probably safe to assume, nevertheless, that the exchange parts will not be very different from their Gaussian counterparts since in O^{17} the range of the force is of the same order as the nuclear radius, and matrix elements of the interaction should not be very sensitive to what is essentially the fine structure of the interaction. This assumption is borne out by the calculations with a Yukawa interaction on the direct parts.

It might be possible to remove the discrepancy between the first order configuration mixing calculations and the observed values for the E2 and quadrupole moment by varying the shape of the single particle eigen-functions. It is probable that the odd neutron states in a proper self-consistent independent particle model formulation of O^{17} will be more loosely bound than is the case in the harmonic oscillator shell model. We can take this roughly into account by "pushing out" the radial functions for the 1d and 2s states, leaving the core states as before. The simplest way to achieve the "pushing out" is to raise by one the power of r involved in the radial function, that is to write in (15) ρ^{l+1} instead of ρ^{l}, changing the normalization accordingly. In

addition for the radial function of the 2s state one can treat the point at which the node occurs as a parameter. Once again we have only made these variations in the direct parts, but it is reasonable to suppose that if nothing drastic happens to the direct parts as a result of these changes, nothing drastic will happen to the exchange parts. We must now re-evaluate the radial integrals in (26) and (29) with the suitably altered radial functions, but with a Gaussian interaction. The technique for evaluation of the radial integrals is essentially the same as before, and the pertinent integrals are given in Appendix 2. The result for the quadrupole moment may be expressed as the product of the previous result for $\langle 1|Q|1\rangle_{direct}$, times a ratio of two third order polynomials in α. Putting in $\alpha = 1.4$ this ratio comes to 0.78, which is really not much of an improvement. The results for the E2 can be written in a similar manner as a product of $\langle \|E2\| \rangle_{direct}$ and a ratio. In this case, however, the ratio depends both on α and on the cross-over, or nodal, point for the 2s state. In the ordinary harmonic oscillator 2s state, the node occurs for $\frac{r}{b} = 1.5$. For $\alpha = 1.4$ we have investigated the effect of varying the node between $\frac{r}{b} = 1$ and 2, this varies the ratio of the new E2 to the old result from 1.3 to 1 respectively. Thus there seems to be no really significant improvement to be achieved by this form of "pushing out" of the radial functions.

Perhaps a more effective way of "pushing out" the radial functions of the odd particle would be to alter the exponential of the odd particle states compared with the core states. This can be done in a reasonable way by taking a smaller b for the odd particle states than for the core states, that is to say by taking the core states as eigen-functions in a narrower well than the odd particle states. Once again such a variation will only affect the radial integrals, and once again we only consider the direct terms with a Gaussian interaction. A discussion of the evaluation of radial integrals for this case is given in Appendix 4. The expressions will now clearly depend on two α's, α_1 for the core and α_2 for the odd particle. For the direct part of the quadrupole moment one gets

$$\langle Q' \rangle_{direct} = - \frac{8 \beta a^2 \alpha_2^{\frac{7}{2}} \alpha_1^{\frac{3}{2}}}{\bar{E} (\alpha_1 \alpha_2 + \alpha_1 + \alpha_2)^{\frac{11}{2}}} \times$$

$$(6\alpha_1^2 \alpha_2 + 6\alpha_1^2 + 5\alpha_1 \alpha_2 + 8\alpha_1 - \alpha_2) \qquad (44)$$

Taking for the core states b = 1.5 and for the odd particles 1.7 (both in units of 10^{-13} cm.) gives $\alpha_1 = 1.6$ and $\alpha_2 = 1.3$. Putting this into (44) one gets

$$\langle Q' \rangle_{direct} = -1.2 \frac{\beta}{\bar{E}} \times 10^{-26} \text{ cm}^2 \qquad (45)$$

which is rather a disappointing fruit for our toil. In the case of the E2 we again treat the nodal point, Θ, as a parameter. (Θ is defined as the value of $\frac{r}{b}$ for which the 2s radial function vanishes. In the harmonic oscillator case, $\Theta = 1.5$) Evaluating the radial integrals gives

$$\langle 11\, E2'\, 11\rangle_{direct} = \frac{3\,B\,a^2\,\alpha_1^{\frac{3}{2}}\,\alpha_2^{\frac{5}{2}}}{\bar{E}\,(\alpha_1+\alpha_2+\alpha_1\alpha_2)^{\frac{11}{2}}}\sqrt{\frac{5}{\pi\,\textcircled{H}}}\times$$

$$\Big[42\,\alpha_1^2\alpha_2^2 + 42\,\alpha_1^2\alpha_2 + 35\,\alpha_1\alpha_2^2 + 56\,\alpha_1\alpha_2 - 7\,\alpha_2^2 - \Theta\,(12\,\alpha_1^2\alpha_2^2 + 10\,\alpha_1\alpha_2^2 + 24\,\alpha_1^2\alpha_2 + 12\,\alpha_1^2 - 2\,\alpha_2^2 + 10\,\alpha_1\alpha_2)\Big] \qquad (46)$$

where $\textcircled{H}$ arises from the normalisation of the 2s radial function and is given by

$$\textcircled{H} = 15 - 12\,\Theta + 4\,\Theta^2 \qquad (47)$$

The most convenient quantity to investigate is the ratio of (46) to (44). Experimentally this ratio should be -5, and we have seen that the calculation with a Gaussian interaction, and ordinary harmonic oscillator functions gives for the ratio -0.8. For the formalism with "pushed out" radial functions, the

ratio can be written

$$-\frac{3.3}{\sqrt{(1)}}\left(1-\frac{\Theta}{7}y\right) \qquad (48)$$

where y is a ratio of polynomials in α_1 and α_2. Varying α_1 from 1.4 to 1.8, and α_2 independently from 1.0 to 1.4 only changes y between the limits 2.7 and 3.1. For any reasonable value of Θ, the term in y will be less than one, and we want it to be much less than one.* To make the ratio (48) large, then, we require that (1) be small. (1) has no real roots, and has a minimum for the oscillator value, $\Theta = 1.5$. Hence the best that can be done is done with $\Theta = 1.5$, and this is fairly independent of α_1 and α_2.

Thus any reasonable assumption (and a few unreasonable ones) about the interaction or the single particle eigen-functions seems to give roughly the same result, and that result is about a factor of six or seven away from a consistent account of the experimental results. That variations in the shape of the radial functions do not improve the agreement is easy to understand. Nothing we do to the functions will make the 2s - 1d overlap as good as the 1d - 1d overlap in the quadrupole moment matrix elements. Further since the range of the force is of the order of the nuclear

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* The sign of the reduced matrix element is not determined by the experimental data, but any reasonable assumption about collective mechanism will predict that it should be plus, in which case there is reason to ask that the term in y always remain smaller than one.

radius, all of the overlaps are essentially complete in O^{17} as long as one does not change the functions by too much. Hence although changing our assumptions will vary the results by factors of order unity, nothing we do within the framework of the first-order configuration mixing approach with closure seems to give a consistent account of the experimental data. Relative to the transition probability, the predicted quadrupole moment is always six or seven times too large.

3.4 Direct Evaluation of the Configuration Mixing Sum

We have seen that the closure formulation is exact in O^{17}, neglecting spin-orbit splittings, and further that it does not give the right answer, even for reasonable variations of the parameters and assumptions involved. Before we abandon hope, it is of interest to investigate the configuration mixing sum in j-j coupling without closure, in order to see which excitations are most important. In this way we can perhaps find a reasonable set of assumptions about the excitations that will give a consistent fit with experiment. If we cannot do this for harmonic oscillator eigen-states and a Gaussian interaction with a Rosenfeld exchange mixture, then it is indicated by the closure calculation that reasonable departures from any of these will not drastically improve the fit.

We wish to evaluate the configuration mixing expression (3) for the same model wave functions and interactions that we used in the first closure calculation, except that this time we evaluate the sum term by term and save the sum over i for last. It is convenient to separate the matrix elements of the interaction and of Q, and to consider first those of the interaction. We are interested in matrix elements of the form

$$M_{2+} = \langle 0\,J \mid V \mid (2+\,J_1)\,J \rangle \tag{49}$$

That is matrix elements between the state 0 of the core and J of the odd particle, and 2+ of the core and J_1 of the odd particle coupled up to angular momentum J. The 2+ state of the core is made by exciting a proton from the core state j to an excited state j_1 of the same parity and then coupling up the hole and the particle in the excited state to angular momentum 2. An elegant formalism for manipulating holes and particles in terms of creation and annihilation operators is given by Brink and Satchler (1956).

Writing in the couplings in terms of Wigner coefficients in the usual way, it is possible to perform the sums over z-components, and reduce (49) to a sum over particle matrix elements of the interaction. Thus for a particular excitation of a proton from the core state j, to the excited state j_1, we have for (49)

$$M_{2+jj_1} = \sum_{J'} (-1)^{j+J_1+J'} (2J'+1) \sqrt{\frac{5}{(2J+1)}} \times$$

$$W(jj_1 J J_1; 2 J') \langle (Jj) J' | V | (J, j_1) J' \rangle \qquad (50)$$

where now the matrix element of V is between the particle states, neutron in state J, proton in j coupled to J', and neutron in J_1 proton in j_1 coupled to J'. W(abcd;ef) is the usual Racah coefficient (Biedenharn, 1952). It is convenient to evaluate the matrix elements of V in L-S coupling since V is a scalar in both orbital angular momentum and spin space, and hence matrix elements of V will be diagonal in total L and total S. The matrix element of V appearing in (50) can be transformed into an L-S representation by making use of the LS-jj transformation coefficients (e.g. Edmonds, 1955), thus

$$\langle (Jj) J' | V | (J, j_1) J' \rangle$$

$$= \sum_{LS} \langle (Jj) J' | (LS) J' \rangle \langle (LS) J' | (J, j_1) J' \rangle \times$$

$$\langle [L(l, l') S] J' | V | [L(l_1, l_1') S] J' \rangle \qquad (51)$$

where

$$J = l \pm \tfrac{1}{2}, \; J_1 = l_1 \pm \tfrac{1}{2}, \; j = l' \pm \tfrac{1}{2}, \; j_1 = l_1' \pm \tfrac{1}{2}.$$

Each term in the interaction (20) splits up into a space part, V_x, and a spin part, V_s which is either one or P_B. Uncoupling L and S in (51) into the single-particle-orbital and spin states, and expending the interaction in spherical harmonics as in (23) one finds that making use of (25) and the techniques of Racah (1942) one can write for (50)

$$M_{2+ j j_1} = \sum_{J' L S} (-1)^{j_1 + J_1 + J'} (2J'+1) \sqrt{\frac{S}{2S+1}} \times$$

$$W(j j_1 J J_1; j 2J') \langle (J_j) J' | (L S) J' \rangle \langle (L S) J' | (J_1 j_1) J' \rangle \cdot$$

$$\langle S | V_s | S \rangle \langle L(l l') | V_x | L(l_1 l_1') \rangle \qquad (52)$$

where for the matrix elements of V_x we have

$$- B \langle L(l l') | f(r_{12}) | L(l_1 l_1') \rangle$$

$$= - B \sum_k (2k+1) [(2l_1+1)(2l'+1)]^{\frac{1}{2}} C^{l\, k\, l_1}_{0\, 0\, 0} \cdot$$

$$C^{l_1'\, k\, l'}_{0\, 0\, 0} W(l' k L l_1; l_1' l) F_k(l l' l_1 l_1')$$

$$- B \langle L(l l') | f(r_{12}) P_R | L(l_1 l_1') \rangle$$

$$= - B \sum_k (-1)^{l'+l-L} (2k+1) [(2l_1'+1)(2l'+1)]^{\frac{1}{2}} \times \qquad (53)$$

$$C^{l\, k\, l_1'}_{0\, 0\, 0} C^{l_1\, k\, l'}_{0\, 0\, 0} W(l_1' k L l'; l l_1) F_k(l l' l_1' l_1)$$

where the F_k's are the radial integrals

$$F_k(a\,b\,c\,d) = \langle R_a^{(1)} R_b^{(2)} | f_k(12) | R_c^{(1)} R_d^{(2)} \rangle \qquad (54)$$

For the spin matrix elements of V_B one gets

$$\langle s | s \rangle = 1 \qquad \langle s | P_B | s \rangle = (-1)^{1-S} \qquad (55)$$

Unfortunately it does not seem possible to do the sum over J' in (52) before doing the sums over L and S, and thus one cannot further reduce (52) before putting in the expressions (53) and (55) and first summing over L and S. In order to do this it is convenient to re-write the Racah coefficients and the LS - jj coefficients in terms of the 6-j and 9-j symbols as given by Edmonds (1955), and use the expressions given by him for sums over the symbols. Since the sums over L and S must be done first, we must consider four separate cases, corresponding to the four types of exchange terms in the interaction (20). Evaluation of the sums by repeated application of the identities given by Edmonds is straight-forward. One gets for the Wigner term, that is the term with no exchange interaction.

$$M_{2+j1'w} = (-1)^{J_1+j+l_1+l_1'} B\, F_2(l l' l_1 l_1') \times$$
$$\left[5(2j+1)(2J_1+1)(2j_1+1)(2l_1+1)(2l'+1)\right]^{\frac{1}{2}} \times$$
$$C^{l\,2\,l_1}_{0\,0\,0}\, C^{l_1'\,2\,l'}_{0\,0\,0}\, W(l_1 l J_1 J; 2\tfrac{1}{2})\, W(l_1' l' j_1 j; 2\tfrac{1}{2}) \qquad (56)$$

In the course of the calculation one finds that only the term with k = 2 contributes. For the Majorana exchange term, the one in P_M only, one gets

$$M_{2+jj'M} = (-1)^{j+J_1+l_1'+l_1} \sum_k (2k+1) F_k(ll'l_1'l_1) \times$$
$$B\left[5(2l_1'+1)(2l'+1)(2J_1+1)(2j+1)(2j_1+1)\right]^{\frac{1}{2}} \times$$
$$C^{l\,k\,l_1'}_{0\,0\,0} C^{l_1\,k\,l'}_{0\,0\,0} W(l_1 l J_1 J\,;\,2\tfrac{1}{2}) \times$$
$$W(l_1' l' j_1 j\,;\,2\tfrac{1}{2})\; W(l l_1' l_1 l'\,;\,k\,2) \qquad (57)$$

and similarly for the term in $P_M P_B$, the Heisenberg term,

$$M_{2+jj'H} = (-1)^{j_1-J+l+l'} \sum_k (2k+1) F_k(ll'l_1'l_1)$$
$$B\left[5(2l_1'+1)(2l'+1)(2J_1+1)(2j_1+1)(2j+1)\right]^{\frac{1}{2}} \times$$
$$C^{l\,k\,l_1'}_{0\,0\,0} C^{l_1\,k\,l'}_{0\,0\,0} W(j j_1 J_1 J\,;\,2k) \times$$
$$W(l J l_1' j_1\,;\,\tfrac{1}{2} k)\; W(l_1 J_1 l' j\,;\,\tfrac{1}{2} k) \qquad (58)$$

We have found no way of doing the summation for the Bartlett term, the one in P_B only. However the expression for this sum can be greatly simplified by noting the relation between the Bartlett sum and the one for the Wigner case (J.P. Elliott, Private Communication). We see from (55) that if the sum in the Wigner case is schematically written as

$$a = \sum_s f(s) \qquad (59)$$

then the sum in the Bartlett case is

$$b = -\sum_{S} (-1)^{S} f(S) \tag{60}$$

But since S is the sum of two spins of 1/2, it can only take the value 0 or 1. Thus

$$b = a - 2 f(0) \tag{61}$$

With the condition S = 0, f(S) simplifies considerably, in particular the 9-j symbols, that is essentially the LS-jj coefficients, reduce to Racah coefficients, and the sum over L,S, and J' reduces to a single sum that must be evaluated numerically. We can write for the Bartlett term

$$M_{2+jj'B} = (-1)^{l+l'+j_1+J} \, 5B \, F_2(ll'l_1l_1') \times \left[5(2j+1)(2J_1+1)(2j_1+1)(2l_1+1)(2l'+1)\right]^{\frac{1}{2}} \times C^{l\,2\,l_1}_{0\,0\,0} \, C^{l_1'\,2\,l'}_{0\,0\,0} \, \mathcal{L} + M_{2+jj'W} \tag{62}$$

where $\mathcal{L}$ is the sum that we evaluate numerically and is given by

$$\mathcal{L} = \sum_{L} (2L+1) \, W(j j_1 J J_1; 2 L) \, W(l'l_1'l l_1; 2L) \times W(l_1' j_1 l J_1; \tfrac{1}{2} L) \, W(l' j l J; \tfrac{1}{2} L) \tag{63}$$

As one might expect one finds empirically that $\mathcal{L}$ vanishes unless k = 2, and this fact has been written into (62) and (63).

The quadrupole matrix element in (3) can be written in the notation of (49)

$$Q_{jj'} = \langle (2+J_1)\, J\, M \mid Q \mid 0 J_1 M' \rangle \tag{64}$$

where the M's represent the z-component of angular momentum of the states.* Using the formalism for holes and particles of Brink and Satchler (1956), one gets in the usual way for (64)

$$Q_{jj'} = C^{J\ 2\ J_1}_{M\ M-M'\ M'} \langle R_{l_1'} \mid r^2 \mid R_{l'} \rangle \cdot \left(\frac{(2l_1'+1)(2j+1)(2j_1+1)}{4\pi}\right)^{\frac{1}{2}} (-1)^{\frac{1}{2}+l'-j} \cdot C^{l'\ 2\ l_1'}_{0\ 0\ 0}\ W(j\, l_1'\, j\, l'\, j\, \tfrac{1}{2}\, 2) \tag{65}$$

The radial integral in (65) is a standard one for three dimensional harmonic oscillator radial functions (Shaffer, 1944) and has very stringent selection rules. These combined with the angular momentum selection rules specified by the Wigner coefficients drastically limit the possible excitations, as we have discussed before. In j-j coupling, the possible excitations of protons from the O^{17} core that will contribute to (65) are

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* The z-components are important here since Q is not a scalar. V is a scalar and hence it follows from the Wigner-Eckart theorem that (49) does not depend on the z-components.

$1s_{1/2}$ to $1d_{3/2}$, $1s_{1/2}$ to $1d_{5/2}$, $1p_{1/2}$ to $2p_{3/2}$, $1p_{3/2}$ to $2p_{1/2}$, $1p_{3/2}$ to $2p_{3/2}$, $1p_{1/2}$ to $1f_{5/2}$, $1p_{3/2}$ to $1f_{5/2}$ and $1p_{3/2}$ to $1f_{7/2}$. Neglecting the spin-orbit splitting, these excitations all have the same energy, but now we wish to keep in the spin-orbit splitting, and clearly this is the reason for doing the calculation in j-j coupling.

We shall be interested in three types of terms in the combination of the interaction and quadrupole matrix elements - those for which $J = J_1 = \frac{5}{2}$, those for which $J = \frac{5}{2}$ and $J_1 = \frac{1}{2}$, and those for which $J_1 = \frac{5}{2}$ and $J = \frac{1}{2}$. These three correspond to diagonal mixing for the ground state moment, and the two case for the E2, mixing into the ground state and excited state respectively. For each of these three cases we must evaluate the contribution of each of the four types of exchange interaction, and this must be done for the eight possible excitations enumerated above. Fortunately the radial integrals, F_k, arising in these cases, may all be expressed in terms of the radial integrals that were needed in the closure calculation, and hence the general results of Appendix 2 can be used.

After considerable manipulation, we can get an expression for the contribution of each of the excitations to each of the three terms; let us call them Q for the quadrupole moment, E_D

for the E2 reduced matrix element with admixtures into the ground state, and E_g for the E2 with admixtures into the excited state. The result will depend upon the exchange character of the force. Since we are interested in comparing this calculation with the closure case, we take a Rosenfeld mixture for the exchange. We have not investigated the variation in contribution of each of the possible excitations with variation of the exchange character. The parameter α is taken as before to be 1.4. We can make a table of the contribution of each of the excitations before dividing by the energy denominators. In units of $\frac{Bb^2\alpha^{3/2}}{(\alpha+2)^{11/2}}$ the contribution of each of the terms, without energy denominators is

	1s - 1d		1p - 2p			1p - 1f		
	$\frac{1}{2}-\frac{3}{2}$	$\frac{1}{2}-\frac{5}{2}$	$\frac{1}{2}-\frac{3}{2}$	$\frac{3}{2}-\frac{1}{2}$	$\frac{3}{2}-\frac{3}{2}$	$\frac{1}{2}-\frac{5}{2}$	$\frac{3}{2}-\frac{5}{2}$	$\frac{3}{2}-\frac{7}{2}$
-Q	22.2	33.5	3.6	3.6	3.8	52	12.8	84.4
E_S	7.1	18	12	8.7	10	8.3	4.9	17
E_D	-8.8	-6.5	2.5	2.8	2.8	19	4.7	36

It is easily verified that the sum of terms gives the closure results.

The calculation yields no very surprising results. We see that in general the relative contribution of each excitation, or groups of excitations to Q, E_D and E_S is roughly of the same order in each case, and thus we cannot get a fit by simply disallowing some particular excitation, or giving it an anomalously low or high energy denominator. It is interesting to note how small is the contribution of the 1p to 2p excitations. It is usually argued that excitations involving a change in principal quantum number only will be large because of the large overlap of the angular parts, but in our case this seems to be cancelled by the small overlap of the radial parts. The largest contributions come from the 1p to 1f excitations, particularly $1p_{3/2}$ to $1f_{7/2}$. But for the quadrupole moment the relative contribution of this excitation is not so large that excluding the excitation will reduce the quadrupole moment to the required value.

In order to get energy denominators for the excitations we take the usual form for the oscillator splitting,

$$E_0 = \frac{\hbar\omega}{2\pi} = \frac{\hbar^2}{4\pi^2 M b^2}$$

where M is the nucleon mass. Taking $b = 1.6 \times 10^{-13}$ cm. gives $E_0 = 16$ mev. The spin-orbit energy is taken in the usual way to be $-\lambda\ \underline{\ell}\cdot\underline{s}$, and we take $\lambda = 2$ mev consistent with the

$d_{5/2} - d_{3/2}$ splitting in O^{17} (Elliott and Flowers, 1955). In addition we depress the $2s_{1/2}$ state by 1.125 mev in order to get it in the observed place. The computation of energy denominators is now simply a problem in subtraction. All of the energies are of the order of 30 mev. Putting them in and combining the contributions of the various excitations, one finds that one needs a B of the order of 15 mev to fit the ground state moment, and one of the order of 120 mev to fit the E2 reduced matrix element. Neither of these values is consistent with other two-body data, the one being too large and the other too small.

A more reasonable procedure may be to pick the excitation energies semi-empirically. The first excited state of O^{16} occurs at 6 mev, and in O^{17} there is a group of negative parity states at about 4 mev (Ajzenberg and Lauritsen, 1955). These must correspond to excitations involving a change in the oscillator principal quantum number, i.e. to excitations of the order of E_0. It is clear then that for the determination of excitation energies, rather than wave functions, E_0 should be more of the order of 6 than 16 mev. This difference reflects the well known fact that the ordinary shell model gives a very bad account of zero order energies. Taking 6 mev as a reasonable mean value for E_0 in O^{17}, and taking the closure expressions (38) and (40)

once again since we are now using an average excitation energy, we find that B = 40 mev fits the E2, whereas we need B = 6 mev for the quadrupole moment. 40 mev is quite a reasonable value for the strength of the interaction, and fits in well with other work that has been done with configuration mixing around A = 19 (Elliott and Flowers, 1955), but taking B = 40 mev, we are left with a ground state quadrupole moment seven times larger than the one measured by Geschwind et al. A remeasurement of this moment is therefore of considerable interest.†

Since the total E2 reduced matrix element is of the order of one half the contribution from a single proton transition, and since the E2 contribution from each excitation is roughly of the order of a single proton transition, the amplitudes of the admixtures must be of the order of $\frac{1}{16}$th. The sum of the squares of the amplitudes is thus about $\frac{1}{30}$th, and one would guess that the zero order shell model state is quite pure, and that first order perturbation theory is fairly good. We have investigated the form of the terms in second order. In particular we have investigated the phases of the contributions to the ground state quadrupole moment that are diagonal in the admixture. We thus avoid ambiguities in the sign of the admixture. We find that these terms alternate in phase, and hence give little hope of all combining together to cancel out the first order contribution to the

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† See Addendum p.67a.

quadrupole moment.

3.5 Other Models

Other attempts from different points of view have been made to explain the weak collective effects in O^{17} and have been equally unsuccessful. Perks (1955) and Horie and Arima (1955) have looked at the configuration mixing without closure. In particular Horie and Arima have evaluated the first order configuration mixing contribution to the quadrupole moment for a large number of nuclei. They make the two simplifying assumptions of a zero range interaction and harmonic oscillator radial functions. The first assumption makes the calculation of the interaction matrix elements very much simpler than it is with finite range forces, and the second, as we have seen, drastically limits the number of excitations that can contribute. Unfortunately these two assumptions are mutually exclusive since harmonic oscillator functions are only good for light nuclei, and zero range forces only good for heavy nuclei. Nevertheless because of the independence of the results in O^{17} on the range of the force, they get an answer for the ground state moment similar to ours. Taking an interaction strength from other data they get a quadrupole moment that is ten times larger than the experimental one. They suggest that a finite range force would improve

the agreement. They do not calculate transition probabilities, but in view of our calculation, one would guess that their method would give reasonably good agreement with the E2 in O^{17}.

The two collective effects have been investigated by Barker (1956) from the point of view of weak surface coupling (Bohr and Mottelson, 1953). In the weak surface coupling formalism the odd particle is coupled parametrically to the surface of the closed shell core. Barker finds that ten times stronger coupling is needed for the E2 as for the ground state moment.

Kamemy (1956) has investigated the problem using semi-empirical admixtures of 2+ states of the O^{16} core. He is able to fit the experimental results but only by neglecting to consider admixtures into the ground state of O^{17} of those states for which the core is in a 2+ state and the odd particle in the $d_{5/2}$ state. In this way he gets first order contributions from his admixtures to the E2, but only second order contributions to the ground state moment. But there is no reason to believe that the admixtures with the neutron in the $d_{5/2}$ state will be small, let alone zero, and one can only assume that Kamemy's success is due to an oversight. A proper semi-empirical calculation taking into account the ground state admixture diagonal in the odd particle (Fallieros and Ferrell, 1957) fails as we might expect.

Thus no calculation for O^{17} that starts with the zero order shell model state of one neutron outside the extremely stable O^{16} doubly closed shell seems able to account for the observed weak electric quadrupole effects. Reasonable calculations seem to fit the E2 but give a ground state moment many times the accepted value. The various predictions are not completely model independent, however, and if remeasurement of the quadrupole moment should reveal a very much larger moment, it will be very interesting to see which if any of the predictions are able to fit it.

The possibility that the shell model state is not a good approximation in O^{17}, even in zero order, must be considered. We have seen that apart from weak collective effects, there are many reasons to believe that the shell model state is a very good approximation indeed, and Elliot and Flowers (1955) use single particle model states in O^{17} as the starting point for a configuration mixing calculation for A = 18 and 19 getting very good results. Any new zero order model we introduce would have to account for the many successes of the single particle model as well as for weak collective effects. The most likely candidate is the strong coupling model of Bohr and Mottelson (1953). In this model the nuclear core is assumed to have an equilibrium deformation, and the motion of the odd particle is

strongly coupled to the core. The core, being deformed, can rotate, and it is the central assumption of the weak coupling formalism that the energy associated with the rotation is small compared with the separation of single particle states. To each single particle configuration there will correspond a rotational band. States of the same spin and parity in different bands will interact strongly if they are close in energy (Kerman, 1956) and will tend to repel each other. In complicated cases the resulting spectrum may look very different from the usual rotational spectrum. In addition to these dynamical properties, the deformed core will give rise to collective quadrupole moments and the like.

This model, although originally constructed to account for the behaviour of heavy nuclei far from closed shells, has recently been applied with surprising success in light nuclei (Cove, et al. 1956), and with success in a nucleus as close to a closed shell as F^{19} (Paul, 1956). In F^{19} the work was done assuming a positive equilibrium deformation, and there may be some reason to believe that the tendency to positive equilibrium deformation extends as far as O^{17} (Mosskowski, 1955). A positive equilibrium deformation for the charged core corresponds to a positive collective quadrupole moment. Calculation with the deformation used in F^{19} gives a collective quadrupole moment for O^{17}

of about + 0.03 barns. This is about the same order as the configuration mixing result but of opposite sign. Thus if in some way we could use both the configuration mixing result and the strong coupling result, we could arrange to have a very small quadrupole moment. If these two effects are not coherent, they will cause no cancellation in the transition probability, since this depends on the square of the matrix element, and there will be no cross terms.

There is a great deal that is unsatisfactory about this mixed model. In F^{19} the collective model approach of Paul is considered as an <u>alternative</u> formulation to the configuration mixing calculation of Elliott and Flowers. Furthermore it is not clear in what way the two effects are incoherent. There is certainly no doubt that O^{16} is spherically symmetric. Thus if the core in O^{17} is to take up an equilibrium deformation, it does so by virtue of the odd particle. It is difficult to see in what way we can say that the odd particle first causes a deformation of the core, and then through the residual interaction wipes that deformation out, and further say that these two effects, both due to the odd particle, are incoherent. A further difficulty arises in the selection of zero order states. O^{17} is usually considered to be spherically symmetric, and thus the levels in O^{17} can be used to adjust the shell model parameters.

The effect of deformations on the levels is then not too difficult to calculate since the position of the levels for zero deformation is known empirically. But if O^{17} is already deformed, we cannot read off the position of the zero deformation levels from it, and in fact it would be likely that the levels in zero deformation would be quite different from those in O^{17}. This would cause a drastic revision in our ideas of the shell model, and would probably change the agreement of the calculation of Paul for F^{19} since the position of the levels in F^{19} depends on the position of the levels for zero deformation.

The final test of a strong coupling model for O^{17} must be the energy levels. Taking the parameters that Paul used in F^{19} and leaving free the positions of the zero order particle levels for the reasons discussed above, we have tried to fit the energy levels in O^{17} using the formalism of Kerman (1956) for the interaction between levels from different rotational bands.* It seems possible to get the proper ordering for the positive parity levels in O^{17} with a reasonable set of zero order particle levels, but no reasonable parameters or zero order ordering of levels will give the observed level spacing. Further it seems impossible to fit the negative parity levels in O^{17} in strong coupling, whereas Rakavy (1957) fits the negative parity levels in F^{19} quite well

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* We are indebted to Dr. Paul for a number of interesting conversations and private communications on this work.

within this formalism.

Thus the strong coupling collective model does not seem to be a better zero order model for O^{17} than the shell model. To use the strong coupling formalism to explain the weak collective effects in O^{17} would indeed seem to be cutting off our nose to spite our face, but with our nose still intact and with no remeasurement as yet available for the ground state moment, the weak collective effects remain unresolved.

3.6 Addendum

Recent preliminary experiments by Stevenson on the hyperfine structure of HDO^{17} (M. J. Stevenson, CRL Quarterly Report, March 15, 1957) give a quadrupole moment for the ground state of O^{17} of -0.03 ± 0.01 barns. This is in complete agreement with our calculation and allows a consistent account of the ground state moment and of the M2. A similar preliminary value has been obtained by R. A. Kamper and C. D. Lustig (Private Communication) from the hyperfine structure of atomic O^{17}.

CHAPTER 4

THE LEAD CLOSED SHELL

4.1 Evaluation of the Matrix Elements

In the region of the lead closed shell (Z = 82, N = 126),[+] there are weak collective quadrupole effects much as in oxygen, and the formalism of configuration mixing can be applied in an attempt to understand these effects. For heavy nuclei the nuclear density distribution is more "square" than in oxygen and hence harmonic oscillator radial functions are no longer a good approximation. We are thus no longer helped by the strong selection rules imposed on the configuration mixing sum by these functions, and the evaluation of the proper first order configuration mixing sum taking all possible contributions into account

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[+] The fact that the lead closed shell is only closed in the j-j sense rather than the L-S sense does not materially alter the formalism since the operator Q does not affect spin-space.

would be very difficult indeed. On the other hand application of the closure formalism is relatively simple.

Let us consider an electric quadrupole transition in the odd neutron hole nucleus Pb^{207} between the states J' and J. We wish to evaluate an expression of the type given in (9). Making use of the fact that in lead the range of the force is short compared with the nuclear radius, the interaction can be treated in a range expansion. In Appendix 5 we discuss the relative contribution of the three-body terms in (9) particularly for zero-range forces. We see that although an exact evaluation of these terms is extremely difficult, and although the terms may in fact contribute quite a bit to the weak collective effects - perhaps even as much as 50% - the dependence of this contribution on the state of the odd particle is very much the same as for the two-body terms. Thus the weak collective effects calculated with the two-body terms only may well be too large, but they will be too large by a roughly constant factor, independent to within 20% of the odd particle state. Hence neglecting the three-body term will not greatly change the validity of the closure assumption, i.e. the assumption that the mean excitation energy is a property of the core roughly independent of the odd particle state.

Taking $\bar{E}' = \bar{E}$ as is consistent with the closure assumption, and using only the two-body term in (9), the matrix element for

the transition from J' to J in Pb^{207} can be written

$$\langle J'|E2|J\rangle = -\frac{2}{E}\sum_i \langle \phi_i(1)\,\nu^{(2)}_{J'M'} \mid V(12)\,Q^{(1)}_{M'-M} \mid \phi_i(1)\,\nu^{(2)}_{JM}\rangle \qquad (66)$$

In the limit of zero range, the space exchange part of the interaction gives just the same thing as the direct part, and as we saw before, spin exchange simply gives a factor of 1/2, thus the interaction in (66) can be treated as purely central, in which case the matrix element contains the sum of squares of the single particle proton states, ϕ_i. Such a sum is just the nuclear charge density distribution. Hence assuming that we can interchange the order of summation and integration, and using a purely Wigner type interaction, we can re-write (66) in the form

$$\langle J'|E2|J\rangle = -\frac{2Z\zeta}{E}\int_0^\infty\int_0^\infty \nu^{*(2)}_{J'M'}\,\nu^{(2)}_{JM}\,\rho(1)\,V(12)\,Q^{(1)}_{M'-M}\,d\tau_1\,d\tau_2 \qquad (67)$$

where ρ is the charge density distribution normalised to unity, and ζ is a numerical factor depending on the exchange mixture.

The introduction of a density distribution instead of a sum over core states is a considerable computational simplification. Further it reduces the physically difficult problem of having to choose single particle eigen-functions for the 82 protons in lead.

to the problem of choosing a density distribution, and the recent high energy electron scattering experiments at Stanford have yielded much information about this distribution (Hofstadter, 1956). The density obtained in these experiments has a rather complicated form, and we take a simpler one, but one that still retains the gross features of the Stanford distribution. We take the spherically symmetric distribution

$$\rho(r,t) = \rho_o \quad \text{for} \quad 0 \leq r \leq R(1-t)$$

$$\rho(r,t) = \rho_o \frac{(R-r)}{Rt} \quad \text{for} \quad R(1-t) \leq r \leq R \qquad (68)$$

$$\rho(r,t) = 0 \quad \text{for } r \leq R$$

The normalisation is $4\pi \int_0^R \rho(r) r^2 \, dr = 1$, giving $\rho_o = \frac{3}{R^3(4-6t+4t^2-t^3)\pi}$

This density has been used by Elton-Swayle (1955), but with slightly different normalisation. If one treats $R_o = r_o \times A^{1/3}$ as the radius of the square density distribution that has the same mean square radius as ρ, then R_o is related to R by

$$R^2 = R_o^2 \beta^2(t)$$

where

$$\beta^2(t) = \frac{3(4 - 6t + 4t^2 - t^3)}{2(6-15t + 20t^2 - 15t^3 + 6t^4 - t^5)}$$

In order to evaluate the integral (67) we expand the integrand in a power series in the range of force (Brink, 1954).

Going to the first non-vanishing term beyond zero range gives for (67)

$$\langle J'|E2|J\rangle = +\frac{2Z}{E}\rho\, a\Big[\int_0^\infty \nu^*_{J'M'}\,\nu_{JM}\,\rho\, Q_{M'-M}\,d\tau + B\int_0^\infty \nu^*_{J'M'}\,\nu_{JM}\,\nabla^2(\rho\, Q_{M'-M})\,d\tau\Big] \tag{69}$$

where

$$a = -4\pi\int V(s)s^2\,ds \quad \text{and} \quad B = \frac{\int V(s)\,s^4\,ds}{3!\int V(s)\,s^2 ds}$$

Using (68) it is easy to show that

$$\nabla^2(\rho Q_m) = -\frac{6\rho_0 Q_m}{Rtr} \quad \text{for } R(1-t)\le r\le R$$
$$= 0 \quad \text{for } 0\le r\le R(1-t) \tag{70}$$

Taking for the odd neutron eigen-states of the type (16), and recalling the definition (17) for the operator Q_m we get for (69)

$$\langle J'|E2|J\rangle = \frac{2Z}{E}\rho\, a\,\langle \mathcal{Y}_{J'l'M'}|Y_{2M'-M}|\mathcal{Y}_{JlM}\rangle \cdot \Big[\int_0^\infty R^*_{N'l'}R_{Nl}\rho\, r^4\,dr - \frac{6\rho_0}{Rt}B\int_{R(1-t)}^{R} R^*_{N'l'}R_{Nl}\,r^3\,dr\Big] \tag{71}$$

The angular part can be evaluated making use of the easily verified relation

$$\langle Y_{J'\ell'M'} | Y_{kM'-M} | Y_{J\ell M} \rangle = (-1)^{J-\ell-\frac{1}{2}} C^{J'\ k\ J}_{M'\ M'-M\ M} \times$$

$$C^{\ell'\ k\ \ell}_{0\ 0\ 0} \left(\frac{(2k+1)(2\ell+1)(2J+1)}{4\pi} \right)^{\frac{1}{2}} W(J'\ell' J\ell; \tfrac{1}{2}k) \quad (72)$$

We take the radial functions, $R_{N\ell}$, solutions of the radial equation for eigen-states in an infinite square well (Schiff, 1949, p.76). These are given by

$$R_{N\ell} = \frac{C_{N\ell}}{(k_{n\ell} r)^{\frac{1}{2}}} J_{\ell+\frac{1}{2}}(k_{n\ell} r) \quad (73)$$

where $J_{\ell+\frac{1}{2}}$ is the usual Bessel function, and $C_{N\ell} = \dfrac{(2k^3_{N\ell})^{\frac{1}{2}}}{\alpha_{N\ell} J_{\ell+\frac{3}{2}}(\alpha_{N\ell})}$.

$\alpha_{N\ell} = k_{n\ell} R$ if R is the radius of the generating potential well, and $\alpha_{N\ell}$ is the nth zero of $J_{\ell+\frac{1}{2}}$ not counting $J(0)$. We assume that the radius of the generating potential is the same as the R that appears in the density distribution; this is a reasonable assumption since it makes the density and the single particle functions go to zero at the same radius. Putting (68), (72) and (73) into (71) we get finally for the reduced matrix element for the transition,

$$\langle J'\|E2\|J\rangle = \frac{2Z^{\nu}a}{\bar{E}}\left(\frac{(2l+1)(2J+1)5}{4\pi}\right)^{\frac{1}{2}} C^{l'\,2\,l}_{0\,0\,0}\,,$$

$$W(J'l'Jl;t2)(-1)^{J-l-t}\,\frac{C_{Nl}\,C_{N'l'}}{\sqrt{k_{Nl}\,k_{N'l'}}}\int_0^{\infty}$$

$$\left[\int_0^{R(1-\tau)} J_{l+\frac{t}{2}}(k_{Nl}r)\,J_{l'+\frac{t}{2}}(k_{N'l'}r)\,r^3\,dr \right. \tag{74}$$

$$\left. +\frac{1}{Rt}\int_{R(1-\tau)}^{R} J_{l+\frac{t}{2}}(k_{Nl}r)\,J_{l'+\frac{t}{2}}(k_{N'l'}r)\left(Rr^3-r^4-6\beta r^2\right)dr\right]$$

Unfortunately the remaining radial integrals must be evaluated numerically. This is done by plotting the integrands for each case and finding the area under the curves as a function of t by counting squares.

If a nucleus has two neutron holes, as does Pb^{206}, the reduced matrix element for transition can still be written in terms of the one neutron matrix elements considered above. Let us consider the reduced matrix element of some one body tensor operator $T(\lambda\mu)$ between a two-particle state with neutrons in states j and j_1 coupled up to a total angular momentum L and a similar state with neutrons in j and j_2 coupled up to L'. Clearly since $T(\lambda\mu)$ is a one-body operator, the two-particle states can only differ in the state of one of the neutrons. It is easily verified that the reduced matrix element of T between L and L' is

given in terms of the single neutron reduced matrix element between j_1 and j_2 by

$$\langle (j j_1) L \| T(\lambda) \| (j j_2) L' \rangle$$
$$= (-1)^{j_2 - j_1 + L' - L} \left[(2j_1+1)(2L'+1) \right]^{\frac{1}{2}} W(\lambda j_2 L j ; j_1 L') \times$$
$$\langle j_1 \| T(\lambda) \| j_2 \rangle \tag{75}$$

We shall be interested in the collective contribution to the quadrupole moment of the odd proton nucleus Bi^{209}. For this case we must use the formalism for the odd proton case developed in Chapter 2. Before doing a range expansion in (13), it is necessary to look at the spin matrix elements. Since we are interested in the quadrupole moment, we want the odd particle state with z-component of angular moment equal to the total angular momentum. We can write for the odd particle state

$$\phi_0 = \sum_m C^{J\ \ell\ \ \frac{1}{2}}_{J\ J-m\ \ m} \varphi_{\ell, J-m} \chi_m$$

and similarly for the core states $\phi_i = \varphi_i \chi_i$ where the φ are space eigen-functions only, and the χ are spin functions. Considering only the Wigner part of the interaction, and evaluating the spin matrix elements, (13) reduces to

$$-\frac{2}{E} \sum_{im} \left(C^{J\ \ell\ \ \frac{1}{2}}_{J\ J-m\ \ m} \right)^2 \left[\langle \varphi_{\ell J-M} \varphi_i | V(Q_1 + Q_2)(2 | \varphi_{\ell J-M} \varphi_i \rangle - | \varphi_i \varphi_{\ell J-M} \rangle) \right]$$
$$+ \frac{2}{E} \sum_{ijm} \left(C^{J\ \ell\ \ \frac{1}{2}}_{J\ J-m\ \ m} \right)^2 \left[\langle \varphi_{\ell J-m} \varphi_j | V(2 | \varphi_{\ell J-M} \varphi_i \rangle - | \varphi_i \varphi_{\ell J-M} \rangle) \langle \varphi_i | Q | \varphi_j \rangle \right]$$
$$+ \frac{2}{E} \sum_{im} \left(C^{J\ \ell\ \ \frac{1}{2}}_{J\ J-m\ \ m} \right)^2 \left[\langle \varphi_{\ell J-m} \varphi_i | V(2 | \varphi_{\ell J-m} \varphi_i \rangle - | \varphi_i \varphi_{\ell J-M} \rangle) \right] \langle \phi_0 | Q | \phi_0 \rangle \tag{76}$$

where now the sums are over the $\frac{2-1}{2}$ different space eigen-functions in the core. The three-body terms in (76) are analogous to those for the odd neutron case, and as discussed in Appendix 5 we do not introduce a very large error by neglecting them. In the limit of zero range, the space exchange terms in (76) will become the same as the direct terms, and neglecting the three-body terms (76) can be written

$$\frac{2\,2\,Q}{E}\int_0^\infty \rho\, Q\,|\phi_0|^2\,d\tau - \frac{2\,Q}{E}\langle\phi_0|Q|\phi_0\rangle\int_0^\infty \rho\,|\phi_0|^2\,d\tau \qquad (77)$$

We assume as in the neutron case that the general form of (77) holds for the first term beyond zero range in the range expansion. Since for zero range space exchange just gives unity, spin exchange becomes equivalent to particle exchange, i.e. Heisenberg exchange, and hence spin exchange will give a minus sign for identical particles. Thus we can write the collective contribution to the ground state quadrupole moment as

$$\frac{4}{E}\sqrt{\frac{\pi}{5}}\,2\,a\,\eta\Big[2\int_0^\infty \rho\,Q\,|\phi_0|^2\,d\tau + 4B\int_0^\infty Q\,|\phi_0|^2\,\nabla^2\rho\,d\tau - \langle\phi_0|Q|\phi_0\rangle\times\Big(\int_0^\infty|\phi_0|^2\,\rho\,d\tau + B\int_0^\infty|\phi_0|^2\nabla^2\rho\,d\tau\Big)\Big] \qquad (78)$$

where η is a factor depending on the exchange character of the force, and where use has been made of the fact that

$$\nabla^2 (Q\rho) = 3 Q \nabla^2 \rho$$

In the approximation of zero range forces that we are using, the exchange factors, ς and η, are easily expressed in terms of the exchange character of (20). P_M is equivalent to unity for zero range, and for the odd neutron case P_B gives a factor of 1/2. Thus we get

$$\varsigma = \gamma + \epsilon + \tfrac{1}{2}(\beta + \delta)$$

In the odd proton case, P_B gives minus the direct part, and we get

$$\eta = \gamma + \epsilon - (\beta + \delta)$$

For a Rosenfeld mixture we find $\varsigma = 0.90$ and $\eta = 0.60$.

For r_0 we take 1.2×10^{-13} cm, (Hofstadter, 1956) which corresponds to an R_0 for lead of 7.1×10^{-13} cm. For the interaction parameters α and B, we take the values given by Brink (1954). $\alpha = 1.3 \times 10^{-36}$ Mev cm^2, which in the usual way is independent of the precise radial form of the interaction; and $B = 0.92 \times 10^{-26}$ cm^2, which is an average for the Yukawa and square well interactions. It should be noted that there is a misprint in the Brink paper; the values given for $\int V(s) s^4 \, ds$ should be multiplied by 6. The precise choice of B is not very important since the range expansion seems to be quite good, the term in B

being only 10% of the first term. This also means that the results are not very sensitive to the assumption that exchange dependence, etc. of the zero range term can be carried over into the term in B.

4.2 Comparison with Experiment

The energy levels and spin assignments for Pb^{207}, one neutron hole in the doubly closed shell, are given by Alburger and Sunyar (1955) and their energy level diagram is reproduced in Figure 1. In particular we take their assignment of $2f_{7/2}$ for the state at 2.35 Mev rather than the $h_{9/2}$ assignment assumed by Lazar and Klema (1955). Reasons for this choice are discussed by Alburger and Sunyar, and further G. R. Satchler (Private Communication) finds the sign of the measured M1-E2 radiation mixing ratio for the 1.78 transition from this state to the $2f_{5/2}$ state to be compatible with an assignment of $f_{7/2}$ but not with $h_{9/2}$.

By assuming a single particle value for the M1 reduced matrix element in this M1-E2 mixed transition, Satchler has calculated the reduced matrix element for the E2 part of this transition, getting 0.15 barns.

The assumption that the M1 part of the transition is well given by the single particle value has been investigated by C. A. Caine (Private Communication). Since both the neutron and

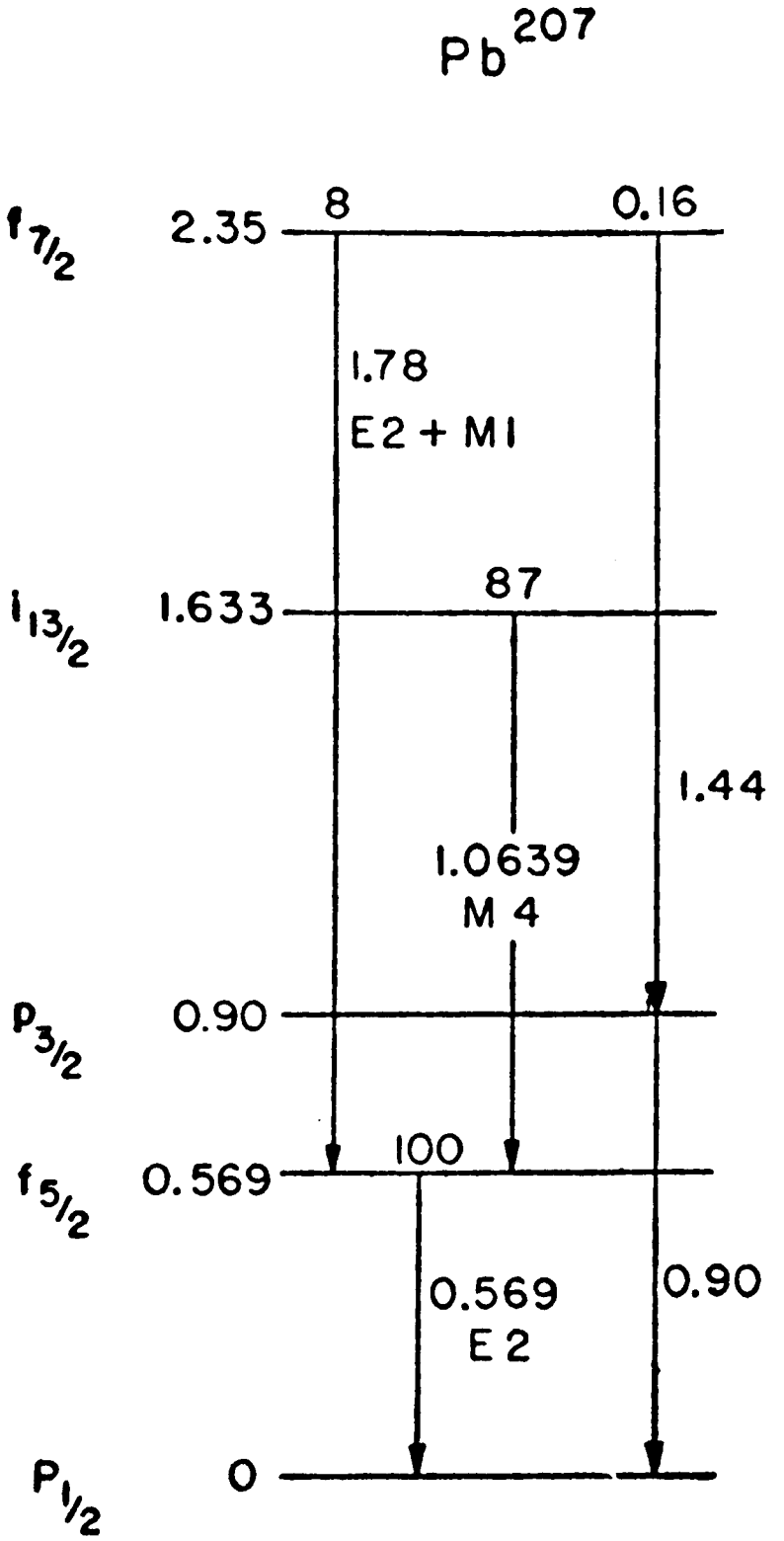

Figure 1: Energy level diagram for Pb^{207} taken from Alburger and Sunyar (1955).

proton closed shells in lead are only closed in the j-j sense, there will be first order configuration mixing contributions to matrix elements of the magnetic dipole operator. There can be no excitations within the 2f spin-orbit doublet, however, since with only one hole in the f shell, one cannot produce first order excitations having the same total angular momentum as the zero order state by exchanging the hole within the spin-orbit doublet. The only excitations that will contribute to the M1 matrix element in first order are proton excitations within the 1h spin-orbit doublet and neutron excitations within the 1i spin-orbit doublet. Caine has calculated the contribution from these excitations using zero range forces and estimating the radial integrals by use of harmonic oscillator functions. He finds that first order configuration mixing reduces the M1 matrix element for the transition by only about 7% of the single particle value. This very small reduction is essentially due to the small overlap between the 2f and the 1h or 1i functions.

The reduced matrix element for the 0.569 Mev E2 transition from the first excited state ($2f_{5/2}$) to the $3p_{1/2}$ ground state has been measured by Stelson and McGowan (1955) using Coulomb excitation, and they get 0.096×10^{-24} cm^2. These two E2 transitions in Pb^{207} must clearly be collective and we can try to fit them to (74). If we equate (74) to the experimental reduced matrix elements in each

case, we get an expression for $\bar{E}$ as a function of t needed to fit the results. Let us call the $\bar{E}$ for the 1.78 Mev transition $\bar{E}'_{207}$ and the one for the 0.569 Mev transition to the ground state $\bar{E}_{207}$. It is convenient to treat t as a parameter in the fitting even though it is given by the electron scattering experiments since it is interesting to see the effect of variation in density distribution. $\bar{E}_{207}$ and $\bar{E}'_{207}$ are plotted in Figure 2 as a function of t.

Alburger and Sunyer also find a 2% branching of the transition from the $2f_{7/2}$ state going by a 1.44 Mev E2 to the $3p_{3/2}$ state. On our model, since we take the space part of the single particle functions to depend only on the orbital angular momentum and not on the total angular momentum, the reduced matrix element for this transition is the same as the one for the 0.569 Mev transition to the ground state apart from angular factors. We find that we can fit the order of magnitude of the branching using the same parameters as for the 0.569 Mev and 1.78 Mev transitions, but an attempt at a detailed fit does not seem justified in view of the many uncertainties, both theoretical and experimental, involved.

In Pb^{206} the first excited state, 2+, decays to the 0+ ground state by a 0.803 Mev E2 gamma ray. The reduced matrix element for the transition, measured using Coulomb excitation by

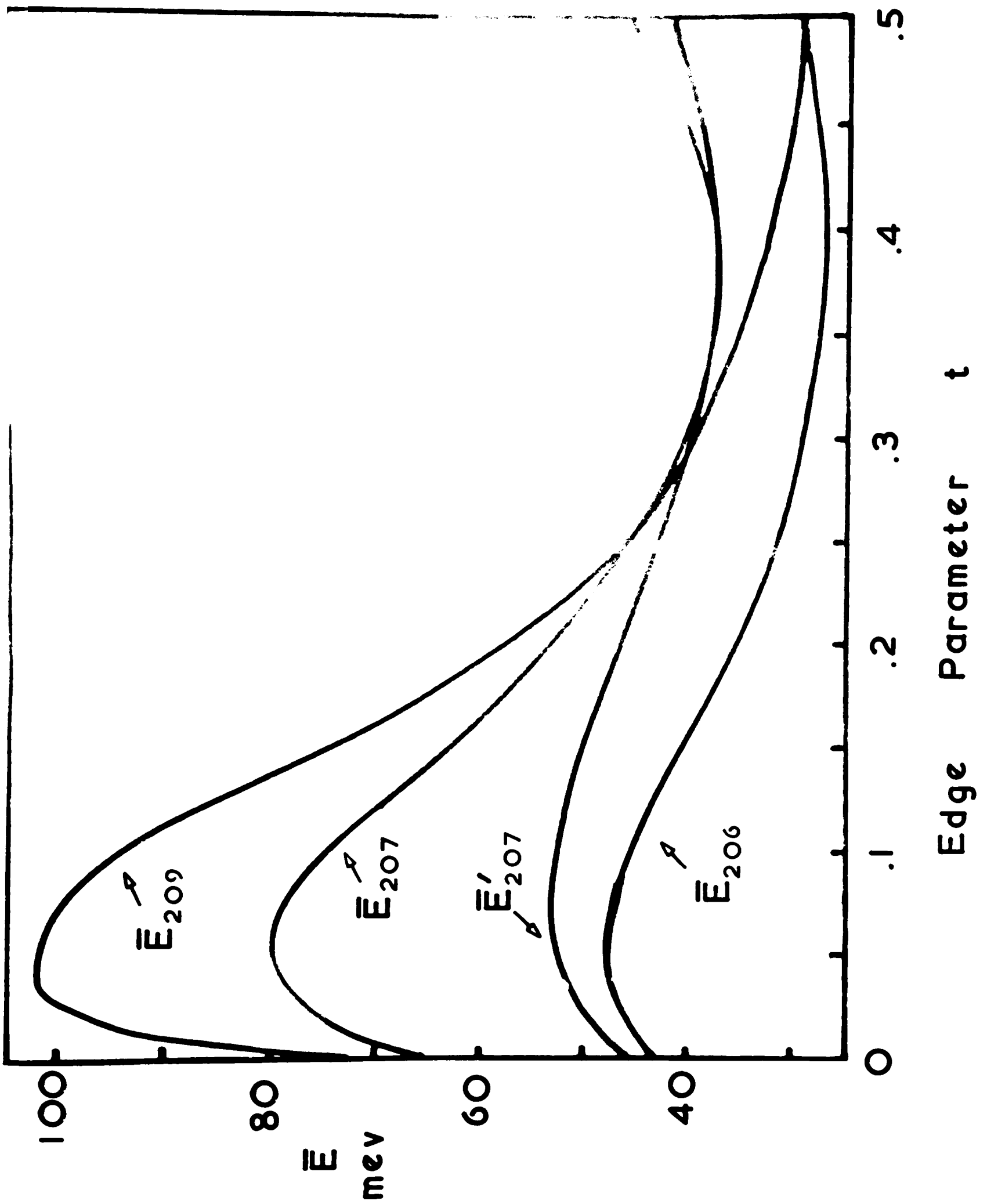

Figure 2: The mean excitation energies plotted as a function of the edge thickness parameter, t.

Stelson and McGowan (1955), is 0.158 barns. Alburger and Bryce (1954) assign configurations for the two neutron holes involved of $(3p_{1/2})^2$ for the 0+ state and $(3p_{1/2}, 2f_{5/2})$ for the 2+ state. In a recent calculation Miss Mary Kearsley (Private Communication) has taken into account the interaction between the two holes. She has calculated the interaction between a large number of the single hole states as observed in Pb^{207} and diagonalised the energy matrix in the usual way. She finds that the 0+ ground state is quite pure $(3p_{1/2})^2$, but that the wave function for the 2+ state can be written schematically as

$$0.80(3p_{1/2},2f_{5/2})-0.56(3p_{1/2},3p_{3/2})+0.03(2f_{5/2})^2+0.11(3p_{3/2},2f_{5/2})$$
$$-0.17(3p_{3/2})^2 \qquad (79)$$

Only those configurations differing in one particle from the ground state will contribute to the transition; thus in addition to the $(3p_{1/2},2f_{5/2})$, we must consider the $(3p_{1/2},3p_{3/2})$ state. This will give a large contribution to the reduced matrix element because of the large overlap with the p state in the ground state. Using the formalism of (75) and (74) one can evaluate the contribution from the two configurations, and one finds that they have opposite signs so that when these contributions are combined with the appropriate factors from (79) they do in fact add. The mean

excitation energy $\bar{E}_{206}$ needed to fit the transition with the wave function (79) is plotted in Figure 2 as a function of t.

The only measured electric quadrupole effect in Bi^{209} is the ground state quadrupole moment of -0.4 barns (Blin-Stoyle, 1956). The contribution of the odd proton in the state j to this moment is given by (cf. Blin-Stoyle, 1956)

$$- \frac{2j - 1}{2(j + 1)} < r^2 > \qquad (80)$$

where $< r^2 >$ is the mean value of r^2 in the odd particle orbit and is usually approximated by 3/5 the square of the nuclear radius. For Bi^{209} the odd particle is in a $1h_{9/2}$ state. For such a state, the radial function is strongly "pushed out" and hence the mean value of r^2 is not well approximated in this way. Calculating $< r^2 >$ with the radial functions (73) one gets for the single proton contribution to the moment, - 0.28 barns. Thus even taking into account the large value of $< r^2 >$ for the odd proton in Bi^{209} there is still a residual moment of - 0.12 barns that must be attributed to collective effects. Applying (78) to the case of Bi^{209} one gets in the usual way a relation between the mean excitation energy $\bar{E}_{209}$ needed to fit the collective contribution and t. This relation is plotted in Figure 2.

4.3 Discussion

In Figure 2 we see that there is surprisingly good agreement between $\bar{E}_{207}$, $\bar{E}'_{207}$, and $\bar{E}_{209}$. This agreement occurs for t = 0.3, a value also consistent with the results of the electron scattering experiments (Hofstadter, 1956). It is interesting to note that the agreement does not occur for values of the edge parameter, t, very different from 0.3. This is striking evidence for the necessity of taking a density distribution with a reasonably diffuse surface. For t = 0.3 the three mean excitation energies are about 40 Mev. $\bar{E}_{206}$ comes out some 25% smaller but we might expect this since, differing by two particles from a closed shell, Pb^{206} should have a "softer" core than those nuclei differing by only one. In addition there is a certain arbitraryness introduced by taking the particle mixtures (79), and more important there is the uncertainty arising from the neglect of the three-body term.

We note that the mean excitation energies come out somewhat larger than four times the spacing to the next shell, as was anticipated. One can take the energy of the maxima for the giant dipole photo-electric effect in nuclei as a rough measure of twice the splitting between shells. (Once more the factor of two comes in because of the velocity dependence of the potential.) In the region of lead, the maxima occur around 14 Mev, and Rand (1955) has

given a successful account of this and other features of the effect using a velocity dependent shell model. One expects results larger than twice this due to the neglect of the three-body terms. A further uncertainty is introduced by the fact that the energy scale in Figure 2 can be slid up and down somewhat corresponding to an uncertainty in the choice of interaction parameters.

The agreement between the mean excitation energies of Pb^{207} and Bi^{209} is perhaps more gratifying than significant. We have made a large number of simplifying assumptions, some even about the data, and it would seem that any relative result should carry an uncertainty of some 20%. But even with this the results indicate that the closure assumption is a good one, i.e. that the mean excitation energy is a property of the core, independent of the odd particle state. To give a complete justification for this assumption, apart from the empirical justification, would of course entail being able to do the configuration mixing sum exactly, or at least knowing a good deal about the contribution of each term in that sum. Since it is precisely the lack of this information that led us to the closure formulation, we cannot hope to give the results anything but a certain plausibility.

Horie and Arima (1955) have calculated the ground state quadrupole moment of Bi^{209} and they get for the collective con-

tribution, that is the part due to configuration mixing, - 0.14 barns, which is in quite good agreement with our closure result. They do not get a good answer for the total quadrupole moment however because the oscillator wave functions they use give much too large a mean value of r^2 in the ground state, and their single particle contribution is - 0.39 barns. The fact that their calculation for the collective contribution to the moment in Bi^{209} agrees so closely with ours perhaps sheds some light on the success of the closure assumption. We have seen that in the approximation of a harmonic oscillator potential the closure assumption is exact because all of the excitations have the same energy. If in a more realistic model of the lead closed shell the excitations responsible for the major contributions still cluster about some particular energy, with a spread small compared with the excitation energy, then we would expect the closure assumption to be a good one. In the light of the work of Horie and Arima, this might in fact seem to be the case.

On the other hand the closure assumption might be good for some reason. We saw in 2.2 that if the relative contribution of each excitation is independent of the odd particle state except for an all over scale, then the closure assumption is fully justified. The closure assumption will still be a good approximation if the relative contribution from groups of excitations is the

same, so long as we consider groups with an energy spread small compared with the mean excitation energy. This is likely to be the case if in the range of important contributions, there are a large number of excitations of different types in each small energy interval. If the number in each interval is large enough and diverse enough, then we can perform a sort of average over the contributions in each interval, and assume that the relative values of each average do not depend on the odd particle state. This is a kind of statistical approach to the problem, and it is likely to be fairly good in heavy nuclei like lead because the large number of particles in the nucleus will make for a large number of diverse possible excitations in each small energy interval.

It is probable that near the lead closed shell the two factors work together to justify the closure assumption. Firstly the energy width of the distribution of excitations giving the major contribution is probably fairly small compared with the mean excitation energy, and secondly the distribution of excitations in each small interval is probably relatively statistical, so that violent fluctuations in the contributions can be effectively averaged out in an interval large enough to be statistically valid and still small compared with the mean excitation energy.

4.4 Comparison with the Weak Surface Coupling Method

It is of interest to compare the formalism for weak collective effects using configuration mixing and closure with the quasi-hydrodynamical method of Bohr and Mottelson (1953). (See also Rainwater, 1950 and Feenberg and Hammack, 1951). They assume that the nucleus may be represented by a spherical core with small compressibility, in which case the collective degrees of freedom which have the lowest energy will be shape deformations with approximate preservation of volume. The normal coordinates of these oscillations will be the expansion parameters, α_μ , of the nuclear surface given by

$$R' = R(1 + \sum_\mu \alpha_\mu Y_{2\mu}) \qquad (81)$$

where R is the equilibrium radius, and where we have restricted ourselves to deformations of the quadrupole type. Bohr (1952) and Bohr and Mottelson (1953) have developed an elegant quantum field-theoretical formalism for treating these surface deformations. They quantize the surface oscillations, or phonons and find that α_μ is essentially the creation and annihilation operator for these phonons. The phonons energy $\hbar\omega$ is easily expressed in terms of the surface tension and mass transport parameters for the nuclear "fluid" of the core, and, as one would expect from the quadrupole nature of the deformation, the phonons have angular momentum 2 and

positive parity. The zero order shell model core state is then considered to be a state with no phonons present, and the effect of the interaction between the odd particle and the core is to mix in states with one phonon (in lowest order). In such a formalism the interaction with the core is most conveniently treated through the modal generating potential U. With a square density distribution and zero range forces, the self-consistent one body potential will also be square, and will have the same radius as the density distribution. The effect of deformations of the type (81) can be treated by expanding U(R') and only going to first power in α_μ. The interaction is U(R') - U(R) and is clearly given by

$$- \sum_\mu r \frac{\partial u}{\partial r} \alpha_\mu Y_{2\mu} \qquad (82)$$

In (82) only α_μ refers to core coordinates and as we saw this will essentially create one phonon. The remainder of the interaction refers to the coordinates of the odd particle. Since U(R) is a square well, the derivative appearing in (82) will give a delta function at the surface, and the admixture of one phonon state will depend on the amplitude of the odd particle state at the surface only. This arises because we have considered the core to be locally incompressible, and hence the odd particle can only affect the core at the surface in first order. The

operator for the quadrupole moment can also be written in terms of α_μ and one gets for the weak surface coupling contribution to the ground state quadrupole moment of a nucleus with one particle in a state J outside the closed shell core

$$Q_B = \frac{6\,a\,Z\,R^2}{7\sqrt{5\pi}\,\hbar\omega}\,\mathcal{Y}_{JJ}\,|R_J(R)|^2 \qquad (83)$$

where we have assumed that U comes from a zero range interaction taken over the core density, and hence a is the strength of the interaction as before, and where $R_J(R)$ is the radial function of the odd particle evaluated at the surface and $\mathcal{Y}_{JJ}$ is an angular matrix element of the type in (72). The expression for Q_B is normally not written as in (83) but rather in a form in which the explicit introduction of the odd particle radial function and the two body interaction is not made. The radial matrix element of (82) is usually treated as a parameter, k. The other dubious quantities in (83) can be grouped together into the surface tension energy, C, and the expression written

$$Q_B = \frac{3}{\sqrt{5\pi}}\,\mathcal{Y}_{JJ}\,\frac{k}{C}\,Z\,R^2 \qquad (84)$$

C is normally treated as a fitting parameter, and like $\bar{E}$ is expected to be a constant for a given core.

It is instructive to compare (83) with the corresponding expression in the configuration mixing formalism with closure. In order to make the comparison valid we must consider the case with t = 0 and take only the first term in the range expansion. We then get for the quadrupole moment of some odd neutron nucleus

$$ {}_J\langle |Q| \rangle_J = \frac{6 Z a}{\sqrt{5\pi}\, R^3 E}\, \gamma_{JJ} \int_0^R |R_J|^2 r^4 \, dr \qquad (85) $$

It is interesting to note that this is just the expression we would get if we assigned to the neutron an effective charge of magnitude $\frac{3Z\,a}{2\pi R^3 E}$, so long as the single particle functions vanish at the core radius. We might expect this effective charge result from the assumptions of the formalism, since we are considering a particle moving in a uniformly charged core and only locally affecting the core. In other words the effect of the perturbation is to add to the uniform charge density of the zero order core, a density just proportional to the odd particle density. The essential difference between this and the weak surface coupling formalism being that we no longer consider the core as incompressible and hence the odd particle can affect the core throughout rather than only at the surface. The surface part is still there as can be easily seen by doing a partial integration in (85). One gets in terms of (83)

$$\langle 1Q1 \rangle_J = \frac{7\hbar\omega}{5\bar{E}} Q_0$$

$$- \frac{6ZQ}{5\sqrt{5\pi}\, R^3 \bar{E}} \gamma_{JJ} \int_0^R r^5 \frac{d}{dr}(|R_J|^2)\, dr \qquad (86)$$

The second term in (86), the bulk term, is in fact larger than the first for the cases we have considered.

The expression for the quadrupole moment in (85) would seem to depend in a more natural way on the odd particle function than does (83). The result in (84) is even less sensitive to the odd particle state since k is normally taken as about 40 Mev for all nuclei and all single particle states, and it is hoped that C will be constant for a given core. The weak coupling formalism of (84) is easily generalized to E2 transitions as well as ground state moments, and has been applied by True (1956) to the transitions to the ground state in Pb^{206} and Pb^{207} as well as to the ground state quadrupole moment of Bi^{209}. He finds values of the surface tension parameter, C, of 1100 Mev for the transition in Pb^{207} but only 520 Mev for the transition in Pb^{206}. In Pb^{206} he uses the $(3p_{1/2}, 2f_{5/2})$ configuration only for the 2+ state. Using a wave function of the form (79), one can raise C to 715 Mev for Pb^{206}, but this is still too large a discrepancy to be explained on the surface coupling formalism. The better fit obtained with the configuration mixing and closure approach can be explained in that it allows one to take into account the

radial integrals and thus the large overlap that arises in Pb^{206} between the $2p_{1/2}$ and $3p_{3/2}$ states. Also since in the configuration mixing formalism one is dealing with a more familiar mechanism than surface coupling, the remaining discrepancies can be more easily accounted for.

Calculations on the 1.78 Mev transition in Pb^{207} indicate that very different parameters would be necessary to fit the transition on the surface coupling model from those used by True for the transition to the ground state. Once more this is largely due to radial integrals. The surface coupling approach since it attributes the collective effect to the surface, and makes all particle states equally good "stimulators" of these surface disturbances, has no way of taking into account the strong overlap that occurs between the $2f_{7/2}$ and $2f_{5/2}$ states.

For the ground state quadrupole moment of Bi^{209}, True finds a collective contribution of - 0.25 barns using C = 1100 Mev. He evaluates the single particle contribution using 3/5 the nuclear radius as an approximation to the mean value of r^2 and gets - 0.21 barns. We have seen that this approximation is not good in bismuth, and if one uses a more realistic estimate of the single particle contribution, one finds that True's results predict much too large a quadrupole moment. In this case an important contribution to the configuration mixing approach is the introduction of

anti-symmetry, which cannot be done conveniently in the weak coupling formalism. Further since the $1h_{9/2}$ state in bismuth is strongly "pushed out", the collective contribution will be very sensitive to the edge of the core density. We see in Figure 2 that we need a very large $\bar{E}$ to fit the quadrupole moment in Bi^{209} if t is small. This corresponds to a large charge density in the region of the odd particle, and hence a large quadrupole moment. As t is increased, the charge density in the region of the odd particle goes down, and so does the $\bar{E}$ needed to fit the experiment. Similarly the rise in $\bar{E}_{207}$ and $\bar{E}'_{207}$ for large t can be attributed to a node in the radial functions.

APPENDIX I

CENTRE OF MASS RECOIL AND MOMENTS IN O^{17}

We have seen that since the shell model eigen-states are generated by an external fixed potential they contain three extra internal degrees of freedom that are not internal degrees of freedom of the actual nuclear system. Thus in the shell model, the internal wave function contains a part that refers to the centre of mass. Such internal wave functions may still be used to calculate multipole moments as long as one is careful to exclude the part of the state corresponding to motion of the mass centre, that is as long as one calculates with operators relative to the centre of mass and not relative to a space-fixed axis. It has been pointed out by Elliott and Skyrme (1955, 1956) that if the internal shell model wave function is a proper one, then the three ostensibly extra degrees of freedom will in fact be internally redundant, and the part of the shell model wave function

referring to motion of the centre of mass will be an S-state. In such a case it makes no difference whether multipole moment operators are referred to the centre of mass or a space fixed axis.*

It is easy to see why shell model states with the centre of mass in an S-state, give no recoil contribution to nuclear moments. Let us look for example at the nuclear magnetic dipole operator. Any recoil contribution to it will clearly come from the orbital angular momentum part. Referred to the centre of mass the orbital angular momentum of the particle i is given by

$$\underline{l}'_i = \underline{r}'_i \times \underline{p}'_i \qquad (A1)$$

where the primes refer to the coordinate system fixed in the centre of mass. The relation between the primed coordinates and the un-primed space fixed coordinates is

$$\underline{r}'_i = \underline{r}_i - \frac{1}{A}\sum_j \underline{r}_j \qquad (A2)$$

$$= \underline{r}_i - \underline{R}$$

and similarly for the momentum $\underline{p}'_i = \underline{p}_i - \underline{P}$.

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* Some precautions are necessary in the case of sum rules since then one generally sums over all states, spurious and proper, and one must refer the operator to the centre of mass so that only the proper states will be picked out or restrict the sum only to proper states (Lane, 1956).

The operator for the orbital magnetic moment referred to the centre of mass is given by

$$\underline{\mu} = \sum_i \frac{1}{2}(1 - \tau_i)\,\underline{l}'_i \qquad (A3)$$

where τ_i is the third component of the isotopic spin operator and the isotopic factor $\frac{1}{2}(1 - \tau_i)$ is 1 for protons and 0 for neutrons. Putting in (A1) and (A2) one gets for (A3)

$$\underline{\mu} = \sum_i \frac{1}{2}(1 - \tau_i)(\underline{r}_i \times \underline{p}_i - \underline{R} \times \underline{p}_i - \underline{r}_i \times \underline{P}) + Z(\underline{R} \times \underline{P}) \qquad (A4)$$

The last term is just the angular momentum operator for the centre of mass, and gives zero since the centre of mass is in an S-state. Similarly the terms in $\underline{R}$ and $\underline{P}$ will vanish since these are vectors in the space of the centre of mass, and it is well known that the matrix element of a vector between S-states must vanish. This leaves only the term $\underline{r}_i \times \underline{p}_i$ which is the magnetic moment operator referred to the external fixed axis.

Similarly it can be shown that if the shell model state is a proper state of the internal motion, and hence the centre of mass is in a S-state, it makes no difference whether we refer the operator for the electric quadrupole moment to the centre of mass or the space fixed origin. Since we are interested in O^{17}, it is of interest to investigate the case of one neutron outside a doubly closed shell in some detail for the quadrupole moment case. Elliott

and Skyrme (1955) show that harmonic oscillator shell model states in this case are proper states of the internal motion, and hence we expect the recoil contribution to vanish, but looking at O^{17} in detail will allow us to investigate departures from the harmonic oscillator.

Referred to the centre of mass, the operator for the ground state quadrupole moment can be written

$$Q = \sum_{i\lambda} C^{2\,1\,1}_{0\,\lambda-\lambda}\, r_{i\lambda}' r_{i-\lambda}' \quad \tfrac{1}{2}(1-\tau_i) \tag{45}$$

where $$r_\lambda = \sqrt{\frac{4\pi}{3}}\, |r|\, Y_{1\lambda}$$

Putting in (A2) one finds that the operator, referred to the space fixed axis, can be split up into three parts.

$$\begin{aligned} Q &= Q(0) + Q(1) + Q(2) \\ &= \sum_{i\lambda} C^{2\,1\,1}_{0\,\lambda-\lambda}\ \tfrac{1}{2}(1-\tau_i)\, r_{i\lambda}\, r_{i-\lambda} \\ &+ \tfrac{1}{A^2} \sum_{i\lambda} \left(2 - A(1-\tau_i)\right) C^{2\,1\,1}_{0\,\lambda-\lambda}\, r_{i\lambda}\, r_{i-\lambda} \qquad (A6) \\ &+ \tfrac{1}{A^2} \sum_{i\neq j\,\lambda} \left(2 - A\left(1 - \tfrac{1}{2}\tau_i - \tfrac{1}{2}\tau_j\right)\right) r_{i\lambda}\, r_{j-\lambda}\, C^{2\,1\,1}_{0\,\lambda-\lambda} \end{aligned}$$

The first term is the ordinary shell model operator for the quadrupole moment. For an odd neutron nucleus like O^{17} this vanishes. The second term is the "classical recoil" (cf. Lipkin, de Shalit,

and Talmi, 1955) operators. For an odd neutron nucleus the index i can only refer to the odd particle by symmetry, and in that case the isotopic spin factor vanishes. Thus the expectation value of Q(1) is Z/A^2 times the single particle quadrupole moment for the odd particle state, i.e. an expression of the form (80). The third term would vanish if it were not for anti-symmetry. Matrix elements diagonal in single particle states of an operator of the form $r_i r_j$ with $i \neq j$ vanish by parity, but this is not true of the exchange matrix elements arising from anti-symmetry in the case that i and j refer to identical nucleons. By symmetry either i or j must refer to the odd neutron and thus the isotopic spin factors will vanish. Treating the core neutrons as a determinant of single particle states, one can expand the matrix elements of Q(2) into a sum over core states (Condon and Shortley, 1935, p.169 et seq.). Keeping only the exchange term one gets

$$\langle Q(2) \rangle = - \frac{2Z}{A^2} \sum_{\alpha} \langle \alpha J | \sum_{\lambda} C^{2}_{0\,\lambda-\lambda} T^{11}_{1\lambda} T_{2-\lambda} | J\alpha \rangle \qquad (A7)$$

where α refers to the core states and J to the odd particle state.

The angular parts of the matrix elements in (A7) can be evaluated in the usual manner. It is most convenient to express

the results in terms of matrix elements of Q(1) since we are interested in the extent that Q(2) cancels the contribution from Q(1). If the radial parts of the single particle states are completely specified by the principal oscillator quantum number, N, and the orbital angular momentum, ℓ, as is the case for harmonic oscillator states, then we can write

$$\frac{\langle Q(2)\rangle}{\langle Q(1)\rangle} = -\sum_{N'} \frac{\left((2\ell+3)\left|\langle N\ell\,|r|\,N'\ell-1\rangle\right|^2 + (2\ell-1)\left|\langle N\ell\,|r|\,N'\ell+1\rangle\right|^2\right)}{(2\ell+1)\langle N\ell\,|r^2|\,N\ell\rangle} \quad (A8)$$

where N is the principal quantum number and ℓ the orbital angular momentum of the odd particle, and N' the principal quantum number of the core states. The matrix elements in (A8) are radial integrals. It is easily verified that for harmonic oscillator radial functions, the radial integrals are such (Shaffer, 1944) that the ratio in (A8) is minus one, as we expect for no recoil contribution.

We can estimate the effect of departures from the harmonic oscillator by calculating the radial integrals in the numerator of (A8) with radial functions other than those of the harmonic oscillator. In O^{17} the odd particle is in a 1d state, and since there is no f state in the core, the second radial matrix element in the numerator of (A8) will not contribute. The only matrix element we need consider in the O^{17} case is

$$\langle 1d\,|r|\,1p\rangle \quad (A9)$$

For harmonic oscillator functions this is 1.58b (Shaffer, 1944), where b is as defined in Chapter 3. For a drastic departure from the harmonic oscillator case we can calculate (A9) with radial functions for an infinite square well (73). The radial integrals in this case must be evaluated graphically, and one gets for (A9) 0.66R, where R is the radius of the square well generating the functions.

In order to estimate the effect of introducing the square well functions, we must be able to relate R and b. A possible way of doing this is through the energy eigen-values. Both R (Feenberg, 1955, p.15) and b may be related to the eigen-value of the odd particle and by equating these one finds that for the 1d state, R = 2.2b. This gives for (A9) calculated with infinite square well functions, 1.45 b. Taking the square of this and comparing it with the square of the result for the harmonic oscillator case, one finds that the ratio in (A8) is reduced by about 10% so there will be a recoil contribution of 0.1 times the "classical recoil". R can also be related to b by making a rough equation of the density distribution for the particle states in the two cases. Brink (Private Communication) finds that the two potential wells may be made approximately equivalent for a given principal quantum number by using a relation $R = b\sqrt{2N + 3}$. Taking an average of this for the 1d and 1p one gets R = 2.5 b.

Putting this in as before one finds that the ratio in (A8) is now increased by about 10%, and thus the recoil value will be -0.1 times the "classical recoil."

This calculation to estimate the effect of departures from the harmonic oscillator is only a rough approximation. A proper calculation with eigen-states in an infinite square well would require that we first pick out the proper states of internal motion using the complicated procedure outlined by Elliott and Skyrme (1955), and then calculate the quadrupole moment using the proper operator. But it is likely that the general trend of such a calculation is indicated by the rough calculation that we have already carried out. In particular we note that even though eigen-states in an infinite square well are very different from harmonic oscillator eigen-states, the recoil contribution is still very small, and further that the sign of the contribution is uncertain.

APPENDIX 2

HARMONIC OSCILLATOR RADIAL INTEGRALS WITH A GAUSSIAN INTERACTION

A procedure for evaluating the radial integrals arising from the expansion of the Gaussian or Yukawa interaction in spherical harmonics and the results for a few cases are given by Swiatecki (1951). Since we wish to generalise this procedure, and since there are a few misprints in the general formula given for f_k by Swiatecki, we will go through the calculation from the beginning.

If we expand the radial dependence of the interaction as in (23), then

$$f_k(r_1, r_2) = \frac{\int f(r_{12}) P_k(\cos\theta_{12}) \, d\Omega}{(2k+1) \int P_k^2(\cos\theta_{12}) \, d\Omega}$$

$$= \frac{1}{2} \int_0^\pi f(r_{12}) P_k(\cos\theta) \sin\theta \, d\theta \qquad \text{(A10)}$$

Putting in a Gaussian dependence for $f(r_{12})$ as in (31), and noticing that $r_{12}^2 = r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta$, the integral in (A10) can be written

$$f_k = \frac{1}{2} e^{-\frac{1}{a^2}(r_1^2 + r_2^2)} \int_{-1}^{1} e^{xz} P_k(z)\, dz \qquad \text{(A11)}$$

where we have put $z = \cos\theta$ and $x = \dfrac{2r_1 r_2}{a^2}$. (A11) can be evaluated for any value of k by making use of the well known relation for the Legendre polynomials, (cf. Churchill, 1941)

$$P_k(z) = \sum_{r=0}^{\pm k \text{ or } \pm(k-1)} \frac{(-1)^r (2k-2r)!}{2^k r!\,(k-r)!\,(k-2r)!}\, z^{k-2r} \qquad \text{(A12)}$$

Using (A12) the integral over z can be done in a straight-forward manner, and one gets for the general f_k

$$f_k = \frac{1}{2} e^{\frac{-r_1^2 + r_2^2}{a^2}} \sum_{r=0}^{\pm k \text{ or } \pm(k-1)} \sum_{s=0}^{k-2r} \frac{(2k-2r)!\ (-1)^s}{2^k r!\,(k-r)!\,(k-2r-s)!} \cdot \left(\frac{(-1)^s e^{x} - (-1)^k e^{-x}}{x^{s+1}} \right) \qquad \text{(A13)}$$

which expression differs in phase factors and by a factor of 1/2 from the result quoted by Swiatecki (1951). The particular values of f_k given by Swiatecki in fact agree with (A13).

Evaluation of radial matrix elements with harmonic oscillator wave functions of the general form (15) always reduces to evaluation of radial integrals of the form

$$ {}_k I_{m\,n} = \int_0^\infty \int_0^\infty f_k\, r_1^m\, r_2^n\, e^{-\frac{r_1^2+r_2^2}{b^2}}\, dr_1\, dr_2 \qquad \text{(A14)} $$

where from parity considerations one always finds that if k is even, m and n are even, and if k is odd, m and n are odd. In view of this, the general integrals (A14) can be generated from the integrals with m = n by repeated use of the relation

$$ \frac{\partial}{\partial\left(\frac{1}{b^2}\right)}\, {}_k I_{m\,n} = -\left({}_k I_{m+2,\,n} + {}_k I_{m\,n+2} \right) \qquad \text{(A15)} $$

Thus we need only use (A13) to evaluate (A14) for the case m = n.

Putting (A13) and (A14) with m = n and changing variables to u and v

$$ u = \frac{r_1 + r_2}{a} \qquad v = \frac{r_1 - r_2}{a} \qquad x = \frac{u^2 - v^2}{2} $$

$$ dr_1\, dr_2 \longrightarrow \frac{a^2}{2}\, dv\, du $$

we get, with $\alpha = \left(\frac{a}{b}\right)^2$

$$ {}_k I_{m\,m} = \frac{a^{2m+2}}{2^{2m+k+1}} \sum_{r=0}^{\frac{1}{2}k \text{ or } \frac{1}{2}(k-1)} \sum_{s=0}^{k-2r} \frac{(2k-2r)!\,(-1)^r\, 2^s}{r!\,(k-r)!\,(k-2r-s)!}\, \alpha^{\,} $$

$$ \int_{r=0}^{\infty} \int_{\xi=0}^{\infty} e^{-\frac{u^2+v^2}{2}(1+\alpha)}\, (u^2 - v^2)^{m-s-1} \left[(-1)^s e^{x} - (-1)^k e^{-x} \right] du\, dv $$

(A16)

Since $(-1)^m = (-1)^k$, the integrand in (A16) is symmetric under interchange of u and v or u and -v as well as being even in u and v; therefore we can take the integral over any quadrant in the u-v plane and hence we can change the limits from r_1, r_2 from 0 to ∞, to u, v from 0 to ∞. (A16) can then be written

$$*I_{mm} = \frac{a^{2m+2}}{2^{2m+k}} \sum_{\tau=0}^{\frac{1}{2}k \text{ or } \frac{1}{2}(k-1)} \sum_{s=0}^{k-2\tau} \frac{(2k-2\tau)!\,(-1)^{\tau+s}\,2^s}{\tau!\,(k-\tau)!\,(k-2\tau-s)!} *$$

$$\int_0^\infty \int_0^\infty (u^2-v^2)^{m-s-1} e^{-\frac{u^2+v^2}{2}(1+\alpha) + \frac{u^2-v^2}{2}} du\,dv \quad \text{(A17)}$$

Assuming that m-s-1 is always positive, and this is the case in the integrals we are interested in, we can expand $(u^2 - v^2)^{m-s-1}$ in an ordinary binomial series, and then the integrals over u and v may be done making use of standard formula

$$\int_0^\infty x^{2n} e^{-ax^2} dx = \frac{(2n-1)!!}{2^{n+1} a^n} \sqrt{\frac{\pi}{a}} \quad \text{(A18)}$$

where we define $(-1)!! = 1$. Putting this in one finally gets for $_kI_{mm}$

$$_k\overline{I}_{mm} = \frac{\pi a^{2m+2}}{2^{2m+k+1}\sqrt{\alpha(\alpha+2)}} \sum_{\tau=0}^{\frac{1}{2}k \text{ or } \frac{1}{2}(k-1)} \sum_{s=0}^{k-2\tau} \sum_{p=0}^{m-s-1} *$$

$$\left\{ \frac{(2k-2\tau)!\,(m-s-1)!\,(2m-2s-2p-3)!!\,(2p-1)!!\,(-1)^{p+\tau+s}\,2^s}{p!\,(m-s-p-1)!\,\alpha^{m-s-p-1}\,(\alpha+2)^p\,\tau!\,(k-\tau)!\,(k-2\tau-s)!} \right\}$$

(A19)

This expression combined with (A15) can be used to evaluate all the radial integrals that arise in the O^{17} calculation with ordinary harmonic oscillator functions and a Gaussian interaction. Swiatecki has evaluated, by direct integration, ${}_kI_{m\,m}$ for $k = 0$, $m = 2$, for $k = 0,2$, $m = 4$, and for $k = 0,2,4$, $m = 6$. In addition the following integrals are needed for O^{17}

$$ {}_0I_{62} = \frac{15\, b^{10}\, \pi\, \alpha^{3/2}}{2^6 (\alpha+2)^{7/2}} (\alpha^2 + 2\alpha + 1) \qquad (A20) $$

$$ {}_0I_{64} = \frac{15\, b^{12}\, \pi\, \alpha^{3/2}}{2^7 (\alpha+2)^{9/2}} (3\alpha^3 + 9\alpha^2 + 13\alpha + 7) $$

$$ {}_1I_{33} = \frac{3\, b^{9}\, \pi\, \alpha^{3/2}}{2^5 (\alpha+2)^{5/2}} $$

$$ {}_1I_{53} = \frac{15\, b^{10}\, \pi\, \alpha^{3/2}}{2^6 (\alpha+2)^{7/2}} (\alpha+1) $$

$$ {}_1I_{55} = \frac{15\, b^{12}\, \pi\, \alpha^{3/2}}{2^7 (\alpha+2)^{9/2}} (5\alpha^2 + 10\alpha + 7) $$

$$ {}_1I_{57} = \frac{15\, b^{14}\, \pi\, \alpha^{3/2}}{2^8 (\alpha+2)^{11/2}} (35\alpha^3 + 105\alpha^2 + 133\alpha + 63) $$

$$_1I_{73} = \frac{105\, b^{12}\pi\alpha^{3/2}}{2^7(\alpha+2)^{9/2}}(\alpha^2+2\alpha+1)$$

$$_2I_{64} = \frac{105\, b^{12}\pi\alpha^{3/2}}{2^7(\alpha+2)^{9/2}}(\alpha+1)$$

$$_3I_{55} = \frac{105\, b^{12}\pi\alpha^{3/2}}{2^7(\alpha+2)^{9/2}}$$

$$_3I_{57} = \frac{945\, b^{14}\pi\alpha^{3/2}}{2^8(\alpha+2)^{1/2}}(\alpha+1)$$

For the calculation with "pushed out" wave functions of the first kind for the odd particle, i.e. those in which we increase by one the power of r in radial function, we also need the following integrals

$$_2I_{48} = \frac{945\,\pi\alpha^{3/2}\, b^{14}}{2^8(\alpha+2)^{1/2}}(\alpha^2+2\alpha+1) \qquad \text{(A21)}$$

$$_2I_{68} = \frac{945\, b^{16}\pi\alpha^{3/2}}{2^9(\alpha+2)^{13/2}}(7\alpha^3+21\alpha^2+25\alpha+11)$$

APPENDIX 3

A RADIAL INTEGRAL FOR THE YUKAWA INTERACTION

To calculate the direct part of the closure expression in O^{17} with a Yukawa form for $f(r_{12})$

$$f(r_{12}) = \frac{e^{-r_{12}/a}}{r_{12}/a} \tag{A22}$$

we need the radial integrals $_2I'_{4\,4}$, $_2I'_{6\,6}$, and $_2I'_{4\,6}$. The first two of these, as well as the expression for f_2 are given by Swiatecki (1951). The third can be calculated by use of (A15) and the results of Swiatecki. This gives

$$_2I'_{6\,4} = \frac{b^{12}}{2^9\alpha^2}\sqrt{\frac{\pi}{2\alpha}}\left(1+13\alpha-11\alpha^2+27\alpha^3 - Z(1+19\alpha)\right) \tag{A23}$$

where

$$Z = e^{\frac{1}{2\alpha}}\sqrt{\frac{\pi}{2\alpha}}\left(1-\mathrm{erf}\frac{1}{\sqrt{2\alpha}}\right)$$

APPENDIX A

RADIAL INTEGRALS WITH A GAUSSIAN INTERACTION AND HARMONIC OSCILLATOR FUNCTIONS FROM DIFFERENT POTENTIALS

In the case in which the odd particle state is "pushed out" by taking it as an eigen-state in a wider potential than the potential used to generate the core states, the general radial integral becomes

$$ {}_{k}\mathrm{II}_{m\,n} = \int_0^\infty \int_0^\infty f_k \, r_1^{\,m} r_2^{\,n} \, e^{-r_1^2/b^2} \, e^{-r_2^2/c^2} \, dr_1 dr_2 \qquad (A24) $$

rather than (A14). Once again given one such integral others can be generated by differentiation, but now we can differentiate separately either with respect to $1/c^2$ or $1/b^2$ and hence vary n and m independently. In particular this means that we can generate ${}_{k}\mathrm{II}_{m+2\;m+2}$ from ${}_{k}\mathrm{II}_{m\;m}$, which cannot be done for ${}_{k}\mathrm{I}_{m\;m}$.

hence we need only calculate (A24) for one particular value of m and n for a given k. Since we are interested only in the direct contribution to the collective effects in O^{17}, we need only evaluate the case $k = 2$.

We choose to evaluate (A24) for $k = 2$, $m = n = 4$. f_2 may be taken from Swiatecki (1951) or from (A13). Putting it in (A24) one gets

$$ {}_2\Pi_{44} = \frac{a^6}{2^4} \int_0^\infty\int_0^\infty e^{-\beta^2 T_1^2 - \gamma^2 T_2^2} T_1 T_2 \times $$

$$ \left[e^{x}(x^2 - 3x + 3) - e^{-x}(x^2 + 3x + 3)\right] dT_1 dT_2 \quad (A25) $$

where

$$ x = \frac{2 T_1 T_2}{a^2} \qquad \beta^2 = \left(\frac{1}{a^2} + \frac{1}{b^2}\right) \qquad \gamma^2 = \left(\frac{1}{a^2} + \frac{1}{c^2}\right) $$

We can make a change of variable to u and v

$$ T_1 = \frac{1}{r_2}\,\frac{u - v}{\beta} \qquad T_2 = \frac{1}{r_2}\,\frac{u + v}{\gamma} \qquad dT_1\, dT_2 \to \frac{du\, dv}{\beta\gamma} $$

and once again since the integrand is symmetric in u and v as well as even in u and v, we can change limits to u and v from 0 to ∞. This gives

$$ {}_2\Pi_{44} = \frac{a^6}{2^4 \beta^3 \gamma^2} \int_0^\infty \int_0^\infty e^{-(u^2 + v^2) + \mu(u^2 - v^2)} $$

$$ \left[\mu^2 (u^2 - v^2)^3 - 3\mu (u^2 - v^2)^2 + 3(u^2 - v^2)\right] du\, dv \quad (A26) $$

where we have called $\mu = \frac{1}{\beta\gamma a^2}$. The integral in (A26) can now be evaluated in a straight-forward manner giving finally

$$ {}_2\Pi_{44} = \frac{15\, a^6 \pi \mu^5}{2^6 \beta^2 \gamma^2 (1-\mu^2)^{\frac{7}{2}}} \qquad \text{(A27)} $$

If we put $\alpha_1 = \frac{a^2}{b^2}$ and $\alpha_2 = \frac{a^2}{c^2}$ this can be re-written

$$ {}_2\Pi_{44} = \frac{15\, a^{10} \pi}{2^6 \left[\alpha_1 + \alpha_2 + \alpha_1\alpha_2\right]^{\frac{7}{2}}} \qquad \text{(A28)} $$

One can easily verify that this reduces to ${}_2I_{4\,4}$ for $\alpha_1 = \alpha_2$.

The other integrals that we need can be obtained from (A28) by differentiation, and we find

$$ {}_2\Pi_{64} = \frac{105\, a^{12} \pi\, (\alpha_2 + 1)}{2^7 \left(\alpha_1 + \alpha_2 + \alpha_1\alpha_2\right)^{\frac{9}{2}}} $$

$$ {}_2\Pi_{66} = \frac{105\, a^{14} \pi}{2^8 \left(\alpha_1 + \alpha_2 + \alpha_1\alpha_2\right)^{\frac{11}{2}}} \left(7\alpha_1\alpha_2 + 7\alpha_1 + 7\alpha_2 + 9\right) \qquad \text{(A29)} $$

APPENDIX 5

THREE-BODY TERMS IN THE LEAD CLOSED SHELL

We saw in 2.3 that the expansion of the wave functions in the closure matrix elements into sums over single particle states gives rise to three-body as well as two-body terms, and that there is a non-vanishing contribution from these three-body terms essentially due to anti-symmetry. The function of this three-body term in (9) is easily understood if we use the fact that the proton states ϕ_i form a complete set to expand the two-body term. We can then write for (9)

$$\sum_{ij} \langle \phi_i | Q | \phi_j \rangle \langle \nu_J, \phi_j | V | \nu_J \phi_i \rangle - \sum_{ij} \langle \phi_i | Q | \phi_j \rangle \langle \nu_J, \phi_j | V | \nu_J \phi_i \rangle \quad (A30)$$

where the sum over j in the first term goes over all states, and not just those of the core as does the sum over j in the second term and both sums over i. Introducing the complete set ϕ_j in

in the first terms has effectively "undone" the closure, and the first term in (A30) is just the sum over all single particle excitations. The second term, coming from the original three-body term, subtracts from the first all those excitations in which the intermediate state, j, is in the core. This is simply the operation on the Pauli principle.

Unfortunately exact calculation of the three-body term is extremely difficult in the region of lead, particularly if we wish to use a density distribution instead of a sum over single particle states for the core. Some formal progress may be made by defining a two particle correlation density, $\rho(12)$, as

$$\rho(12) = \sum_{ij} \left[|\phi_i(1)|^2 |\phi_j(2)|^2 - \phi_i^*(1)\phi_j(1)\phi_j^*(2)\phi_i(2) \right] \qquad (A31)$$

This correlation function is the probability density for finding two particles a distance r_{12} apart, and hence the double integral and sum over spin states of $\rho(12)$ must be normalised to $Z(Z-1)$. It is clear from (A31) that we can write (Lane, Thomas, Wigner, 1955)

$$\rho(12) = Z^2 \rho(1)\rho(2) - Z\rho(1)J(12) \qquad (A32)$$

where $\rho(r)$ is the usual one particle density distribution normalised to unity, and where J represents the correlations introduced by the anti-symmetric form of (A31). The double integral over ρJ is unity, thus preserving the normalisation of $\rho(12)$.

We can express the sum over core states in the three-body parts of (8) in terms of $\rho(12)$, in which case we notice that the first term in (A32) gives no contribution since

$$\int \rho\, Q\, d\tau = 0$$

just as the first three-body term in (8) vanishes. We can then write for the three-body term in (9)

$$-\tfrac{1}{2}\iiint \rho(1)\, J(12)\, \chi^{*}_{j'}(3)\, \chi_{j}(3)\, V(13)\, Q(2)\, d\tau_1\, d\tau_2\, d\tau_3 \qquad (A33)$$

An explicit form for J is given for free electrons by Wigner and Seitz (1933). They find that J is unity for $r_{12}=0$ and falls off to zero within a range of the order of the average particle spacing. Since in a lead nucleus this spacing is small compared with the nuclear radius, we might try approximating J with a delta function in (A33). If we do this we get a disastrous result, for (A33) is then simply the two-body term, but with opposite sign, and the collective contribution to the quadrupole effects becomes zero. This can be understood in terms of

the form for J in the case of free fermions, i.e. plane waves. The range of J is related to the maximum momentum of the free fermions, (cf. footnote 17, Lane, Thomas and Wigner, 1955) and the limit in which the range of J tends to zero corresponds to the limit in which the maximum momentum tends to infinity. Such a limit means simply that all possible states are filled, and thus by the Pauli principle we expect no contribution.

Other methods of calculation with J in (A33) are extremely difficult, particularly since we would wish to compare any calculation of the three-body terms with the results obtained for the two-body terms using a one particle nuclear density distribution. We can gain some information about the three-body terms from the calculation in O^{17}, where for both the ground state moment and the E2, the three-body terms are slightly less than 20% of the two-body terms. The contribution from the three-body terms in lead should probably be somewhat smaller than this, since for eigen-states in an infinite square well the selection rules will allow many more excitations to states outside the closed shell to contribute to the collective effects than are allowed by the stringent selection rules in the harmonic oscillator case.

We can get further information about the terms by actually writing (9) for zero range forces with a determinant of single particle states of the form (14) for the core, odd particle states of the type (16), and using the definition (17) for Q. After

evaluating the angular matrix elements in the core, we get for (9)

$$\frac{a}{2\pi}\langle \psi_{J'\ell'M'} | Y_{2M_Q} | \psi_{J\ell M}\rangle \sum_{n_i\ell_i} (2\ell_i+1)\times$$

$$\Big\{\langle R^{(i)}_{n_i\ell_i} R^{(j)}_{n'\ell'} | r_i^{-2} | R^{(i)}_{n_i\ell_i} R^{(j)}_{n\ell}\rangle \qquad (A34)$$

$$- \sum_{n_j\ell_j} \begin{pmatrix} \ell_j & 2 & \ell_i \\ 0 & 0 & 0 \end{pmatrix}^2 \langle R^{(i)}_{n_i\ell_i} R^{(j)}_{n'\ell'} | R^{(j)}_{n_j\ell_j} R^{(j)}_{n\ell}\rangle \langle R_{n_j\ell_j} | r^{-2} | R_{n_i\ell_i}\rangle\Big\}$$

It is clear that if the sum over j is extended over all n_j and ℓ_j rather than only those in the core, then (A34) will vanish, as we would expect. The factor $(2\ell_i+1)$ is a population factor giving preference to the core states of high angular momentum. For a given ℓ_i the Wigner coefficient will only couple in those states with $\ell_j = \ell_i, \ell_i \pm 2$. For large ℓ_i there will be no $\ell_j = \ell_i+2$ in the core. Those states with $\ell_j = \ell_i-2$ will have rather small radial matrix elements for large ℓ_i since the states of low angular momentum will either have many nodes, or will be rather strongly concentrated about small r and in either case the overlap with the core states of large ℓ_i, which have a single node and are peaked out toward the nuclear radius, will be rather small. Thus the largest contribution can be expected to come from the terms with $n_j\ell_j = n_i\ell_i$. The contribution from these terms will be reduced by a factor of about 1/4 from the

Wigner coefficient. It seems fair to assume, then, that at worst the three-body term should not exceed 50% of the two-body term, and the results for O^{17} make 25% a very reasonable claim as an upper limit.

On the other hand something can be said about the three-body terms with much greater certainty than simply a rough factor of 50%. Firstly it is clear from symmetry considerations as well as from (A34) that the three-body term must depend in the same way on the angular properties of the odd particle states as does the two-body term. But this will be true of any theory that has the zero order shell model state as a starting point. More particular to the configuration mixing approach with closure is the fact that the three-body term has roughly the same dependence on the odd particle radial function as the two-body term. Both terms depend on the product of the odd particle radial functions and some sort of overlap of this product with the radial functions of the core states. The similarity in the radial dependence of the two- and three-body terms is particularly strong for those states with $n_j l_j = n_i l_i$, and we expect the largest contribution from these. Thus although the three-body term could conceivably alter the already dubious zero of the energy scale in Fig. 2 by as much as 50%, it would have a very much smaller effect on the relative positions of the curve. In as much as the closure

assumption is that the mean excitation energies are independent of the odd particle state, then, it seems safe to say that the three-body terms would not affect by more than 15% or at most 20% the extent to which Fig. 2 corroborates this assumption.

The argument thus far has been given for the three-body terms in the odd neutron case, but it is clear that the same will hold for the odd proton case (13), *mutatis mutandis*.

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