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A Mass-Dependent Effective Interaction for Shell-Model Calculations Derived for the *fp* Shell

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Abstract

An effective interaction suitable for shell-model calculations for the fp shell is derived from the Reid soft-core potential folded with two-body correlation functions. These correlations were designed to take into account the short-range repulsion in the nucleon-nucleon force and also the large tensor component in the Reid force. The interaction when compared with the experimentally fitted data of Van Hees and Glaudemans in the fp - shell region of the nuclei show reasonable agreement.

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1.0 Introduction

For sometime now a lot of interest has been generated in the study of nuclei far above the calcium region. In particular the work of Van Hees and Glaudemans [1], Johnstone and Skouras [2], Zuker and co-workers [3,4], Novoselsky and Vallieres [5], Richter et al. [6] etc, have shown that shell-model calculations in the fp-shell can be performed quite successfully to describe the energy spectra, electromagnetic properties and single transfer reactions as well as rotational properties of these nuclei.

The input data to these calculations is a suitable two-body effective interaction and the starting point usually is to consider all (or some) of the two-body matrix elements of the effective two-body interaction as free parameters to be adjusted empirically to fit experimental results. Another useful modification of the matrix elements of an effective interaction in the fp-shell is suggested by Zuker and co-workers [3,4] who suggest an isospin - dependent energy shift to the diagonal matrix elements of the form

$$V'_{ijij} = V_{ijij} - 0.3(-1)^T \, MeV \tag{1.1}$$

Where V_{ijij} represent an original diagonal matrix element of the effective interaction. Van Hees and Glaudemans [1] have shown that to fully account for all configurations in the predominantly $0f_{7/2}$ states one has to take into account excitations from the $0f_{7/2}$ orbit into the other three *fp*-shell orbits in an extended configuration space.

Several years ago, Fiase et al., [7] generated a simple mass-dependent effective interaction for *sd* shell – model calculations by folding together a Hamiltonian for the rest-frame of the nucleus, based on the Reid [8] soft-core potential, with a simple set of two-body correlation functions. They compared their data with the fitted data of Wildenthal [9] which was designed for this region of the nuclei. They found excellent agreement besides reproducing exactly the mass dependence of the matrix elements (ME) of the form

$$\frac{ME(A)}{ME(18)} = \left(\frac{18}{A}\right)^{0.3} \tag{1.2}$$

In the present work we have examined the mass - dependence of this interaction for the *fp*-shell region of the nuclei and have demonstrated that they show remarkable similarity with the fitted data of Van Hees and Glaudemans [1] designed for this region of the nuclei.

2.0 The Effective Interaction

In order to clarify the method and approximations used we shall briefly outline the method developed by these authors. This approach involves two stages. In the first stage the Hamiltonian is formulated in the rest-frame of the nucleus (Fiase et al., [7]) as:

$$H = \sum_i {p_i^2}/{2m} + \sum_{i>j} V_{ij} \rightarrow H' = \sum_{ij} \left({p_{ij}^2}/{M} + V_{ij} \right) \tag{2.1}$$

where the relative momentum of the two-particle system is defined by $\mathbf{p}_{ij} = (1/\sqrt{2})(\mathbf{p}_i - \mathbf{p}_j)$ and M = Am is the total mass of the nucleus while V_{ij} was taken to be the Reid [8] soft-core potential. Having found the bare Hamiltonian defined in the rest-frame of the nucleus, we next defined an effective two-body Hamiltonian in the form [10,11])

$$H_{eff}^{(2)} = \sum_{\lambda, i>j} f_2^{\lambda}(ij) \left({p_{ij}^2}/{M} + V_{ij} \right) f_2^{\lambda}(ij) \tag{2.2}$$

where the $f_2^{\lambda}(ij)$ are the two-body correlation operators and λ is a summation over all the reaction channels. In studies regarding nuclear matter and finite nuclei the correlation functions were found to have three features. These were: (i) the 'wound' induced in the two-body wave function by the repulsive core of the N-N interaction, (ii) the tensor correlations and (iii) the meson-exchange corrections. Of these the most important feature was found to be the tensor correlations. Thus a simplified and parameterized form of the two-body correlation functions was designed to take the form [10,11]:

$$\begin{aligned} f_2^{\lambda}(ij) &= 0, & r < r_c \\ &= (1 - e^{-\beta(r_{ij} - r_c)^2})(1 + \alpha^{\lambda} S_{ij}), & r \geq r_c \end{aligned} \tag{2.3}$$

where $r_c = 0.25$fm and $\beta = 25\text{fm}^{-2}$. The parameter α^{λ} defines the strength of the tensor correlations and is non-zero only in the $^3S_1$ - $^3D_1$ channel. In equation (2.3), S_{ij} is the usual tensor operator. Using the effective interaction of equation (2.2) together with the correlation functions defined by equation (2.3) we have a mass-dependent two-body interaction containing no free parameters with which to perform shell-model calculations. Fiase et al., [7] carried out such calculations for the *sd*-shell nuclei in a harmonic oscillator basis. They also compared their results with the fitting routines of Wildenthal and collaborators [9,12] for the various values of α^{λ} and the oscillator size parameter $b = \sqrt{((m\omega)/\cong)}$ contained in the harmonic oscillator wave function and found an excellent agreement between the two sets of results besides offering explanation to some of the salient features inherent in the fitting routines.

3.0 Results for the *fp* shell.

We now report on the extension of the work of Fiase et al., [7] to the fp shell. We use the same effective interaction as in the *sd* shell defined by equation (2.2) with the two-body correlation functions of equation (2.3). From the work of Van Hees and Glaudemans [1], it is clear that in order to fully account for the low-lying states in the predominantly $f_{7/2}$ configurations one must include excitations from the $f_{7/2}$ orbit into the other three *fp*-shell orbits i.e., $1p_{3/2}$, $0f_{5/2}$ and $1p_{1/2}$ in an extended shell-model configuration space. In this study we report on a similarly motivated work by allowing excitations from the $f_{7/2}$ orbit into the other three *fp*-shell orbits. There are 60 Pauli - allowed two-body matrix elements that can be formed by any such combination, comprising 32 diagonal and 28 non-diagonal matrix elements. In an earlier analysis for the *sd* shell, Fiase et al., [7] have shown that agreement between their calculated matrix elements and those of the fitting routines of Wildenthal and collaborators [9,12] could be greatly improved if a constant shift is applied to all the diagonal

two-body matrix elements, the off-diagonal matrix elements remaining the same. We shall investigate that finding further in this work.

In Figure 1 we present a scatter diagram of our calculated matrix elements and those of Van Hees and Glaudemans [1] for A = 55 nuclei. From the figure we can see an immediate agreement between the two sets of data especially for the off-diagonal two-body matrix elements. To obtain a comparable agreement for the diagonal two-body matrix elements we applied a constant shift of 0.7MeV to all the diagonal matrix elements. In an earlier prescription for the *sd*-shell, Fiase et al., [7] introduced the variance $\chi_f(A)$, which gives the measure of the quality of agreement of the two sets of data in the form:

$$\chi_f(A) = \frac{\sum_{i=1}^{NP} (ME_c(i) - ME_f(i))^2}{\sum_{i=1}^{NP} (ME_f(i))^2} \tag{3.1}$$

where $ME_c(i)$ are the calculated matrix elements while the $ME_f(i)$ are those taken from the fitting routines. For the *sd*-shell, NP represents the 63 Pauli-allowed two-body matrix elements formed by the combination of the angular momentum of the two-particle system and their isospin counterparts. They investigated this as a function of a constant shift, Δ_D, to all the diagonal two-body matrix elements of the form

$$V_{ijij}' = V_{ijij} - \Delta_D \tag{3.2}$$

where V_{ijij} is an original diagonal matrix element and Δ_D is the shift in the diagonal two-body matrix element. With this shift they found comparable agreement with the fitted data of Wildenthal and collaborators [9,12] giving $\chi_W(A)$ of the order ≈ 0.03. In Figures 2(a) - 4(a) we plot $\chi_{VH}(A)$ for the fitted data of Van Hees and Glaudemans based on equation (3.2) as a function of a constant shift, Δ_D, to all the diagonal two-body matrix elements for $50 \le A \le 55$ for $\omega = 9$MeV appropriate for this region of nuclei and the values of α^λ in the range $0.07 \le \alpha^\lambda \le 0.09$. In the present case, NP = 60. From each of these figures we obtained a smoothly varying mass-dependent energy shift, Δ_D, as a function of the variance. The optimised variances for $\cong \omega = 9$MeV and $\alpha^\lambda = 0.07$, 0.08 and 0.09 are approximately 0.19, 0.14 and 0.11 respectively, which show a good agreement between the two sets of data. We considered further the suggestion of Zuker and co-workers [3,4] who suggest a phenomenological cure to all the diagonal matrix elements of the form

$$V_{ijij}' = V_{ijij} - \Delta_T \tag{3.3}$$

where Δ_T is an isospin - dependent shift to the diagonal matrix elements. In Figures 5, 6 and 7 we investigated this by choosing a range of values for Δ_T and then searching for the minimum point in the variance for ω 9MeV and $\alpha^\lambda = 0.08$, 0.085 and 0.09 respectively. This yielded optimised values of χ_{VH} between 0.25 and 0.35 which are clearly higher than the previous analysis and the agreement therefore not so good. However, when we combined the prescriptions of equations (3.2) and (3.3) in the form

$$V'_{ijij} = V_{ijij} - \Delta_T - \Delta_D \tag{3.4}$$

the results of these investigations in the form of plots of the variances, χ_{VH} against shifts in energy Δ_T and Δ_D for the various values of ω and α^λ are shown in Figures 2(b) - 4(b). In Figure 2(b) we used $\Delta_T = 0.45(-1)^T$ MeV as the shift in the diagonal matrix elements while in Figures 3(b) and 4(b), Δ_T was respectively $0.3(-1)^T$ and $0.2(-1)^T$ MeV. I

In these figures we notice further reduction in the values of the variances which now lie in the range $0.08 \le \chi_{VH} \le 0.14$ which confirm the validity of using the prescription of Zuker and co-workers [3,4] but more importantly in making appropriate shifts to the diagonal two-body matrix elements in order to obtain reasonable agreement with the fitted data.

In Table 1 (i) we give a sample set of our calculated matrix elements for A = 50, $\hbar\omega$ = 9.0 MeV and α^{λ} = 0.09. One should note the excellent agreement between our calculated off-diagonal matrix elements and those of the fitted data of Van Hees and Glaudemans [1]. The agreement between the diagonal matrix elements is not so good. These observations can also be seen in Figure 1 for the A=55 case.

Conclusion

We have produced an effective interaction for the *fp*-shell nuclei by folding a Hamiltonian for the rest-frame of the nucleus. This interaction when compared to the work of Van Hees and Glaudemans [1] in the *fp*-shell region of nuclei show reasonable agreement with the fitted values. As in the earlier prescription for the *sd*-shell, it was found that an improvement in the agreement between the diagonal matrix elements could greatly be achieved if we make a constant shift to the diagonal matrix elements, the off-diagonal matrix elements remaining the same. Furthermore, we considered the suggestion made by Zuker and co-workers [3,4] who suggest a phenomenological cure to the diagonal matrix elements of the form of equation (3.3). By combining this suggestion with our earlier prescription we obtained further reduction in the variance as can be seen from Figures 2(b) – 4(b). While the overall agreement between our calculated matrix elements and the interaction of Van Hees and Glaudemans [1] is good, there is some problem in the diagonal matrix elements. One may trace this to some underlying physics which includes core polarisation. In a first approximation this should affect the widths of our eigenvalue distributions and so we may have to further account for this phenomenologically by applying a multiplicative parameter to all the diagonal matrix elements. A further investigation using this interaction to calculate energy levels and other properties of nuclei such as electromagnetic properties and single transfer reactions etc, for the *fp*-shell nuclei using a suitable shell-model code and taking these observations into account is being undertaken and will be presented elsewhere.

Acknowledgment

One of the authors (J.O.F) wishes to thank Professor J.M. Irvine who introduced him to nuclear structure theory including several of the techniques reported here.

Figure Captions

1(a) Two-body off-diagonal fp- shell matrix elements for T =1 and T = 0 isospin. Van Hees and Glaudeman's interaction, present . 7 = of $_{7/2}$, 5 = 1f $_{5/2}$, 3 = 2p$_{3/2}$ and 1 = 1p$_{1/2}$. The J in the bracket denotes the total angular momentum of the two- particle system. Calculation parameters are w = 9MeV,α^{λ}=0.09, A = 55.

1(b) As in (a) for diagonal matrix elements. The calculated diagonal matrix elements are shifted by 0.7MeV. Calculation parameters are as in (a).

2(a) - 4(a). Variance χ_{VH} between our calculated matrix elements and the interaction of Van Hees and Glaudemans as a function of a constant energy shift, Δ_D to all the diagonal matrix elements, equation (3.2).

2(b)-4(b). Calculated variance is based on equation (3.4). Notice the lowering in the values of the variance.

5-7 Here calculated values of the variances is based on equation (3.3) alone which is not good enough.

Table 1: A Sampie List of Calculated Matrix Elements for A = 50, $\hbar\omega$ = 9.0 MeV and α^{λ} = 0.09. 7 = of $_{7/2}$, 5 = 1f $_{5/2}$, 3 = 2p$_{3/2}$ and 1 = 1p$_{1/2}$.

Table 1: A Sample List of Calculated Matrix Elements for A = 50, $\hbar\omega$ = 9.0 MeV, α^{λ} = 0.09.(i) Present (ii) Van Hees and Glaudemans [1].

(a) Diagonal

T = 0

						(i)	(ii)
1	7	1	7	3	0	-0.8127	-2.14
1	7	1	7	4	0	0.7439	-1.18
3	7	3	7	2	0	0.3489	-1.07
3	7	3	7	3	0	-0.0650	-1.18
3	7	3	7	4	0	0.5862	-0.62
3	7	3	7	5	0	-1.6710	-2.67
5	7	5	7	1	0	-3.5839	-5.26
5	7	5	7	2	0	-2.1080	-2.87
5	7	5	7	3	0	-0.3799	-1.99
5	7	5	7	4	0	-1.1990	-1.48
5	7	5	7	5	0	-0.1006	-0.58
5	7	5	7	6	0	-2.4950	-3.27
7	7	7	7	1	0	0.3404	-0.99
7	7	7	7	3	0	0.4379	-0.61
7	7	7	7	5	0	-0.1696	-0.15
7	7	7	7	7	0	-2.290	-2.51

T = 1

1	7	1	7	3	1	0.7439	0.23
1	7	1	7	4	1	0.2236	-0.07
3	7	3	7	2	1	0.0786	-0.66
3	7	3	7	3	1	0.6759	0.17
3	7	3	7	4	1	0.5402	0.15
3	7	3	7	5	1	0.4021	0.35
5	7	5	7	1	1	0.8729	-0.09
5	7	5	7	2	1	0.7770	0.10
5	7	5	7	3	1	0.7225	0.22
5	7	5	7	4	1	0.4265	0.23
5	7	5	7	5	1	0.2174	0.36
5	7	5	7	6	1	-0.8830	-0.69
7	7	7	7	0	1	-0.4950	-2.60
7	7	7	7	2	1	0.1487	-1.11
7	7	7	7	4	1	0.4875	-0.20
7	7	7	7	6	1	0.2285	0.23

(b) Off-Diagonal

T = 0

						(i)	(ii)
1	7	3	7	3	0	-1.1981	-1.15
1	7	3	7	4	0	0.2576	-0.06
1	7	5	7	3	0	-0.6626	-0.93
1	7	5	7	4	0	-0.8680	-0.92
1	7	7	7	3	0	-0.7156	-0.64
3	7	5	7	2	0	0.9023	0.48
3	7	5	7	3	0	-0.4475	-0.16
3	7	5	7	4	0	0.0721	-0.11
3	7	5	7	5	0	-0.5739	-1.01
3	7	7	7	3	0	-0.5483	-0.48
3	7	7	7	5	0	-0.9166	-0.82
5	7	7	7	1	0	-2.1164	-1.89
5	7	7	7	3	0	-0.8807	-1.01
5	7	7	7	5	0	-0.5213	-0.90

T = 1

1	7	3	7	3	1	0.0123	-0.08
1	7	3	7	4	1	0.3878	0.50
1	7	5	7	3	1	0.0176	-0.01
1	7	5	7	4	1	-0.1101	-0.09
1	7	7	7	4	1	0.2747	0.29
3	7	5	7	2	1	0.0173	-0.01
3	7	5	7	3	1	0.0810	0.17
3	7	5	7	4	1	0.1573	0.15
3	7	5	7	5	1	0.0157	0.35
3	7	7	7	2	1	-0.3774	-0.50
3	7	7	7	4	1	-0.1795	-0.31
5	7	7	7	2	1	0.2169	0.00
5	7	7	7	4	1	0.4173	0.41
5	7	7	7	6	1	0.5445	0.72

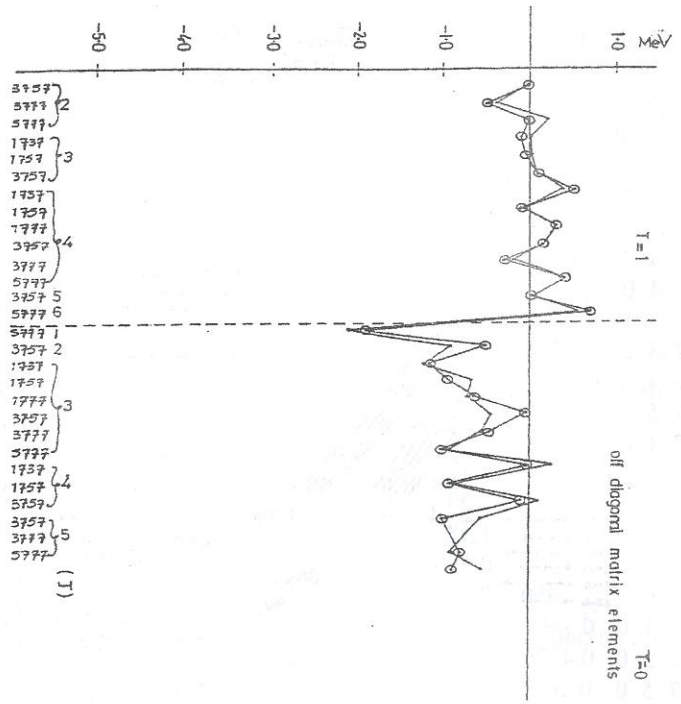

-50
-40
-30
-20
-10
0 MeV
T = 1
T=0
off diagonal matrix elements
(T)

Figure 1(a)

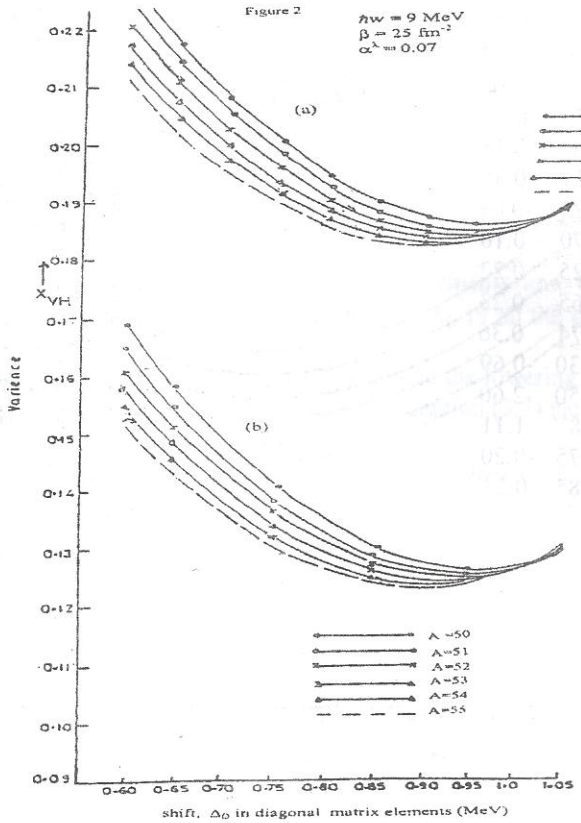


Figure 2
ħw = 9 MeV
β = 25 fm⁻²
α^λ = 0.07
(a)
(b)
A=50
A=51
A=52
A=53
A=54
A=55
Variance
shift, Δ₀ in diagonal matrix elements (MeV)

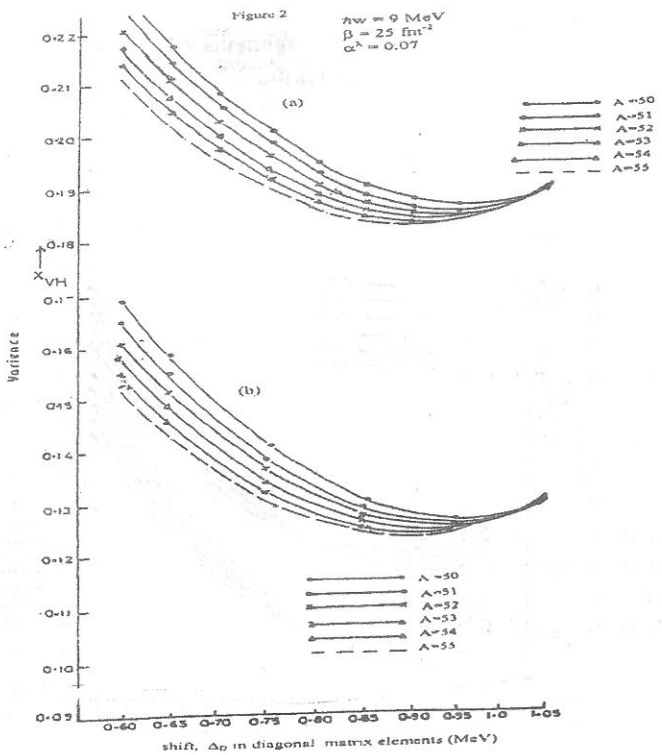


Figure 2
ħw = 9 MeV
β = 2.5 fm⁻¹
α^λ = 0.07
(a)
(b)
A=50
A=51
A=52
A=53
A=54
A=55
X_VH
Variance
shift, Δp in diagonal matrix elements (MeV)

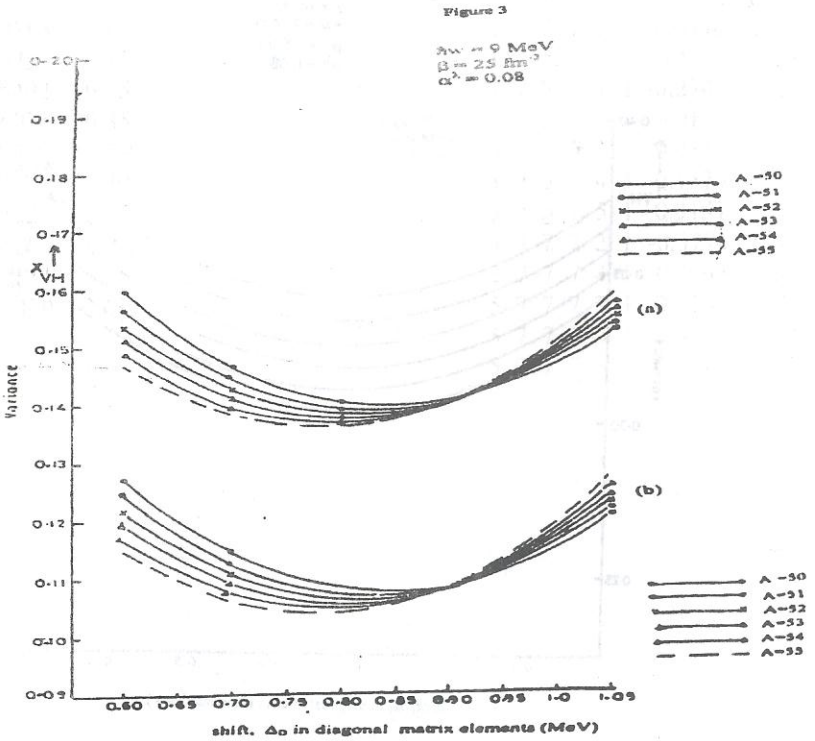


Figure 3
ħw = 9 MeV
β = 2.5 fm⁻¹
α^λ = 0.08
(a)
(b)
A=50
A=51
A=52
A=53
A=54
A=55
X_VH
Variance
shift, Δp in diagonal matrix elements (MeV)

Figure 4

$\hbar w = 9$ MeV
$\beta = 25$ fm^{-2}
$\alpha^{\lambda} = 0.09$

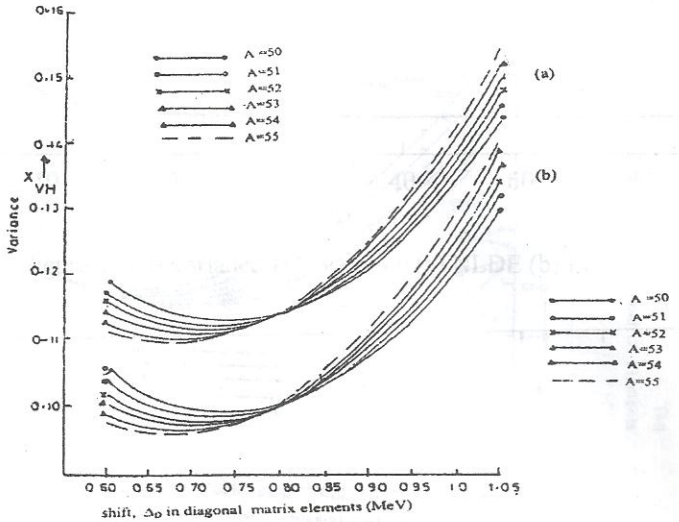


Figure (5)
$\hbar w = 9$ MeV
$\beta = 25$ fm^{-2}
$\alpha^{\lambda} = 0.08$

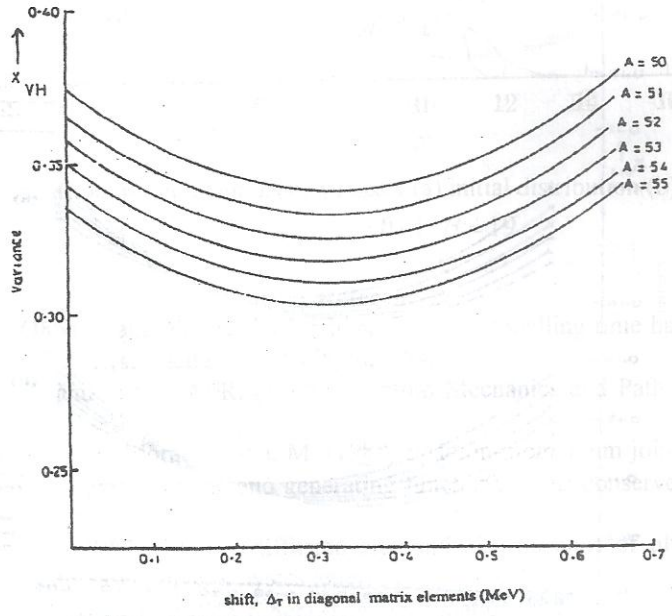
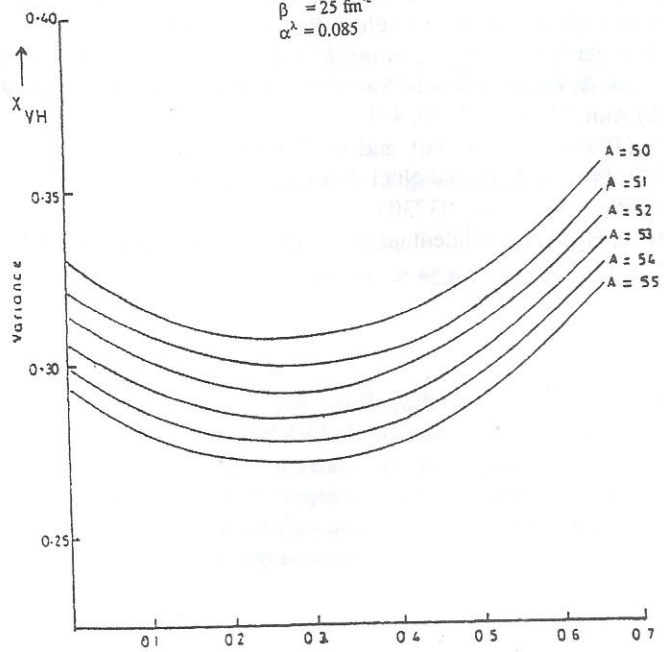
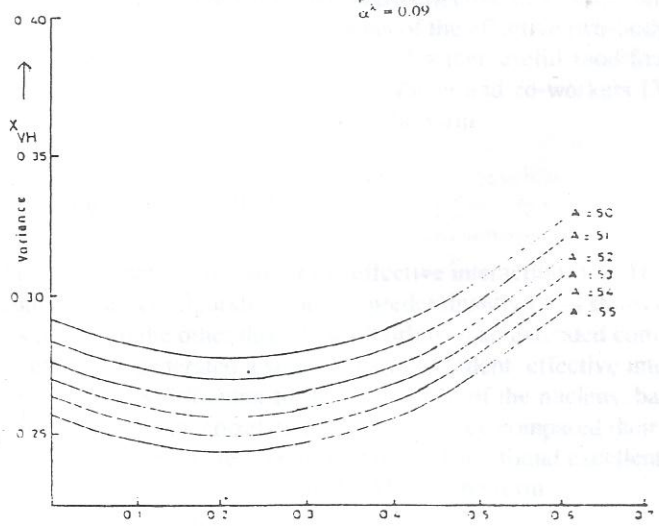


Figure (6)
$\hbar w = 9$ MeV
$\beta = 25$ fm^{-2}
$\alpha^{\lambda} = 0.085$



shift, Δ_T in diagonal matrix elements (MeV)

Figure (7)
$\hbar w = 9$ MeV
$\beta = 25$ fm^{-2}
$\alpha^{\lambda} = 0.09$



shift, Δ_T in diagonal matrix elements (MeV)

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