FR7800345

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Abstract

This paper is divided into two main parts. In the first part we point out that the Hartree-Fock (HF) calculations of the Coulomb displacement (CD) energies miss an important correction term. In the standard HF approach the difference between the neutron and proton densities is replaced by the excess neutron density while the difference between the core neutron and proton densities is neglected in calculating the CD energy. We evaluate the correction due to the core and find that it increases the CD energies by about 2.5 to 4.5 % for the various nuclei considered. We discuss the significance of this correction and of other higher order Coulomb terms, and point out that these are not treated consistently in the existing calculations of CD energies. In the second part of this work we present a new approach to the CD energies. The position of the isobaric analog resonances is calculated using the HF-TDA theory with a complete proton particle-neutron hole basis. The important feature of this approach is the fact that the HF potential and the particle-hole interaction used in the TDA are derived from the same two-body interaction. In this theory all the higher order effects are taken into account in one consistent framework. The calculations are performed for several $N > Z$, closed shell nuclei. For these nuclei good agreement between the experimental and theoretical CD energies is obtained.

1. INTRODUCTION

In the early stages of development of nuclear physics the binding energies of mirror nuclei were the only direct source of information concerning Coulomb displacement (CD) energies. The theoretical treatment of these was usually limited to a parametrization of a Coulomb term in a phenomenological mass equation [1], or alternatively classical models were used [2].

The discovery of isobaric analog resonances (IAR) in the sixties [3] and the large amount of very accurate measurements [4] of the IAR energies have prompted new, more ambitious and more sophisticated calculations of CD energies. The aim was to find in the framework of the shell model, nuclear wave functions of both protons and neutrons which correctly reproduced the CD energies. Usually the procedure was, first to parametrize proton and neutron one-body potentials which then generated the desired wave functions [4-6]. A requirement was added that the proton wave functions correctly reproduce the experimental charge distribution (or at least its radius) in the parent nucleus. The CD energy was usually calculated using first order perturbation theory and then various small corrections were added. These included among others magnetic terms [4-6], second order Coulomb terms [5-7], core polarization contributions [8-11], short range correlations [5,6] and other corrections [4-6]. Nonetheless, in spite of the detailed treatment a serious difficulty arose. The calculated CD energies were not compatible

with the charge distributions obtained from electron scattering data or μ-mesic atoms. In order to reproduce the CD energies one needed potential wells which led to too small charge radii, or conversely the wave functions which gave correct charge radii produced CD energies which were 6-8 % smaller than the experimental ones for all nuclei studied [4].

In the late sixties considerable progress was made in determining one-body nuclear wave functions starting from realistic nuclear interactions, the Hartree-Fock (HF) theory of the nucleus and the local density approximation (LDA) [12]. Later studies led to effective zero-range , density-dependent interactions of the Skyrme type [13] which when used in the HF calculations gave in essence the same results [14,15] as the HF-LDA theory. Thus, there was no longer the need to parametrize one-body potentials, these could be calculated using a two-body effective nucleon-nucleon interaction and the HF theory.

The above calculations reproduced correctly several one-body properties of the nucleus, including the charge radii of most nuclei. It seemed therefore that the HF theory should provide the most reliable calculations of the CD energies. The results of these calculations [16-18] however showed that the discrepancy found in the phenomenological calculations [4] existed also here. The calculated CD energies were too small by 6-8 % as compared with the measured ones. Because of this failure the possibility that a charge asymmetric nuclear force could contribute to the CD energies was suggested [16,17].

We would like to stress however that the HF calculations of the CD energies, especially for non-mirror nuclei

are not complete since they do not treat in a systematic and consistent way higher order Coulomb corrections. In fact the second order Coulomb corrections to the HF results in non-mirror nuclei have never been treated in a systematic manner using the determined HF wave functions. The higher order Coulomb corrections (such as the Thomas-Ehrman shift, isospin mixing, etc.) were taken from other types of calculations [5,6] which used a different basis and a different method.

We shall show in the first part of this paper that in order to achieve some degree of consistency one has to introduce a substantial correction which increases the CD energy. In the second part of this work we shall describe a method of calculation of the CD energy in which the starting point is the HF theory applied to the parent nucleus, but then when describing the IAR a new approach is used [19]. This method enables us to take into account higher order Coulomb corrections and core polarization terms in one consistent way free of problems of double counting.

2. HIGHER ORDER COULOMB TERMS IN HF CALCULATIONS OF CD ENERGIES

2.1 - Higher Order Coulomb Terms and the Role of the Core

In the analysis of experimental data the CD energy is taken as the difference between the energy of the parent state and the peak energy of the observed IAR. When the isobaric analog is bound it is the difference between the energy of the parent state and the physical analog state (as opposed to the theoretical analog state defined below in eq.(1)).

It is clear that a precise calculation of the CD energy is complicated since it requires the knowledge of the peak energy of a resonance. The use of a model state (such as in eq.(1) below) is not always sufficient. Nonetheless we shall start our considerations (as many theories of CD energies do) with the definition of a model state - the analog state

$$|A\rangle \equiv \frac{T_-|\pi\rangle}{\langle\pi|T_+T_-|\pi\rangle^{1/2}} \qquad (1)$$

where $T_-(T_+)$ is the isospin lowering (raising) operator and $|\pi\rangle$ is the parent state. The difference ΔE_A between the energy E_A of the analog state and that of the parent E_π is the starting point of the calculation of the CD energy and makes up the bulk part of it :

$$\Delta E_A \equiv E_A - E_\pi = \langle A|H|A\rangle - \langle \pi|H|\pi\rangle \qquad (2)$$

Using eq.(1) we rewrite eq.(2) in the form :

$$\Delta E_A = \frac{\langle \pi|T_+[H,T_-]|\pi\rangle}{\langle \pi|T_+T_-|\pi\rangle} \qquad (3)$$

This expression can be divided into two parts[6] :

$$\Delta E_A = \frac{\langle \pi|[T_+,[H,T_-]]|\pi\rangle}{\langle \pi|T_+T_-|\pi\rangle} + \frac{\langle \pi|[H,T_-]T_+|\pi\rangle}{\langle \pi|T_+T_-|\pi\rangle} \qquad (4)$$

The second term is zero for a state $|\pi\rangle$ which has a pure isospin quantum number. This term is at least of second order in the Coulomb interaction - V_C. The first Coulomb interaction comes from the commutator while the second one is implicit in the isospin admixture in $|\pi\rangle$. Numerical estimates of this term have been given in several papers (see, e.g., refs. 5-7,20). The contributions are negative and range from a few keV in lighter nuclei to approximately - 100 keV in the heavy ones. We shall not deal with this correction in the present section but concentrate on the first term in eq. (4). We denote it by $\tilde{\Delta E}_A$. Although this term is mainly of first order in the Coulomb interaction it also contains contributions of higher orders in V_C.

In the independent particle model, of which the HF approximation is a special case, the $\tilde{\Delta E}_A$ term can be written as [5-7,16-18] :

$$\tilde{\Delta E}_A = \frac{1}{\langle \pi|T_+T_-|\pi\rangle}\int [\rho_n(\vec{r})-\rho_p(\vec{r})]\frac{e^2}{|\vec{r}-\vec{r}'|}\rho_p(\vec{r}')d\vec{r}d\vec{r}' + \text{Exch.} \qquad (5)$$

where ρ_n and ρ_p are the local densities of neutrons and protons in the parent nucleus. From now on we assume that these densities come from a HF calculation. The symbol "Exch" denotes the exchange term, which for simplicity we shall neglect in our discussion (but not in the calculation). It is important to stress that in this formula :

a) the distributions ρ_n and ρ_p are calculated using the full HF Hamiltonian with the Coulomb interaction included and therefore higher order Coulomb terms are implicit ;

b) the difference $\rho_n - \rho_p$ refers to all the nucleons including the ones in the core and not merely the excess neutrons.

In the past when eq.(5) was applied to calculate CD energies from HF wave functions [16-18] one substituted for $\rho_n - \rho_p$ the distribution of the N-Z excess neutrons- ρ_{exc}. The contribution from the difference between the density of the Z neutrons in the core- $\rho_{n,core}$ and the proton density- ρ_p :

$$\Delta\rho \equiv \rho_{n,core} - \rho_p \qquad (6)$$

was neglected.

It can be argued that this difference is non-zero only when the Coulomb force is present*) and therefore the correction to $\tilde{\Delta E}_A$ from $\Delta\rho$ is a particular second order Coulomb term and should be treated in the same framework as all other second order corrections so as not to double count . To

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*This is not strictly true in the HF approximation for N≠Z nuclei since neutron and proton orbitals may differ because of the nuclear symmetry potential which acts as an isospin breaking term (see section 2.3 and Appendix).

answer this argument two points should be made ; first, the standard HF calculations never go beyond the calculation of eq.(5) with ρ_{exc} replacing $\rho_n - \rho_p$. Higher order terms are not calculated in the HF theories but are taken from other theories which use different sets of wave functions. Therefore consistency is not achieved. The second and even more important point is the fact that although $\Delta\rho$ is left out in the HF calculation of $\Delta\tilde{E}_A$ still the proton charge distribution ρ_p is obtained from a HF calculation in which the Coulomb interaction is present. The HF proton distribution ρ_p (the one that agrees so well with experiment) is the one which contains Coulomb effects to all orders. And so, by leaving out $\Delta\rho$ from the calculation of $\Delta\tilde{E}_A$ in eq.(5) one does not avoid having higher order Coulomb terms. The omission of $\Delta\rho$ in the evaluation of eq.(5) leads to an additional, and as we shall see numerically significant inconsistency in treating higher order Coulomb terms. It is therefore advantageous and more consistent to evaluate $\Delta\tilde{E}_A$ in eq.(5) with both ρ_p and ρ_n determined from a HF calculation in which the Coulomb potential is included. One should then keep in mind that the expression in eq.(5) is not of first order in the Coulomb interaction but contains some special type of higher order contributions.

One can expect that the inclusion of $\Delta\rho$ in the evaluation of $\Delta\tilde{E}_A$ will give larger CD energies. The effect of the Coulomb interaction on the densities is to expand the protons with respect to the neutrons. Therefore,for the core nucleons the neutrons have a smaller radius than the protons. Adding up $\Delta\rho$ to the excess neutrons leads to an effectively smaller excess neutron radius

and therefore a larger $\tilde{\Delta E}_A$. We shall return to these points in a more quantitative way in the next subsection.

2.2 - Calculations of the Core Correction

In this subsection we calculate eq.(5) using the full $\rho_n - \rho_p$ density and compare it with the case when only the excess neutron density ρ_{exc} is used for $\rho_n - \rho_p$.

We rewrite eq.(5) in the form :

$$\tilde{\Delta E}_A = \frac{1}{\beta}\int \rho_{exc}(\vec{r})\,\frac{e^2}{|\vec{r}-\vec{r}'|}\rho_p(\vec{r}')\,d\vec{r}d\vec{r}' + \frac{1}{\beta}\int \Delta\rho(\vec{r})\,\frac{e^2}{|\vec{r}-\vec{r}'|}\rho_p(\vec{r}')\,d\vec{r}d\vec{r}'$$

$$\equiv \tilde{\Delta E}_A^{exc} + \tilde{\Delta E}_A^{core} \qquad (7)$$

where

$$\beta \equiv \langle\pi|T_+T_-|\pi\rangle$$

The second term $\tilde{\Delta E}_A^{core}$ is the correction omitted in the various HF calculations of CD energies [16-18]. We shall refer to it as the core correction.

Our HF computations are performed using the Skyrme type [13] density dependent forces. Two versions are used, the SIII and SIV forces. Both fit quite well the charge distributions and in particular their radii. However, they are rather different in some of their properties. The SIV force leads to a much larger non-locality in the HF field than the SIII force and gives more deeply bound hole states. We use both forces in order to check whether our results depend on the detailed properties of the force. As we shall see most of the results do not depend

on these as long as the proton and neutron radii do not change much when the different interactions are used.

We first calculate the various mean square radii for the nuclei under consideration. These are shown in Table I for forces SIII and SIV.

The definitions are the following :

The r.m.s. radius of protons is

$$\langle r_p^2 \rangle^{1/2} \equiv \frac{1}{Z} \int r^2 \rho_p(\vec{r})\, d\vec{r} \qquad (8.a)$$

The r.m.s. radius of neutrons

$$\langle r_n^2 \rangle^{1/2} \equiv \frac{1}{N} \int r^2 \rho_n(\vec{r})\, d\vec{r} \qquad (8.b)$$

of the excess neutrons

$$\langle r_{exc}^2 \rangle^{1/2} \equiv \frac{1}{N-Z} \int r^2 \rho_{exc}(\vec{r})\, d\vec{r} \qquad (8.c)$$

and of the core neutrons

$$\langle r_{n,core}^2 \rangle^{1/2} \equiv \frac{1}{Z} \int r^2 \rho_{n,core}(\vec{r})\, d\vec{r} \qquad (8.d)$$

And finally we define the <u>modified</u> excess neutron r.m.s. radius $\langle \tilde{r}_{exc}^2 \rangle^{1/2}$ as :

$$\langle \tilde{r}_{exc}^2 \rangle^{1/2} \equiv \left(\frac{N\langle r_n^2 \rangle - Z\langle r_p^2 \rangle}{N-Z} \right)^{1/2} \qquad (8.e)$$

In the last column of Table I we show the experimental proton r.m.s. radii- $\langle r_p^2 \rangle^{1/2}_{exp}$ taken from ref.[21].

As expected the $\langle \tilde{r}_{exc}^2 \rangle^{1/2}$ radii are smaller than $\langle r_{exc}^2 \rangle^{1/2}$. The surprising fact is that the differences are that large, from 4 to 6 percent.

According to the empirical prescription [4] the corresponding change in the CD energies is minus one half of the change in the excess neutron radii, i.e.

$$\frac{\delta(\Delta\tilde{E}_A)}{\Delta\tilde{E}_A} \simeq -\frac{1}{2}\,\frac{\delta\langle r^2_{exc}\rangle^{1/2}}{\langle r^2_{exc}\rangle^{1/2}} \qquad (9)$$

From this rule we obtain a rough estimate that the $\Delta\tilde{E}_A^{core}$ correction will increase the CD energy by 2-3 %.

In Fig.1 we show the excess neutron density $\rho_{exc}(r)$ and the difference $\rho_n(r) - \rho_p(r)$ for ^{208}Pb. The difference between these two : $\Delta\rho = (\rho_n - \rho_p) - \rho_{exc}$, i.e. the excess neutron density in the core [8-11,16-18] is also shown.

The results of the calculations of $\Delta\tilde{E}_A$ once using $\rho_n - \rho_p$ and once ρ_{exc} are shown in the first and third column of Table II (the exchange term is not included in the above results and for the sake of simplicity in presentation and comparison we used $\langle\pi|T_+T_-|\pi\rangle \simeq N-Z$). We note that the increase in the CD energies due to $\Delta\rho$ is even larger than the estimate made above. The corrections range between 300 to 500 keV for the various nuclei considered. Relative to the total CD energy this amounts to about 2.5 to 4.5 % of correction. We stress that this is one of the largest single correction terms considered and was not taken into account in previous evaluations of CD energies.

In column two of Table II are presented results of a calculation of the quantity

$$\Delta\tilde{E}^{\circ}_A \equiv \frac{1}{N-Z}\int [\rho^{\circ}_n(\vec{r}) - \rho^{\circ}_p(\vec{r})]\,\frac{e^2}{|\vec{r}-\vec{r}'|}\,\rho^{\circ}_p(\vec{r}')d\vec{r}\,d\vec{r}' \qquad (10)$$

where ρ_n° and ρ_p° are densities obtained in a HF calculation in which the Coulomb interaction is switched-off. The expression in eq.(11) is a truly first order Coulomb term. It is interesting to note that $\tilde{\Delta E}_A$ and $\tilde{\Delta E}_A^\circ$ are numerically very close. This means that when $\tilde{\Delta E}_A$ is treated consistently (i.e. $\tilde{\Delta E}_A^{core}$ included) it is numerically close to a first order Coulomb term and therefore one can in principle proceed with the evaluation of higher order terms avoiding double counting.

2.3 - Discussion and Summary of Section 2

In this subsection we shall add several comments concerning the HF calculations of CD energies and summarize the results of section 2.

Spurious isospin mixing. A severe limitation of any HF calculation in $N > Z$ nuclei is the appearance of spurious isospin mixing. Even when the Coulomb force (or any charge dependent part of the Hamiltonian) is put to zero the HF ground state for $N > Z$ nuclei does not have pure isospin, i.e. even when $[H,\vec{T}] = 0$ the HF approximation introduces non-physical isospin mixing. The N-Z excess neutrons produce a symmetry potential which in the framework of the HF theory becomes a charge symmetry violating potential since only the $t_z T_z$ component and not the full $\vec{t}.\vec{T}$ product appear in the calculation. (The symbol $\vec{t}$ denotes the isospin operator of a single nucleon and $\vec{T}$ of the entire nucleus). The spurious isospin mixing is a hampering factor in all HF calculations in $N > Z$ nuclei. Also in the present calculation the spurious isospin

mixing is present and leads to some approximations. We believe however that the uncertainties are not large and the main conclusions still hold.

We estimated the amount of spurious isospin mixing in our calculations by evaluating the expression :

$$\varepsilon_0^2 \equiv \frac{\langle \phi^o_{HF} | T_+ T_- | \phi^o_{HF} \rangle - (N-Z)}{N - Z + 2} \qquad (11)$$

where ϕ^o_{HF} is the HF ground state of the parent nucleus calculated for the case when the Coulomb interaction is switched off ($V_c = 0$) and comparing it with the case when V_c is taken into account. We found that ε_0^2 for $V_c = 0$ was small, not exceeding 0.15 % for the SIV interaction and smaller than 0.5 % for the SIII force. For both interactions and especially for the SIV force the values of ε_0^2 were much smaller than ε^2 evaluated for the case when V_c is not suppressed. We shall return to the problem of spurious isospin mixing and its effect on the CD energy also in section 3. In the Appendix a more detailed discussion of this problem is presented.

The second order Coulomb corrections . As already discussed the second order correction terms added to the HF calculations in order that the theoretical results could be compared with the experimental ones, were not evaluated using the same set of wave functions as the lower order term.

The higher order terms of the CD energies are given [6,7,20] schematically by :

$$\Delta_c = \frac{1}{2T} \langle \pi | V_c^{(+)} \frac{Q}{QHQ - E_A} V_c^{(-)} | \pi \rangle \qquad (12)$$

where Q is a projection operator which projects onto all states except the analog i.e. $Q = 1 - |A\rangle\langle A|$ and $V_c^{(\pm)} \equiv [H, T_\pm]$. In practical evaluations of Δ_c it is necessary to choose a set of intermediate states orthogonal to $|A\rangle$ and the value of Δ_c depends on that choice. Calculations [5,6] of Δ_c were performed using parent wave functions calculated with the aid of phenomenological potentials. The intermediate states were then chosen to be orthogonal to the analog state in use. Since the structure of the parent in the HF calculations is somewhat different from the one obtained from a phenomenological shell-model potential it is clear that the addition of a Δ_c term calculated in the shell-model to the HF lowest order result is a rather crude approximation and leads to a lack of consistency. The same arguments apply to the second term in eq.(4) - the isospin mixing term. This term has been estimated only in the framework of a shell-model [5-7,20] and not in the HF calculations.

Summary. We have stressed in this section that the treatment of higher order terms in the HF calculations of CD energies is not satisfactory. We have found a rather large correction which is of higher order in V_c but which has to be treated in the framework of eq.(7) in order to achieve consistency. This correction increases the CD energy.

In a recent paper [22] it was suggested that the discrepancy in the CD energies is due to the compression of the proton core when a neutron is transformed into a proton in

going from the parent to the analog, and the neglect of this effect is somehow connected to the approximation $\rho_n - \rho_p \simeq \rho_{exc}$. The authors of ref.[22] say that the existence of the discrepancy in the CD energies indicates that the HF calculations are inadequate and require the introduction of an additional attractive neutron-proton interaction. We would like to emphasize that the large correction $\Delta\tilde{E}_A^{core}$ we found does not invalidate the HF calculation itself but only the subsequent treatment of the CD energy. In fact the correction $\Delta\tilde{E}_A^{core}$ is calculated from the present HF densities and this correction is a result of a consistent treatment of CD energies and not a consequence of using some additional interaction.

In order to have a more complete treatment of higher order Coulomb terms and core polarization effects [8-11] in the CD energies it is necessary to go beyond the HF approximation and extend the method of calculation. In the next part of this work we deal with such an extension which provides a more systematic and consistent treatment of higher order effects and which we believe gives better results for CD energies.

3. THE PROTON PARTICLE - NEUTRON HOLE SCHEME

3.1 - Introduction to Section 3

Attempts [23,24] were made in the past to describe the analog state starting from a basis which consisted of one particle-one hole (1p-1h) excitations in which the particle is a proton and the hole is in the neutrons. The work in the past delt with 1p-1h states in which the particle occupied only orbits which correspond to the orbits of the excess neutrons. In this space the residual T = 1 particle-hole interaction - V_{ph} was diagonalized. One of the resulting eigenstates had a large overlap with the analog state in eq.(1). The rest were the so called configuration states. The above calculations could not determine the basic properties of the analog, such as for example its width, and failed badly in reproducing the excitation energy of the analog. There are two main reasons for these limitations. First, the space used in the above calculations was too small and did not include such important parts as the particle continuum and therefore was not able to reproduce widths. Secondly the calculations did not fulfil a consistency requirement [25] that the single-particle energies and the residual particle-hole matrix elements derive from the same force. This consistency requirement is very important in the calculation of the position of the analog i.e. in the calculation of the CD energy [19,25].

In a recent paper [19] the proton particle-neutron hole (pn^{-1}) formalism was extended so that it avoids the limitations and difficulties discussed above. In this theory the starting

point consists of a HF ground state which is assumed to provide an adequate description of the parent state - $|\pi\rangle$. The space includes all proton-particle and all neutron-hole HF states, their energies being measured relative to the energy of the HF ground state in the parent nucleus with (N,Z). The excitations in the analog nucleus (N-1,Z+1) are described by all the possible proton particle-neutron hole configurations allowed by the exclusion principle. Since only the isovector excitations are of interest in this work and we deal only with closed shell parent nuclei the particle and hole are coupled to isospin one (T =1) and angular momentum zero ($J=0^+$). In the above space the particle-hole spectrum is calculated using the particle-hole residual interaction derived from the same interaction which enters into the HF potential. The completeness of the particle space insures that the proton continuum is properly accounted for in the calculation and that the collective effects coming from the giant isovector monopole [6-11,18-20] resonance are included.

All these advantageous features of the calculation could not be achieved without the important progress made in the development of an effective nucleon-nucleon interaction which has a zero range and a density dependence and which gives very good results in the HF calculations[14,15]. With this type of a force the residual particle-hole interaction is given by the functional derivative [26,27] of the HF Hamiltonian H_o with respect to the density - $\frac{\partial H_o}{\partial \rho}$. Furthermore the fact that the force is of zero range enables one to calculate the particle-hole (p-h) spectrum using the Green's function method [26,27] for the TDA or

RPA. This method was used recently with considerable success to study giant excitations in nuclei [26-29]. It turns out that the same method is very efficient for our purpose [19] of calculating the position of the IAR in the HF-TDA approach.

3.2 - A Brief Description of the Method

The full p-h Green's function is calculated from the integral equation [26-29] :

$$G(\omega) = G^{(o)}(\omega) + G(\omega)\ V_{ph}\ G^{(o)}(\omega) \qquad (13)$$

where V_{ph} is the antisymmetrized p-h interaction and $G^{(o)}(\omega)$ is the unperturbed p-h Green's function which in the TDA is given by :

$$G^{(o)}(\vec{r},\vec{r}';\omega) = \sum_h \varphi_h^*(\vec{r})\left[\langle\vec{r}|\frac{1}{H_o-\varepsilon_h-\omega-i\eta}|\vec{r}'\rangle - \sum_{h'}\frac{\varphi_{h'}(\vec{r})\varphi_{h'}^*(\vec{r}')}{\varepsilon_{h'}-\varepsilon_h-\omega-i\eta}\right]\varphi_h(\vec{r}') \qquad (14)$$

where the HF Hamiltonian for protons is denoted by H_o. The summation index h runs over the hole (i.e. neutron occupied) states while h' runs over the proton occupied states. The single-particle Green's function $\langle\vec{r}|\frac{1}{H_o-z-i\eta}|\vec{r}'\rangle$ can be written in a closed form in terms of regular v(r) and irregular w(r) solutions of H_o if H_o is local or if the non-locality is described by an effective mass [28,29]. The radial part of the single-particle Green's function is then proportional to :

$$\langle r|\frac{1}{H_o - z - i\eta}|r'\rangle \sim \frac{v(r_<)w(r_>)}{W(v,w)} \qquad (15)$$

where W is the Wronskian of the two solutions and $r_<$, $r_>$ are

respectively the smaller or larger of r and r'.

For a zero range p-h interaction eq. (13) can be solved exactly in coordinate space. In order to "probe" the calculated Green's function and to determine the distribution of strengtn of a one-body operator Q and hence the excitation spectrum, one calculates the strength distribution $S(\omega)$ which is simply related to the p-h Green's function by [26-30] :

$$S(\omega) \equiv \sum_n |\langle 0|Q|n\rangle|^2 \, \delta(\omega-\omega_n)$$

$$= \frac{1}{\pi} \, \mathrm{Im} \int Q^+(\vec{r}) G(\vec{r},\vec{r}';\omega) Q(\vec{r}') d\vec{r} \, d\vec{r}' \qquad (16)$$

The choice of the operator Q is guided by our interest in the particular physical property. It is obvious that in the case of analog excitations the appropriate operator [19] to probe the Green's function is T_-. In coordinate space representation :

$$T_- \equiv \sum_i t_-^{(i)} = \int p^+(\vec{r}) n(\vec{r}) d\vec{r} \qquad (17)$$

where $p^+(\vec{r})$ $(n(\vec{r}))$ creates a proton (destroys a neutron) at point $\vec{r}$. Another operator useful in our study is the isovector monopole [7,19,20] operator whose $T_z = -1$ component is :

$$M_- = \sum_i r_i^2 \, t_-^{(i)} \qquad (18)$$

With the aid of the above two operators we can "probe" the TDA pn^{-1} Green's function.

3.3 - Results of the HF-TDA Calculation in pn^{-1} Space

As in section 2 we emplcyed the two Skyrme forces SIII and SIV. They were used of course in both the HF calculations

and the calculations of the p-h Green's function. As a typical example of our results we show in Fig. 2 the spectrum obtained with the SIII force for the $J = 0^+$, $T = 1$ excitations in ^{48}Sc the analog of ^{48}Ca. We probed the Green's function first with T_-. The lower energy part of the spectrum shows one distinct peak which in general is the isobaric analog resonance while in the case of ^{48}Ca the analog is bound and therefore what we see is the physical analog state which is different from the ideal analog state as defined in eq.(1). The state (or resonance) exhausts nearly all the T_- strength[19]. The position of the state relative to the energy of the parent is the CD energy. Since the calculation is exact within the TDA scheme, the effects of core polarization [8-11] or higher order Coulomb correction [5-7,20] are already contained. The exchange part of the Coulomb energy as well as other small corrections are not included yet and have to be added to the TDA results.

The structure seen at higher energies is the distribution of the isovector monopole strength M_-. The broad peak is identified with the isovector monopole resonance. This resonance plays an important role in many Coulomb effects as was discussed extensively in the literature [5-11,19,20]. It is worthwhile to point out here that the influence of the isovector monopole state on the analog state (the one of eq.(1)) is inherent in the present approach, and the position of the physical analog state which results from our calculation contains already the shift due to the coupling to the isovector monopole state (of course this last statement is already contained in the previous statement that higher order Coulomb and core polarization

corrections are implicit in the HF-TDA result).

The same type of calculations as for ^{48}Ca were performed for several closed shell nuclei in different regions of the periodic table. For these nuclei in which the result is an analog resonance we took the position of the peak of the resonance as the CD energy. This corresponds to the experimental definition of the CD energy.

In the present TDA calculation there is the computational problem of correctly taking into account the Pauli principle. The first term of eq.(14) is calculated in a closed form while the sum in the second term is computed term by term. Because of the different treatment of the two terms, the poles not allowed by the Pauli principle in the first term might not be exactly cancelled by the second term of eq.(14). This could lead to spurious poles and misleading results. We have therefore taken special care to insure that no unwanted pole is present in the calculation.

A more serious limitation is again, as in section 2, the spurious isospin mixing in the HF state. This limitation cannot be avoided in the framework of the theory we deal with. Also, as discussed in detail in the Appendix, the use of the RPA instead of the TDA or RPA like scheme suggested in the literature [31] does not solve the problem.

In the present work we are actually only interested in establishing some procedure which will give us a reasonable estimate of the shift caused by the spurious isospin mixing. The way we proceeded was to repeat in each case the entire HF-TDA computation with the Coulomb force put to zero in the HF part of the calculation. If there is no spurious isospin mixing

then the resulting lowest state must be degenerated with the parent state, i.e. appear at zero excitation energy. This state should coincide with the ideal analog in eq.(1), where $|\pi>$ is the HF parent state obtained in the $V_c \equiv 0$ calculation. Any deviation from E = 0 is due to non-physical isospin mixing caused by the approximations in the HF theory.

It is quite remarkable that the spurious shifts we found in our calculation turned out to be very small compared to the total CD energy. For the SIV force the position of the analog for the case $V_c \equiv 0$ was usually around 100-200 keV and only for ^{48}Ca was it larger, about 350 keV. For the SIII force which causes larger spuriosity as already mentioned in section 2, the shifts were slightly larger. For ^{48}Ca and ^{208}Pb the SIII force gave about 400 keV deviation from E = 0 and in other cases less than 250 keV. Once the above shifts (for $V_c \equiv 0$) were determined we used two procedures to estimate the CD energy free of the spurious shift. (1) We simply subtracted the calculated spurious shifts for $V_c \equiv 0$ from the results obtained in the full calculation in which the Coulomb interaction is not suppressed. (2) Or, we renormalized slightly the interaction V_{ph} so that the spurious shift for $V_c \equiv 0$ is exactly zero. With the renormalized V_{ph} the full TDA calculation of the CD energy is then performed. It turned out that the two procedures gave practically identical results. The results for the CD energies we present here were obtained using method (1) for the removal of the spurious shift.

In column one of table III the HF-TDA results (E_{TDA}) are shown. These contain the correction for the finite size of

of the protons and the above correction due to spurious isospin mixing. They do not include the exchange term or other small size corrections discussed extensively in the literature [4-6,16]. The sum of all the small corrections is shown in column two of table III. The sum is composed of the exchange, magnetic [4-6], vacuum polarization [6] , dynamic proton-neutron mass difference [4-6] and short range correlation [5,6] corrections. These were taken from the work already published [4-6]. We have postulated the existence of a charge-dependent force and estimated its contribution using the approximation of refs. 5 and 6 :

$$\Delta E_A^{cd} = - 750 \frac{N - Z}{A} \text{ keV} \qquad (19)$$

where we assumed a 3 % charge-dependent force. The correction ΔE_A^{cd} is contained in the sum making up the numbers of column two. We assumed that there is no charge asymmetric nuclear force[6,16,17]. As already emphasized the higher order Coulomb terms such as the Thomas-Ehrman shift, shift due to isospin mixing [5,6,20] and core polarization [8-11] to all orders in the Coulomb and strong forces are all contained in the values given in column one of table III. The final theoretical CD energies E_{CD} (sum of columns one and two) are given in column three and are compared to the experimental CD energies (column four). In the last column we show the differences between the experimental and theoretical CD energies (The CD energy of ^{140}Ce is not known experimentally). We see that the deviations between the measured and calculated CD energies are small, less than 2 %. The deviations are not systematic ; the calculated CD energy in ^{48}Ca is smaller than the experimental one while in ^{208}Pb the situation is reversed.

3.4 - Discussion and Summary of Section 3

The results of the previous subsection indicate that the calculated CD energies for non-mirror nuclei are in agreement with the measured ones and it seems that there is no need to invoke [16,17] a charge asymmetric nuclear force in order to achieve this. This is the case for both the SIII and SIV forces. We emphasize that the charge radii obtained in the HF calculation using the above two forces are in reasonable agreement with experiment (see table I) and the values of the excess neutron radii $\langle r^2_{exc} \rangle^{1/2}$ are considerably larger than the values required to fit the CD energies in the phenomenological calculations [4,5] (Of course, as shown in section 2, the inclusion of the core leads to an effective radius $\langle \tilde{r}^2_{exc} \rangle^{1/2}$ substantially smaller than $\langle r^2_{exc} \rangle^{1/2}$).

Why is it that the present calculation does explain the CD energy for non-mirror nuclei while the previous HF calculations [17] produced CD energies too small as compared with experiment ? It is difficult to pin-point one main single factor. There are most probably several reasons that cause the substantial differences between our HF-TDA an.. the older HF calculations. As discussed in section 2 the HF calculations do not include the $\Delta\tilde{E}^{core}_A$ while the present calculation does include it. This is a rather large positive correction which increases the CD energy. We feel that the other second order Coulomb corrections used in the previous HF calculations had too large negative values (for example [6] - 600 keV in ^{208}Pb). In a separate calculation [32] we estimated these to be about one-half of the values used previously, and since this correction is

negative the CD energy is larger than previously estimated. It is also conceivable that some core polarization included in our theory and not contained in the other calculations increases somewhat the CD energies. Whatever the reasons are the important point is that the present scheme of the consistent HF-TDA furnishes an extended and more advanced treatment of the CD energies than the previous HF calculations did.

The present method of calculation is limited to closed shell nuclei and the extension to odd-even systems is not straightforward and requires additional approximations. Therefore it cannot be applied to pairs of mirror nuclei such as ^{41}Sc-^{41}Ca without introducing substantial uncertainties in the calculation of the CD energy. We believe however that the present results for non-mirror nuclei indicate that an appropriate extension of this theory to mirror nuclei will reduce considerably, if not remove completely the discrepancy between the theoretical and experimental CD energies.

Acknowledgements

We wish to thank G.F. Bertsch, O. Bohigas, A.M. Lane, S. Shlomo and M. Vénéroni for helpful discussions. One of us (N.A.) thanks R. Vinh Mau for his hospitality at the Division de Physique Théorique, Institut de Physique Nucléaire and the IN2P3 for financial support.

Appendix : Spurious Isospin Mixing in the HF Approximation and the RPA

We have seen that the weak point of our HF-TDA calculations or HF calculations in general is the appearance of spurious isospin mixing. The ground state in the HF approximation for nuclei with $N > Z$ does not have pure isospin even in the limit when all electromagnetic effects are suppressed. The loss of isospin invariance is a consequence of the HF approximation.

If $[H,T_-] = 0$ and $H|\alpha\rangle = E_\alpha|\alpha\rangle$ then $|\tilde{\alpha}\rangle \equiv T_-|\alpha\rangle/\langle\alpha|T_+T_-|\alpha\rangle^{1/2}$ is also a solution of H and degenerated with $|\alpha\rangle$. It is well known (see for example ref. 31) that the analog state $|A\rangle = T_-|\pi\rangle/\langle\pi|T_+T_-|\pi\rangle^{1/2}$ is not degenerated with $|\pi\rangle$ even when the Coulomb force is suppressed if $|\pi\rangle$ is calculated in the HF approximation.

One of the advantages of the RPA is its property of being able to restore invariances lost in the HF approximation. The correlations introduced by the RPA lead to degeneracies as required by the symmetries of the basic Hamiltonian. For instance, in the HF approximation the translational invariance is not obeyed and therefore the isoscalar (T=0) dipole state (which represents simply a translation of the entire nucleus) is not degenerated with the ground state. In the HF-RPA calculations the symmetry is restored and the isoscalar dipole state appears at zero energy [26,33]. It is important to note that this

nice property of the RPA exists only when the following two conditions are fulfilled : a) the HF single-particle states and the p-h interaction - V_{ph} are generated by the same two-body force b) the particle-hole space is complete. We shall discuss the question of symmetry breaking and the role of the RPA in restoring it by using sum rules.

Let P and Q be one-body operators. Then :

$$\langle 0|[P,[H,Q]]|0\rangle = \sum_n (E_n-E_o)\{\langle 0|P|n\rangle\langle n|Q|0\rangle+\langle 0|Q|n\rangle\langle n|P|0\rangle\} \quad (A1)$$

where $|0\rangle$ and $|n\rangle$ are the exact ground and excited states of H, and E_o, E_n are the corresponding eigenvalues. For the special case of hermitian operators and for $P \equiv Q$ the above relation is reduced to :

$$\langle 0|[Q,[H,Q]]|0\rangle = 2 \sum_n (E_n-E_o)|\langle n|Q|0\rangle|^2 \quad (A2)$$

In the case of the consistent HF-RPA, i.e. the one obeying the conditions a and b, Thouless theorem [33] (see also ref. 34) leads to a similar sum rule :

$$\langle \Phi_{HF}|[P,[H,Q]]|\Phi_{HF}\rangle = \sum_n (E_n-E_o)_{RPA}\{\langle \tilde{0}|P|\tilde{n}\rangle\langle \tilde{n}|Q|\tilde{0}\rangle + \langle \tilde{0}|Q|\tilde{n}\rangle\langle \tilde{n}|P|\tilde{0}\rangle\} \quad (A3)$$

where Φ_{HF} is the HF ground state, $|\tilde{0}\rangle$ and $|\tilde{n}\rangle$ are the RPA ground and excited states and $(E_n-E_o)_{RPA}$ denotes the corresponding energy differences in the RPA. The sum n runs only over the physical eigenvalues $E_n > E_o$. The analog of

eq.(A.2) is :

$$\langle\Phi_{HF}|[Q,[H,Q]]|\Phi_{HF}\rangle = 2\sum_{n}(E_n-E_o)_{RPA}|\langle\tilde{n}|Q|\tilde{0}\rangle|^2 \qquad (A4)$$

From the above relations one notes that if $[H,Q] = 0$ then in order to satisfy the sum rule one must have $(E_n-E_o)_{RPA} = 0$ for all states $|\tilde{n}\rangle$ for which $\langle\tilde{n}|Q|\tilde{0}\rangle \neq 0$. This means that in the consistent HF-RPA scheme degeneracies appear which are due to the fact that the basic Hamiltonian H contains a symmetry. The above considerations hold for both isoscalar and isovector excitations in which charge is conserved , i.e. $\Delta T_z = 0$. What happens when the 1p-1h excitations are of the type pn^{-1} discussed in the present work, i.e. excitations in which $\Delta T_z \neq 0$?

Formally, one can define the RPA problem and set up the equations also for the $\Delta T_z \neq 0$ case. One must treat simultaneously $\Delta T_z = \pm 1$ excitations, which include both proton particle-neutron hole excitations in the nucleus with (N-1, Z+1) and the neutron particle-proton hole excitations in the nucleus with (N+1, Z-1)[35]. The corresponding operators are $p^{+}_{\bar{\alpha}}\, n_{\underline{a}}$ and $n^{+}_{\bar{a}}\, p_{\underline{\alpha}}$ where $p^{+}(p)$, $n^{+}(n)$ are the creation (annihilation) operators for protons and neutrons and $\bar{\alpha}(\bar{a})$, $\underline{\alpha}(\underline{a})$ are respectively the proton (neutron) unoccupied and occupied HF states. The RPA so defined describes small oscillations in which protons change into neutrons and vice versa. The correlated RPA ground state does not possess a definite number of protons or neutrons. Since the equations of such a scheme have the same formal structure as the usual RPA, seemingly one can apply the theorem of Thouless and rewrite eq.(A.3) for the two operators $P = T_+$ and $Q = T_-$. Using the property that $(T_{\pm})^{+} = T_{\mp}$ one obtains formally :

$$\langle\phi_{HF}|[T_+,[H,T_-]]|\phi_{HF}\rangle = \sum_n (E_n-E_o)_{RPA}\{|\langle\tilde{n}|T_-|\tilde{0}\rangle|^2 + |\langle\tilde{n}|T_+|\tilde{0}\rangle|^2\} \qquad (A5)$$

The first thing to note is that in the limit when $[H,T_-] = 0$ one of the solutions of the RPA is the analog state of eq.(1) with $|\tilde{0}\rangle$ being the parent and both the analog and the parent state having the same energy. Thus the solution of the above RPA does not contain spurious isospin mixing and there is no spurious CD energy shift. Moreover, we note that the left-hand side of equation (A.5) is $\Delta\tilde{E}_A$ of eq.(7) times N-2 and it seems as if it provides a better understanding of the relation between the HF-RPA solutions and the CD energy. For example assuming that the lowest RPA state is the isobaric analog resonance and noting that all terms in the sum of eq.(A.5) are positive*) one concludes that $\Delta\tilde{E}_A$ is the upper limit for the CD energy. (Note that we refer here to the energy of the IAR measured relative to the correlated RPA ground state).

Although all the above considerations are formally correct they are unfortunately not very useful since the present HF-RPA scheme breaks down for states which involve $\Delta T_z \neq 0$ excitations. The RPA describes small oscillations around a minimum. The standard HF approximation is based on a restricted variational principle which assumes charge conservation and describes a system with a fixed number of protons and neutrons and therefore the system is stable against particle-hole excitations in which the charge is conserved. In other words there is a substantial gap between occupied and unoccupied states and proton particle - proton hole or neutron particle - neutron hole

*) Note that the derivation of eq.(A5) contains the underlying assumption that all the eigenvalues $(E_n-E_0)_{RPA}$ are real [35].

excitation energies have to be at least of the order of $1\hbar\omega$ or $2\hbar\omega$, and the RPA may work. The situation is different when we consider pn^{-1} excitations. It is not clear whether the system described by the usual HF will be stable against p-h excitations in which a neutron is transformed into a proton. When an excess neutron is transformed into a proton and put in the corresponding orbit it is a zero $\hbar\omega$ excitation. When a neutron is transformed into a proton it looses some binding energy because of the Coulomb interaction, but then the symmetry energy partially and sometimes fully compensates this loss. As a result the HF ground state may be unstable against pn^{-1} excitations and the RPA may not be valid. In our numerical calculations with the SIII and SIV forces we found that the RPA for the $\Delta T_z = 0$ case worked well but for $\Delta T_z \neq 0$ it failed badly. Both the SIII and the SIV force give large symmetry potentials.

We should mention that there was an attempt [31] in the past to define an RPA-like set of equations for pn^{-1} excitations. Since these equations are not really the RPA ones many of the advantages of using the RPA are lost. For example Thouless theorem (eq.A.5) does not hold and there are other unpleasant peculiarities in the above scheme.

We have discussed at some length the rather futile HF-RPA method for pn^{-1} excitations. It was our aim to clarify this problem and to stress that the difficulty of spurious isospin mixing in HF is even more severe than thought. Also, we hope that a better understanding of the difficulties and their source will help to find possible ways of improvement.

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[35] We thank Dr. A.M. Lane for discussions and correspondence concerning this point.

Table Captions

Table I - Nuclear radii from the HF calculations. The radii in the upper line are obtained with the SIII force and the lower with SIV. In the last column are given the experimental proton radii. All the radii are in fm.

Table II - Calculated $\Delta\tilde{E}_A$, $\Delta\tilde{E}_A^0$ and $\Delta\tilde{E}_A^{exc}$ (for definitions see text) using the SIII or SIV forces. The exchange term is not included and $\langle\pi|T_+T_-|\pi\rangle = N-Z$ is used. The results are in MeV.

Table III - Experimental and calculated Coulomb displacement energies in ^{208}Pb. In column one are the eigenvalues E_{TDA} obtained from the HF-TDA calculation corrected for the shift due to spurious isospin mixing. In column two is given the sum of the exchange, magnetic, dynamic p-n mass difference, short range correlations, charge dependence of the nuclear force and vacuum polarization corrections. (The correction for the finite proton size is included in the numbers of column one). The numbers in column three are the sums of the values in column one and two and correspond to the final theoretical CD energies. In column four are given the experimental CD energies and in the last column the deviations. All numbers are in MeV.

- Table I -

Parent Nucleus		$\langle r_p^2 \rangle^{1/2}$	$\langle r_n^2 \rangle^{1/2}$	$\langle r_{exc}^2 \rangle^{1/2}$	$\langle r_{n,core}^2 \rangle^{1/2}$	$\langle \tilde{r}_{exc}^2 \rangle^{1/2}$	$\langle r_p^2 \rangle^{1/2}_{exp.}$
^{48}Ca	SIII	3.47	3.60	4.10	3.38	3.91	3.38
	SIV	3.43	3.60	4.16	3.34	3.98	
^{88}Sr	SIII	4.22	4.29	4.82	4.11	4.53	4.18
	SIV	4.17	4.28	4.88	4.07	4.60	
^{140}Ce	SIII	4.89	4.98	5.42	4.78	5.17	4.82
	SIV	4.84	4.97	5.52	4.73	5.27	
^{208}Pb	SIII	5.53	5.65	6.10	5.39	5.86	5.46
	SIV	5.46	5.65	6.23	5.32	5.98	

- Table II -

Parent Nucleus	$\tilde{\Delta E}_A$		$\tilde{\Delta E}_A^0$		$\tilde{\Delta E}_A^{exc}$	
	SIII	SIV	SIII	SIV	SIII	SIV
^{48}Ca	7.30	7.21	7.24	7.14	7.02	6.96
^{88}Sr	11.70	11.62	11.54	11.43	11.20	11.14
^{140}Ce	15.51	15.41	15.43	15.30	15.06	14.95
^{208}Pb	19.36	19.22	19.32	19.15	18.89	18.71

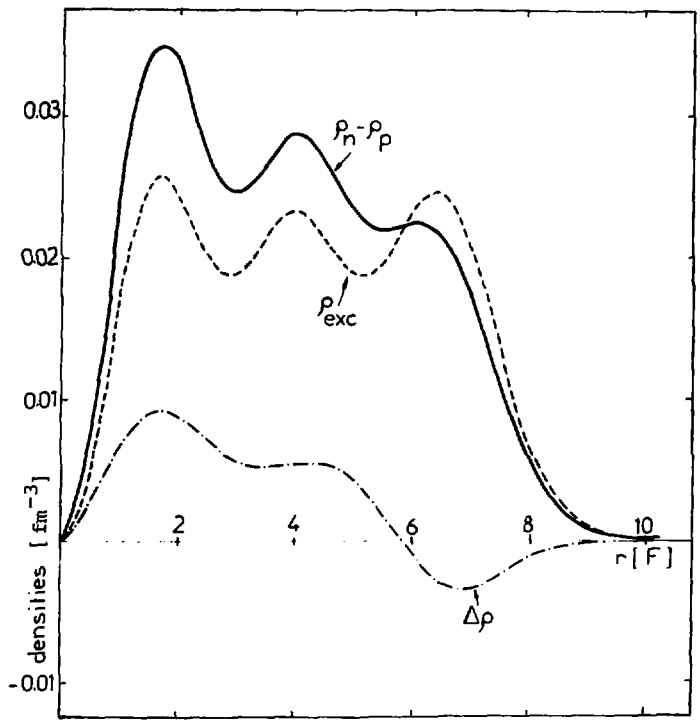
- Table III -

Parent Nucleus	E_{TDA} SIII	E_{TDA} SIV	$\Delta E_{corr.}$	E_{CD} SIII	E_{CD} SIV	E_{CD}^{exp}	$(E_{CD}^{exp} - E_{CD})$ SIII	$(E_{CD}^{exp} - E_{CD})$ SIV
^{48}Ca	7.35	7.26	-.25	7.10	7.01	7.17	.07	.16
^{88}Sr	11.62	11.51	-.25	11.37	11.26	11.45	.08	.19
^{140}Ce	15.58	15.44	-.31	15.27	15.13	-	-	-
^{208}Pb	19.50	19.35	-.33	19.17	19.02	18.83	-.34	-.19

Figure Captions

Figure 1 The densities $\rho_n-\rho_p$ (solid curve), ρ_{exc} (dashed curve) and $\Delta\rho=(\rho_n-\rho_p)-\rho_{exc}$ calculated in ^{208}Pb with the force SIV.

Figure 2 The distributions of the T_- strength (in dimensionless units, l.h.s. scale) and M_- strength (in fm^4 MeV^{-1}, r.h.s. scale) calculated in ^{48}Sc with the force SIII. The excitation energies are relative to the ^{48}Ca ground state. They include the correction for spurious isospin mixing as explained in the text.


0.03
0.02
0.01
densities [fm⁻³]
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2
4
6
8
10
r[F]
$\rho_n - \rho_p$
ρ_{exc}
$\Delta\rho$

Fig.1

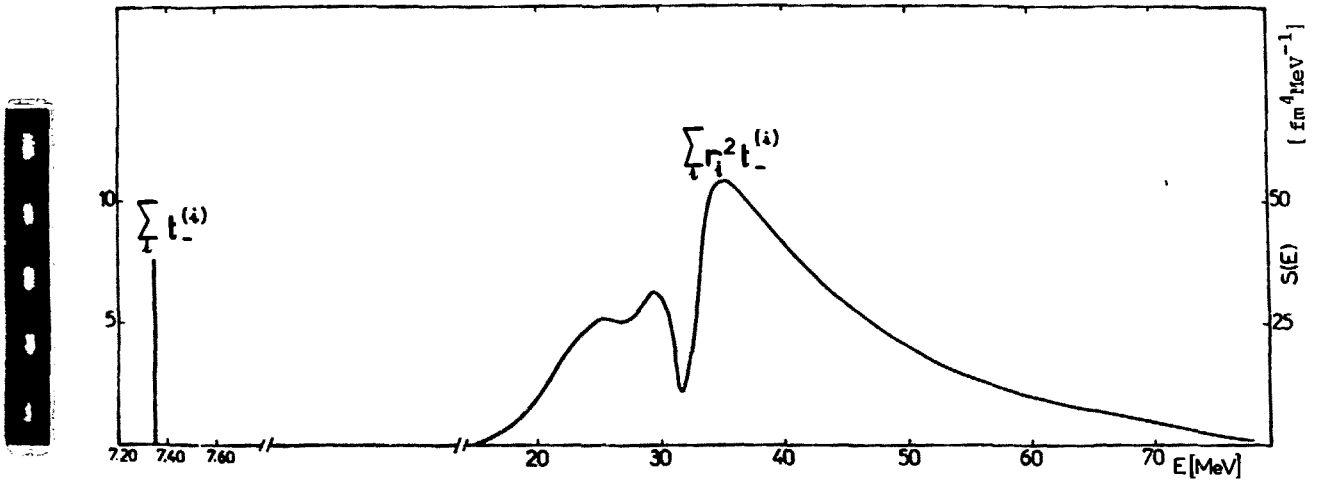
$\sum_i t_-^{(i)}$
$\sum_i r_i^2 t_-^{(i)}$
10
5
50
25
S(E) [fm^{4}MeV^{-1}]
7.20
7.40
7.60
20
30
40
50
60
70
E [MeV]

Fig.2