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**RELATIONSHIP BETWEEN THE SPHERICAL SHELL MODEL
AND THE DEFORMED HARTREE-FOCK MODEL FOR NUCLEI**

by

M. HARVEY

Paper presented at
the Congress of the Canadian Association of Physicists,
Montreal, June 18-21, 1973.

Chalk River Nuclear Laboratories
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RELATIONSHIP BETWEEN THE SPHERICAL SHELL MODEL
AND THE DEFORMED HARTREE-FOCK MODEL FOR NUCLEI*

M. HARVEY

Abstract

A definition of the spherical shell model Hamiltonian is given for nuclei in which the Hartree-Fock field is deformed; this definition is consistent with the usual phenomenological parametrization. Calculated single particle energies in an individual particle model and in a shell model with residual interaction are presented. A new approach to describing deformation effects in the spherical shell model is presented in terms of the deformation of the Hartree-Fock field. A comparison is shown between the results of projected unrestricted Hartree-Fock calculations and the new deformation-renormalized spherical shell model. A "shape-dependent" effective interaction for the spherical shell model is suggested.

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* *This was an invited paper at the Congress of the Canadian Association of Physicists, Montreal, June 18-21, 1973*

Relation entre le modèle à couche sphérique et
le modèle Hartree-Fock déformé, pour les noyaux*

M. Harvey

*Communication sollicitée pour le Congrès de l'Association canadienne des physiciens ayant eu lieu à Montréal du 18 au 21 juin 1973.

Résumé

On donne une définition du modèle Hamiltonien à couche sphérique pour les noyaux où le champ Hartree-Fock est déformé; cette définition est en accord avec la paramétrisation phénoménologique habituelle. On présente les énergies calculées des particules simples dans un modèle pour particule individuelle et dans un modèle à couche avec interaction résiduelle. On présente une nouvelle façon d'aborder la description des effets de la déformation dans le modèle à couche sphérique, laquelle est en fonction de la déformation du champ Hartree-Fock. On compare les résultats de calculs Hartree-Fock non restreints et projetés et le nouveau modèle à couche sphérique à déformation renormalisée. On suggère une interaction efficace "dépendant de la forme" pour le modèle à couche sphérique.

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The spherical shell model for nuclei was proposed over twenty years ago, yet, despite its longevity, the foundations of the model are still under critical discussion. In formulating the model¹⁾ it is assumed that particles move in an average spherical single particle potential generated, self-consistently, by all particles in the system. When the full Hartree-Fock (H-F) field calculation is actually performed, however, it is found that, for most nuclei, the average field is deformed and not spherical. The existence of this deformed field has led to the so-called deformed Hartree-Fock model²⁾. The spherical shell model continues to be used³⁾, however, and we find in the literature calculations for the same nucleus done with both the spherical and deformed field models. This talk is concerned with the compatibility of these two types of calculations. We shall see that the two models are indeed compatible and, indeed, we shall see, through an understanding of the relationship between the two models, how each enriches our understanding of the other.

The first concern is how to formally define the spherical field when the H-F field is deformed. In the phenomenological approach¹⁾ we consider a description of the field in terms of a harmonic oscillator potential perhaps, and choose the parameters such that the eigensolutions have the observed mean square radius. Thus we choose $\hbar\omega_0 \approx 41 A^{-1/3}$. What does the deformed H-F calculation have to say about the

mean square radius? In Figure 1 we show the results of Lee & Cusson⁴⁾ on light nuclei using the Saunier-Pearson⁵⁾ G-matrix #2. Although theory and experiment do not agree in places on a fine scale, it is clear that the $A^{1/3}$ dependence of the root mean square radius is exhibited. How does the mean-square-radius (MSR) arise in a deformed H-F calculation? It can be written in the following form:

$$\begin{aligned}
 \text{MSR} &= \langle \chi_\delta | R^2 | \chi_\delta \rangle & R^2 &= \frac{1}{A} \sum_i r_i^2 \\
 &\equiv \sum_{\alpha\beta} R_{\alpha\beta}^2 \langle \chi_\delta | a_\alpha^\dagger a_\beta | \chi_\delta \rangle & R_{\alpha\beta}^2 &= \langle \alpha | R^2 | \beta \rangle \\
 &\equiv \sum_{\alpha\beta} R_{\alpha\beta}^2 \rho_{\beta\alpha} & \rho_{\beta\alpha} &= \langle \chi_\delta | a_\alpha^\dagger a_\beta | \chi_\delta \rangle
 \end{aligned}$$

where $\rho_{\beta\alpha}$ is the density matrix for the DHF state χ_δ , and α, β is a general single particle representation. If the representation has angular momentum j a good quantum number, then we can write

$$\begin{aligned}
 \text{MSR} &= \sum_{ab} \bar{R}_{ab}^2 \rho_{ba}^0 : & \bar{R}_{ab}^2 &= \langle j_a || R^2 || j_b \rangle \\
 & & \rho_{ab}^0 &= \langle \chi_\delta | (a_a^\dagger a_b)^0 | \chi_\delta \rangle
 \end{aligned}$$

with ρ^0 the spherical density distribution.

What determines the spherical density distribution in a deformed H-F procedure? The H-F field as I have already pointed out is in general deformed but it can always be expanded in terms of spherical tensors.

$$h_{\delta} = T + U$$

$$= T + U^0 + \sum_{\lambda \neq 0} U^{\lambda} = h_0 + \sum_{\lambda \neq 0} U^{\lambda}.$$

The spherical density distribution ρ^0 arises largely from the structure of the spherical part of the completely deformed field. This has been verified from the Hartree-Fock results of Lee & Cusson by showing that the diagonalization of ρ^0 also largely diagonalizes h_0 . The verification was done with the aid of Paul Lee. This immediately suggests that we should define the spherical potential to be just the spherical part of the fully deformed potential. With knowledge of the full H-F potential we can extract the eigensolutions of h_0 . This extraction has also been done for sd-shell nuclei by Paul Lee from the results of the EVALIN Hartree-Fock Program⁶⁾ using the Saunier-Pearson potential. We show in Figure 2 how these energies change as we proceed throughout the sd shell. I don't want to comment too much on the accuracy of these results in this talk but would rather concentrate on the principle. I note however that the $s_{1/2}$ orbit is below the $d_{5/2}$ at ^{16}O and ^{20}Ne probably indicating a deficiency in the potential. We do see the raising of this level throughout the shell in agreement with the experimental data on ^{39}Ca . The numbers on the levels show the occupancy of each spherical level in the H-Fstate (to get the average number of particles in each level one should multiply the occupancy number by $2j+1$).

Having now defined the spherical shell model Hamiltonian, let us examine the usual spherical shell model calculation. In this approach we write the Hamiltonian

$$H = h_0 + V_{\text{res}} \quad (\text{N.B. } V_{\text{res}} \equiv H - h_0 - \text{no more and no less}) \\ \equiv G - U^0.$$

It is usual to consider the residual interaction taken in the space of a few valence shells. To examine the structure of V_{res} it is necessary to consider the actual structure of U^0

$$U_{\alpha\beta}^0 = \sum_{\gamma\delta} G_{\alpha\gamma\beta\delta} \rho_{\delta\gamma}^0.$$

Since $\rho^0 \approx 1$ for core orbits we can write

$$U_{\alpha\beta}^0 = \sum_c G_{\alpha c \beta c} + \sum_v G_{\alpha v \beta v} \rho_{vv}^0 \quad \text{where } c \text{ and } v \text{ indicate core and} \\ \text{valence orbits respectively.} \\ = \bar{U}_{\alpha\beta}^0 + \tilde{U}_{\alpha\beta}^0$$

This has divided the total spherical field into the contribution from the core and the contribution from the valence orbits. Now the matrix elements of the (bare) two-body potential G for shell model states having configuration of a closed shell with a few particles in a few valence orbitals has the structure

$$\langle G \rangle \approx \frac{1}{2} G_{cc'cc'} + G_{vcvc} + \frac{1}{2} G_{vv'vv'}$$

where summations over core (c) and valence (v) orbitals are implied. The factors of $\frac{1}{2}$ are included to avoid double counting. Thus

$$\begin{aligned} \langle G - U^0 \rangle &\approx \frac{1}{2} G_{cc'cc'} + G_{vcvc} + \frac{1}{2} G_{vv'vv'} \\ &\quad - G_{cc'cc'} - G_{vcvc} - G_{vv'vv'} \rho_{v'v}^0 \\ &= \frac{1}{2} G_{vv'vv'} - \frac{1}{2} G_{cc'cc'} - \langle \tilde{U}^0 \rangle. \end{aligned}$$

We see then that if we use the single particle energies of h^0 in a shell model calculation then we have to subtract from the matrix elements of the (bare) residual interaction the contribution that the valence orbits make to the average field. Alternatively one can subtract \tilde{U}^0 from the single particle energies and take the single particle energies as the eigen-solutions of $T + \tilde{U}^0$; this latter approach is then consistent with the standard shell model calculation. We see then that we have to consider the complete potential U^0 in order to be able to get spherical wave functions that have the correct MSR but only that part of it that represents the contribution from a core in order to define the single particle energies that go into the spherical shell model (with residual interaction).

Paul Lee has also extracted the single particle energies of $\bar{h}^0 = T + \bar{U}^0$ from the H-F code. We find that the energy differences $\epsilon_j - \epsilon_{p_{\frac{1}{2}}}$ (where the $p_{\frac{1}{2}}$ level represents the Fermi energy) are linearly dependent on the $\bar{h}\omega$ of the basis states

used in the H-F code.[†] This should not be and indicates that the representation of H-F states in terms of the expansion over 5 oscillator wells (as it is in the EVALIN Program) is not really sufficient for the extraction of single particle energies. We have tried to correct this by the technique

$$(\epsilon_j - \epsilon_{p_{\frac{1}{2}}})_{\text{corrected}} = \frac{(\epsilon_j - \epsilon_{p_{\frac{1}{2}}})_{\text{calc}}}{\hbar\omega_{\text{basis}}} \times 41 A^{-1/3}.$$

The extracted spin-orbit parameter κ and ℓ^2 parameter μ for sd-orbitals is shown in Fig. 3. The spin orbit parameter has an $A^{-1/3}$ dependence which, since we introduced this into the corrected values, suggests that we should be careful in taking a literal interpretation of the results. The ℓ^2 strength does not have any smooth dependence. Whereas the absolute numbers are probably not correct, they do indicate that we should expect a change in the single particle energies throughout a shell and it is not sufficient to simply assume the energies observed at the beginning of the shell as for example in ¹⁷O.

So much for the single particle potential and single particle energies. What about the rest of the shell model calculations? It is well known that it is not sufficient to diagonalize the bare effective interaction within the space of a few valence orbits. In the first place the eigenfunctions are very much governed by their spherical structure obtained

[†] N.B. the total energies do not have such a dependence.

from h_0 . The consequence of this is that such data as enhancements to E2 transitions can be underestimated by often a factor of 4. The correction to the electric multipole matrix elements is usually put into the calculation phenomenologically with the use of effective additional charges on both valence shell neutrons and protons. These effective charges are supposed to derive from the fact that the valence particles polarize the core - in other words they attempt to correct the spherical shell model for the fact that the average field is not spherical but happens to be deformed. The corresponding corrections have also to be included in the effective interaction. Various approximations have been suggested⁷⁾ for how the so called "core-polarization" corrections should be included in the spherical shell model using bubble diagrams, TDA and RPA and higher-order corrections. I want to consider here a much simpler approach.

We recall that in defining the spherical shell model Hamiltonian we first constructed the fully deformed HF field

$$h_\delta = h_0 + \sum_{\lambda \neq 0} U^\lambda$$

but up till now have only used the spherical part of this field. It is the non-scalar tensors, however, that contain all the knowledge there is to know about deformation - they are, by definition, the deformation terms. It is clearly desirable to

somehow make use of these operators in trying to describe the effects of deformation in the spherical shell model.

We consider the following auxiliary Hamiltonian

$$H_A = h_0 + \sum_{\lambda \neq 0} \frac{U^\lambda \cdot U^\lambda}{\langle U_0^\lambda \rangle} (\times \text{ exchange}).$$

The auxiliary Hamiltonian has been constructed such that the Hartree procedure, or with the special exchange term, the H-F procedure, will lead exactly to the single particle field h_δ . In other words both H and H_A have the same single particle fields. If we now write

$$H = H_A + \tilde{V}_{\text{res}} \quad (\tilde{V}_{\text{res}} = H - H_A)$$

we see that the *new* residual interaction does not contribute at all towards the field. If we are interested in properties of H that derive from the field then these should also be properties of H_A . In the first approximation then it makes sense to study the properties of H_A .

Note that this approach is completely parallel to that of the early definition of the spherical shell model¹⁾. Then we wrote

$$H = h_0 + V_{\text{res}} \quad (V_{\text{res}} = H - h_0)$$

and in the first instance ignored V_{res} to derive properties of the nucleus in terms of the properties of the single particle spherical Hamiltonian h_0 . In this way predictions

of ground state spins and parities were determined together with such estimates as the Schmidt values for magnetic moments and the Weisskopf estimates for electromagnetic transitions. We would like to learn now how much of the spectrum we can understand with the auxiliary Hamiltonian H_A which incorporates all parts of the average field (and not just the spherical part as does h_0).

Just as it is convenient to consider a simple form for h_0 in terms of the spherical harmonic oscillator, so is it convenient to consider a simple form for h_δ in terms of the deformed harmonic oscillator:

$$h_\delta = \frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \frac{\hbar^2}{2m} \sum_i \left(\frac{x_i^2}{b_1^4} + \frac{y_i^2}{b_2^4} + \frac{z_i^2}{b_3^4} \right)$$

$$\equiv h_0 + B_0 Q_0 + B_2 (Q_2 + Q_{-2}).$$

The deformed oscillator can be written in terms of a spherical oscillator with quadrupole deforming terms. We shall restrict ourselves to axially symmetric cases ($B_2 \equiv 0$). The auxiliary Hamiltonian then takes the form

$$H_A = h_0 + x \hbar \omega_0 \sum_{i < j} Q_i \cdot Q_j \quad (* \text{ exchange})$$

with x a strength constant and the exchange mixture chosen, for even even nuclei, such that

$$3A^{13} + 3A^{31} = A^{11} + 9A^{33} = 8$$

where $\langle TS | \text{exchange} | TS \rangle = A^{2T+1, 2S+1}$.

With these conditions the H-F procedure on H_A leads *exactly* to the deformed oscillator field.

What are the properties of H_A ? There are now two ways of proceeding. We could take the deformed H-F approach and project states of angular momentum ψ_J from the H-F state χ_δ (i.e. lowest solution to the deformed harmonic oscillator). The energy spectrum can then be estimated by calculating the expectation value $(\psi_J | H_A | \psi_J)$. In Figure 4 I show (by the dots) the result of such a calculation in ^{20}Ne for various strengths of the Q.Q potential. These calculations were done by Pierre Amiot using the EVALIN Hartree-Fock program of Lee & Cusson⁶⁾. Let us consider now the spherical shell model approach. In the first approximation we might consider diagonalizing the Q.Q potential just within the space of configurations having a closed ^{16}O core with four particles in the sd-shell. This calculation is very simple because, as Elliott⁸⁾ has shown, the Q.Q. potential within the space of a major oscillator shell can be written

$$\begin{aligned} \sum_{i < j} Q_i \cdot Q_j &\approx \frac{1}{2} \sum_{ij} Q_i \cdot Q_j - (\text{one-body terms}) \\ &= \frac{1}{2} (C - 3L^2) - (\text{one-body terms}) \end{aligned}$$

where C is the Casimir operator of SU_3 and L is the orbital angular momentum. The coefficient of L^2 is therefore $-\frac{3}{2} \hbar^2 \omega$ from which we can easily deduce the spectrum if we ignore the effects of the single particle terms. The results of such a calculation are shown by the dashed lines in Figure 4. Clearly the energy dependence is linear in x . Clearly also there is disagreement with the projected H-F result. What we should consider in the shell model calculation, however, is not the "bare" Q.Q. potential but a renormalized potential corrected for the polarization of the field. The general procedure for determining the renormalized interaction has been given by Bloch & Horowitz⁹⁾ and the particular renormalization of a Q.Q potential given by Harvey¹⁰⁾. If v_{11} is the effective interaction to be used in a truncated space #1 and V is the fundamental (bare) potential defined for the full space #1+2 then

$$v_{11} = V_{11} + V_{12} \Gamma v_{21}.$$

The second term provides the correction to V in the space #1 for neglect of space #2 in terms of a complicated "coupling" operator⁹⁾ v_{21} . If $V = Q \cdot Q$ and we consider truncation to a major oscillator shell then

$$v_{11} = Q^{11} \cdot Q^{11} + 2Q^{11} \cdot Q^{12} \Gamma v_{21} + \dots$$

where Q^{11} is the part of the quadrupole operator that transforms within an oscillator shell and Q^{12} is the part that

transforms out of an oscillator shell (actually coupling shells differing by $2\hbar\omega$). The factor of 2 arises because of the two quadrupole operators. To estimate $2Q^{12}\Gamma\nu_{21}$ we consider the effective quadrupole operator \tilde{Q}^{11} within an oscillator shell that has the same matrix elements for spherical states(s) as the bare quadrupole operator has for deformed orbits(δ). Again the Bloch-Horowitz procedure⁹⁾ tells us

$$\tilde{Q}^{11} = Q^{11} + 2 Q^{12} \Gamma \nu_{21} + \dots$$

and $\langle \tilde{Q}^{11} \rangle_s \equiv \langle Q \rangle_\delta \equiv \frac{\langle Q \rangle_\delta}{\langle Q \rangle_s} \langle Q \rangle_s$.

We write

$$\tilde{Q}^{11} \equiv \frac{\langle Q \rangle_\delta}{\langle Q \rangle_s} Q^{11} \equiv \alpha Q^{11}$$

with an enhancement factor α . For an N=Z even-even nucleus $\alpha = 1+2\eta$ where η = effective charge. Now it is seen that $2Q^{12}\Gamma\nu_{21} \equiv (\alpha-1)Q^{11}$. Thus the effective residual interaction can be replaced by

$$\nu_{11} = Q^{11} \cdot Q^{11} + (\alpha-1) Q^{11} \cdot Q^{11} \equiv \alpha Q^{11} \cdot Q^{11}.$$

Thus, in the spherical shell model, the effective interaction we should use is the quadrupole-quadrupole interaction renormalized by the factor $\alpha = \langle Q \rangle_\delta / \langle Q \rangle_s$. Since the deformation of the well depends on the strength x , this

renormalization factor is also x -dependent. The results of the renormalized shell model calculation for the spectrum of ^{20}Ne are shown in Figure 4 by the solid curves and we see a remarkable agreement now between these renormalized spherical shell model results and the unrestricted deformed H-F results.

[As a historical note I should explain that the renormalized shell model results were produced first since they involve essentially back-of-the-envelope type calculations. It was with extreme gratification that, when the deformed H-F calculations came out of the 6600 computer, we found that they had this remarkable agreement.]

What is a realistic value for x ? Mottelson¹¹⁾ pointed out some time ago that we should consider a field having the property that the deformation of the field is identical to the deformation of the lowest eigensolution in the field. The argument being that the field is being generated by the particles and we should expect to find a field only where there are particles. If we select this "shape-consistent" deformed oscillator as a realistic estimate of the average field then we find the corresponding $Q.Q$ strength at $x_{s.c.} \approx -3.79 \times 10^{-3}$ for ^{20}Ne . We note now that the spectrum at this shape-consistent point is very similar to that from the full H-F calculation of Lee & Cusson using a G -matrix; in other words this use of an auxiliary Hamiltonian

appears to have extracted the essential features of the more complete calculation.

For the "shape consistent" harmonic oscillator, the enhancement factor $\alpha \approx 2$. In terms of the effective charge formalism ($\alpha = 1+2\eta$) this implies the use of an effective charge η of $\frac{1}{2}$. Thus we see that the polarization corrections we are putting into the spherical shell model for the "realistic" situation are, demonstrably, consistent with our use of an effective charge of about $\frac{1}{2}$.

You will note that there is a discrepancy between the projected and renormalized spherical shell model result for $x > x_{s.c.}$; why is this? In Figure 5 we show the β -deformation of the H-F solution as a function of the O.O strength x . Since the H-F potential has the deformed oscillator structure for any x we can solve the H-F problem exactly. The exact answer for the β -deformation is shown by the solid curve in Figure 5. The crosses show the results from the EVALIN program. Clearly we see that the representation of the H-F' orbits in terms of an expansion over five major spherical oscillator shells (as they are in the EVALIN code) is not adequate beyond $x_{s.c.}$. Even at $x_{s.c.}$ the error in the β -deformation is $\sim 15\%$.

In Figure 6 I show the results of calculations with the auxiliary Hamiltonian H_A for ^{28}Si . In this nucleus the H-F procedure shows two low lying solutions one

oblate and the other prolate. Again we find that in both cases the projected H-F results and the renormalized spherical shell model results agree remarkably well. Again we find reasonable agreement between the spectra for the shape-consistent strengths and those from the (unpublished) H-F calculations of Lee & Cusson using a G-matrix effective interaction; indeed the agreement between the theories is better than the agreement between theory and experiment. We can now perhaps say that field effects are understood and the discrepancy with experiment is due to the ignored (non-field producing) residual interaction \tilde{V}_{res} which (hopefully) can be treated in the spherical shell model by matrix diagonalisation. But this is another story.

Of particular interest is to note that the shape consistent strengths in the prolate and oblate solutions are not the same, i.e., the auxiliary Hamiltonians are not the same; i.e., the renormalization in the spherical shell model should depend on the *shape* of the field. How can such an effect be included in the spherical shell model? In general it would be very difficult to include such an effect - but there is a possibility if one uses an SU_3 basis. The SU_3 states are the remnants in the spherical shell model space of the fully deformed states, the $(\lambda\mu)$ numbers of the SU_3 representations corresponding to the $\beta\gamma$ of the deformed state. If we are to renormalize with respect to deformation, then the effective interaction will have a $(\lambda\mu)$ dependence. What information do

we have that such a dependence is actually needed in a spherical shell model calculation? In Figure 7 I show the recent shell model results of the University of Michigan group¹²⁾ (Draayer & Hecht) for the low energy spectrum of ^{25}Mg . They noted that if they use a Kuo G-matrix with a standard ($(\lambda\mu)$ independent) renormalization then the calculated spectrum doesn't look at all like the calculated spectrum (see spectrum labelled KB(MS)). On the other hand if they allow themselves the freedom of a $(\lambda\mu)$ dependence (spectra labelled with +R) then they are able to reorder states in the spectrum such that the experimental spectrum is more understandable. They also find that the properties of their states (i.e., ground state quadrupole moment and the gross features of E2 and M1 transitions) are in better agreement with the experimental data.

These results are very preliminary and it is too early to say whether a shape dependent renormalization is really necessary to explain the data in ^{25}Mg , but in view of our earlier calculations it is indeed a fascinating - and provocative - possibility.

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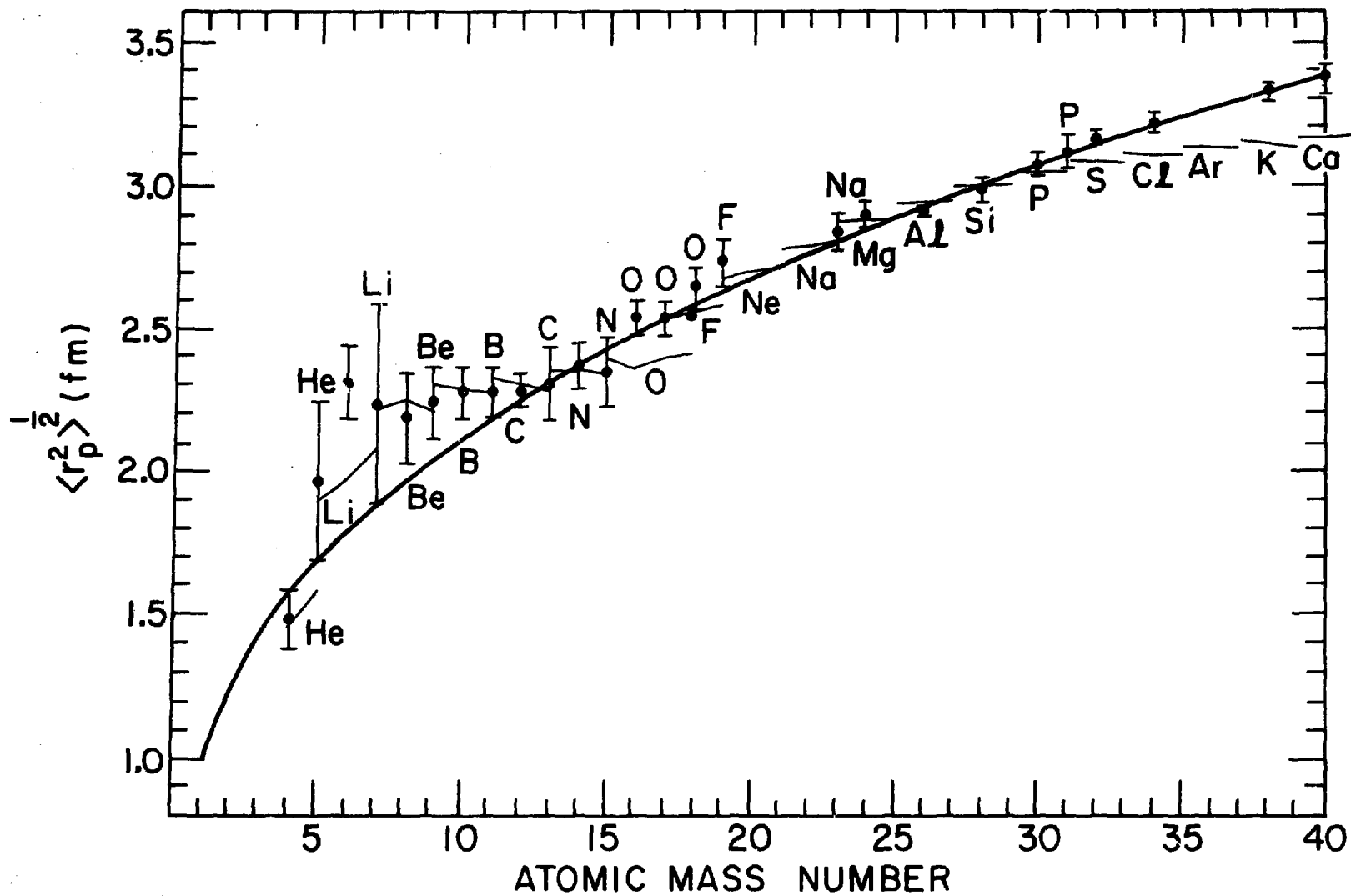


Figure 1

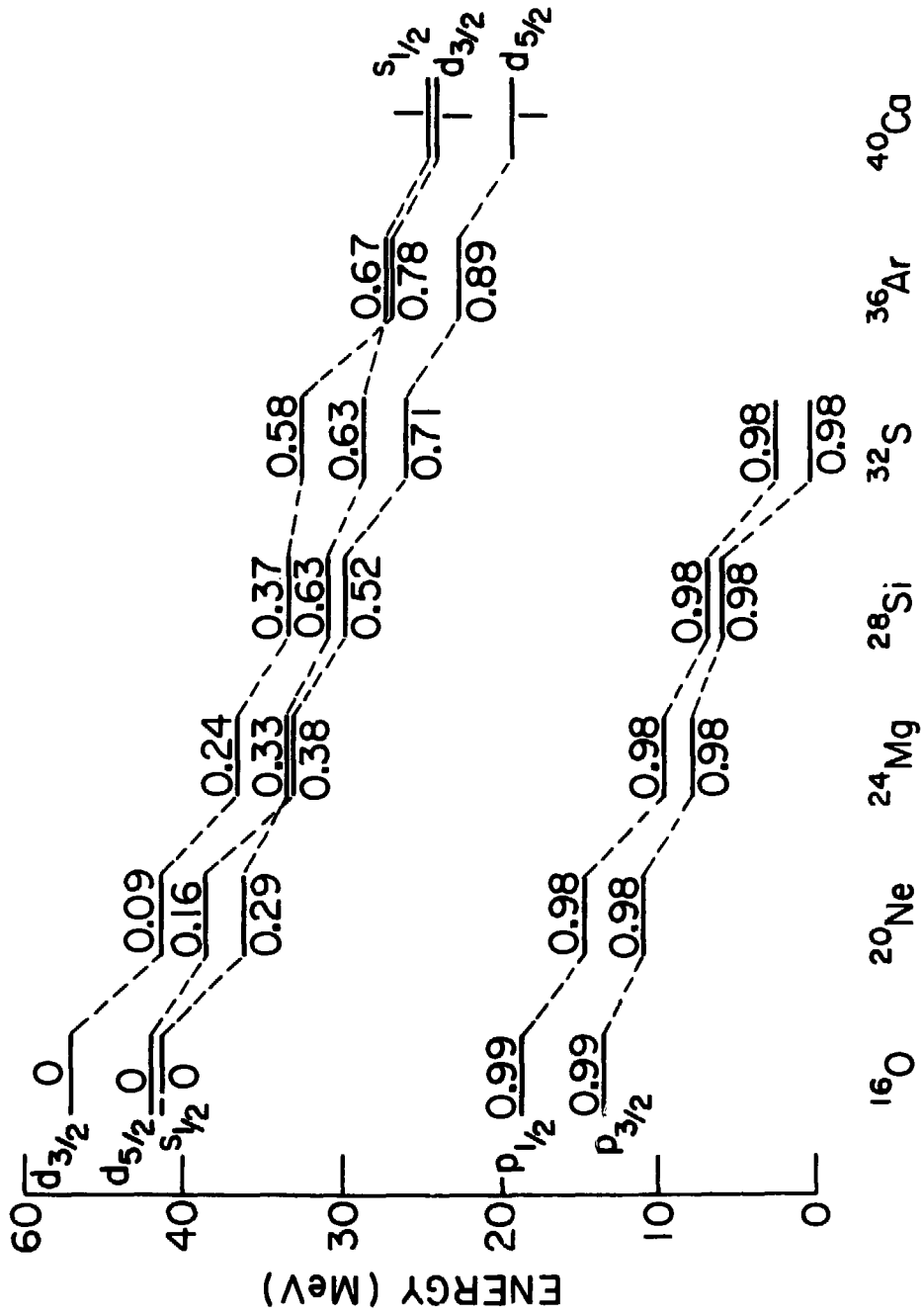


Figure 2

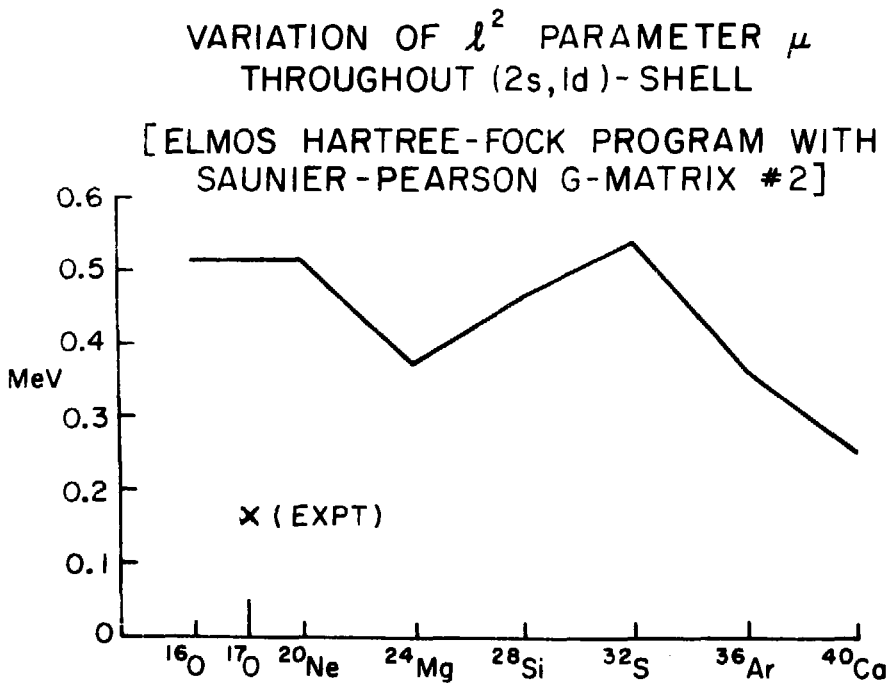
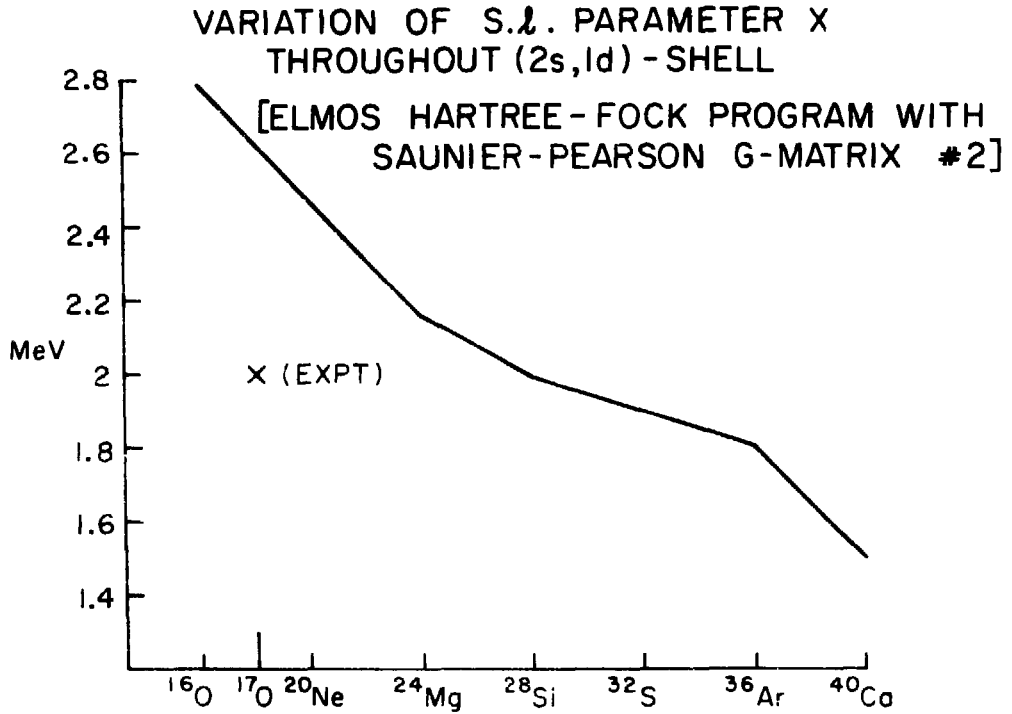


Figure 3

VARIATION OF ^{20}Ne SPECTRUM WITH THE STRENGTH X OF Q.Q. POTENTIAL

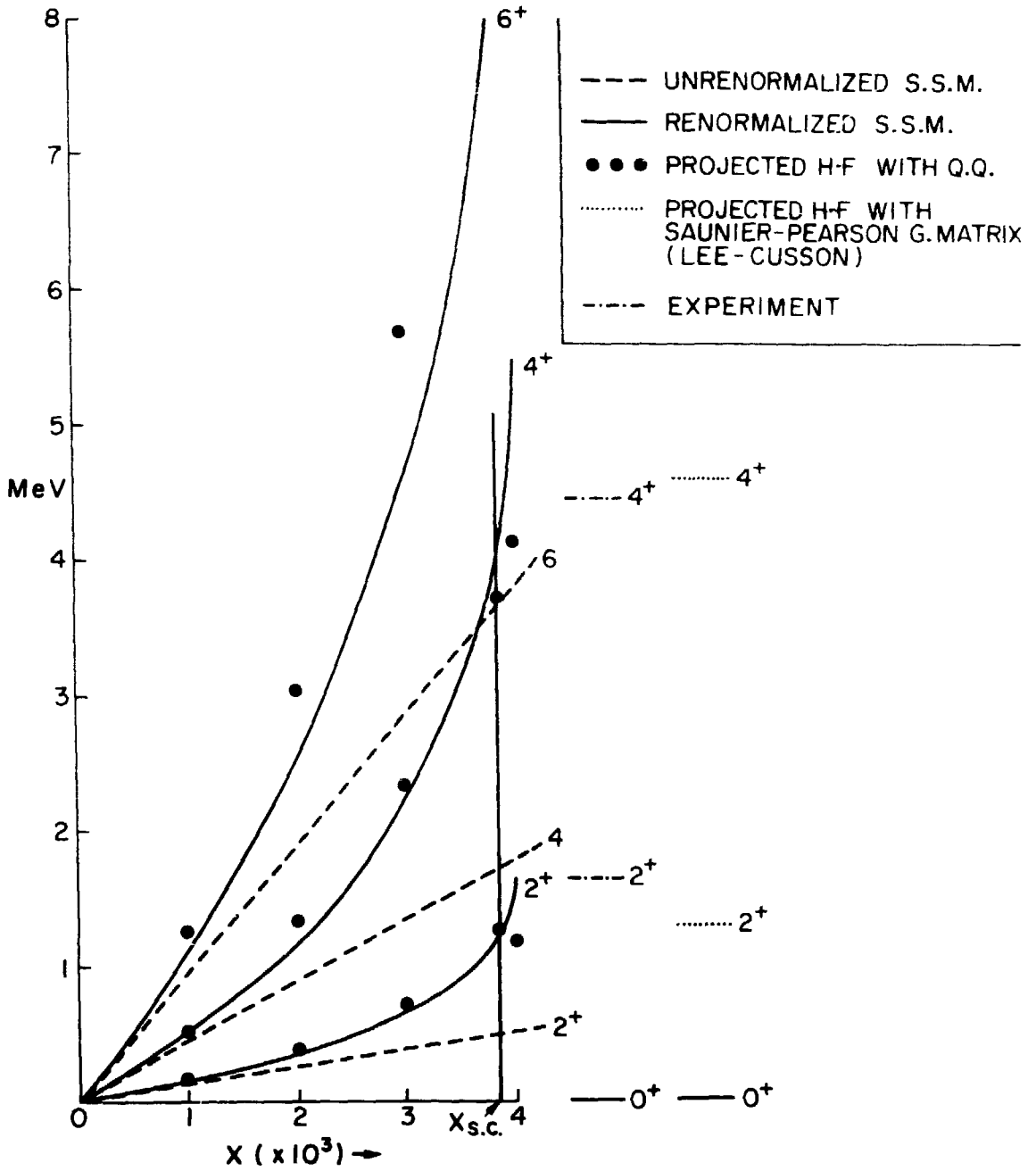


Figure 4

β -DEFORMATION OF ^{20}Ne HARTREE-FOCK STATE AS A FUNCTION OF Q.Q. STRENGTH

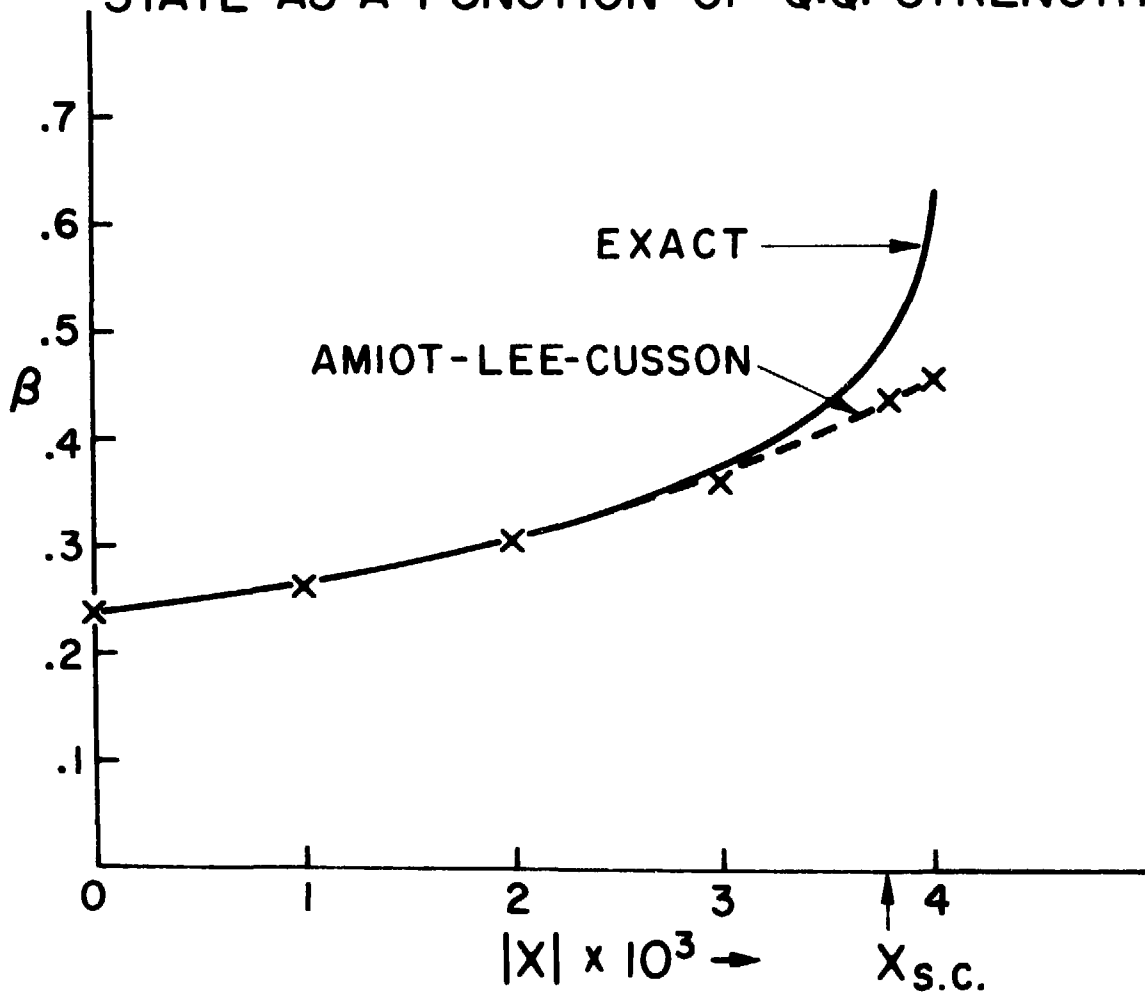


Figure 5

VARIATION OF THE ENERGIES OF THE PROLATE AND OBLATE BANDS IN ^{28}Si WITH Q.Q. STRENGTH

x PROJECTED H-F
 --- UNRENORMALIZED SHELL MODEL
 — RENORMALIZED SHELL MODEL

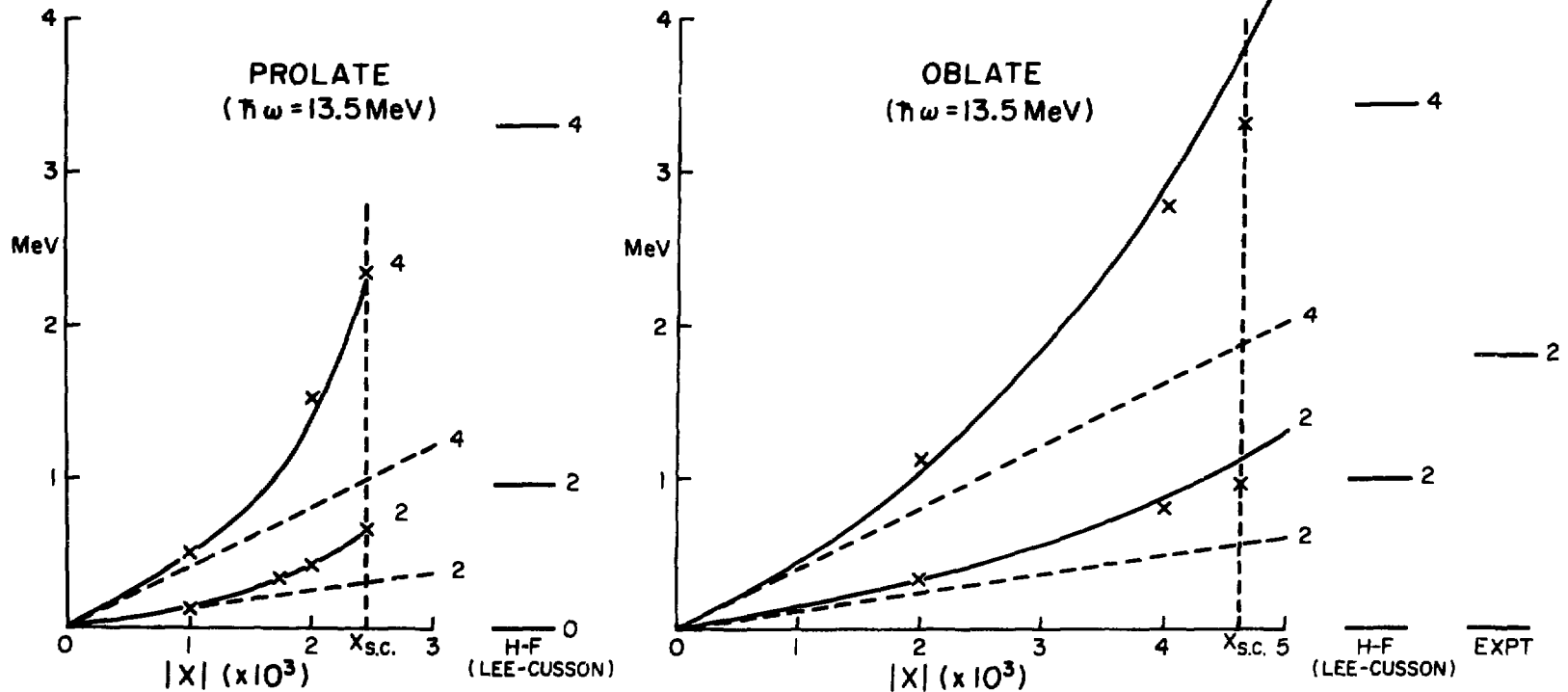


Figure 6

²⁸Mg ENERGY LEVEL SCHEME (SHELL MODEL CALCULATIONS
BY J.P. DRAAYER)

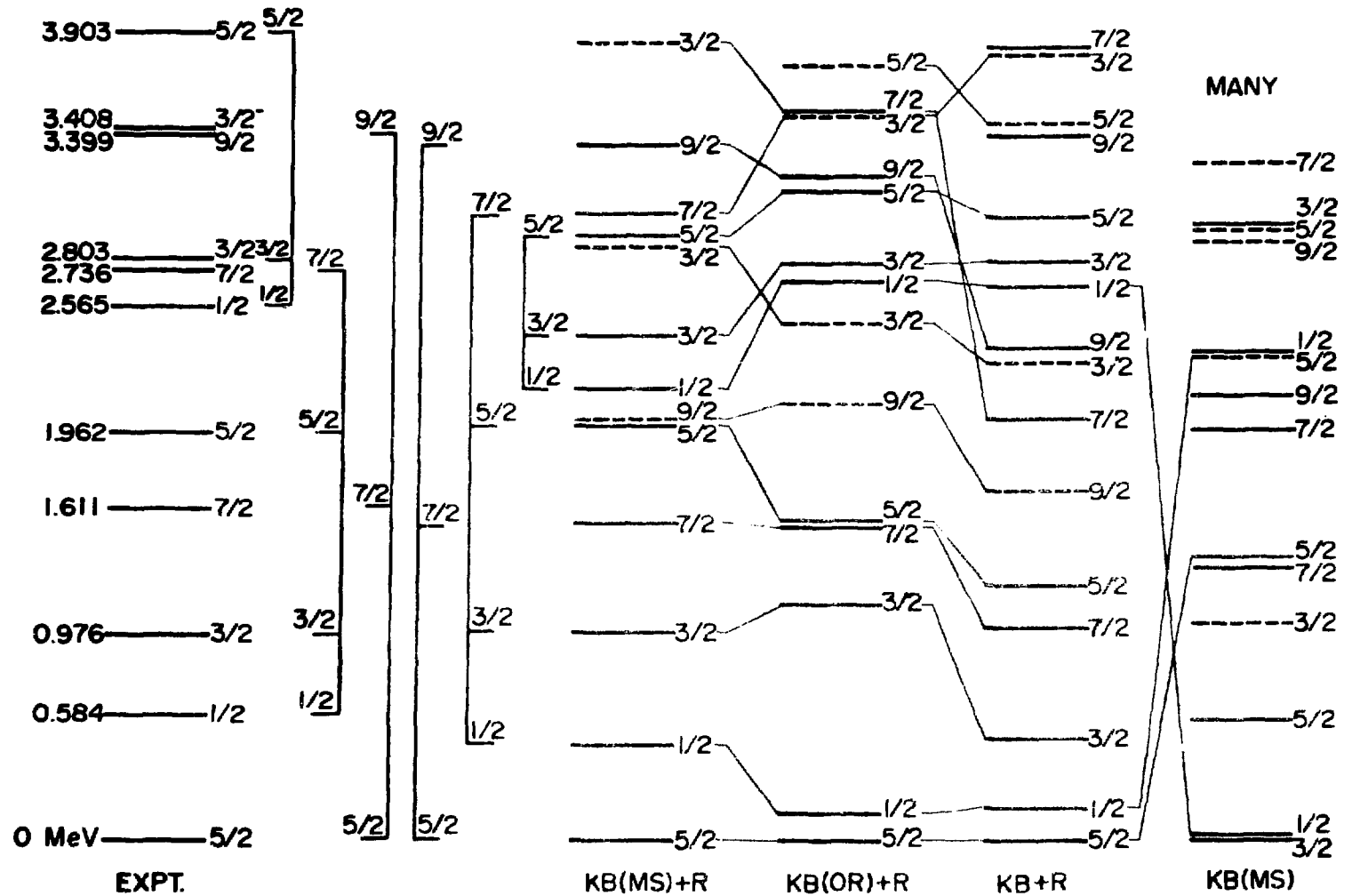


Figure 7

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