T = 0 FREE NUCLEON REACTION MATRIX AS A RESIDUAL INTERACTION IN FINITE NUCLEI

by

Hoong-Chien Lee

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Institute of Theoretical Physics
Department of Physics
McGill University
Montreal 2, Quebec

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ABSTRACT

The isotopic singlet S-wave free nucleon reaction matrix is used as the residual two-nucleon interaction to calculate the low energy spectra of F^{18} and Sc^{42}. The free reaction matrix is determined by the demand that it reproduces the triplet S-wave two-nucleon scattering data. The O^{16} and Ca^{40} cores are assumed to be inert. In the case of F^{18}, the splittings between the excited states and the ground state are generally too large as compared with the experimental spectrum. The possible origin of this discrepancy is discussed. In the case of Sc^{42} the calculated spectrum more closely resembles the experimental one.

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CHAPTER 1

INTRODUCTION

The nuclear shell-model was proposed by Mayer[1] and by Haxel, Jensen, and Suess[2] to explain a large number of measurements of nuclear spins and magnetic moments, and the "magic numbers." Nucleons in a nucleus were treated as single particles moving in an effective potential which represents the average effect on one nucleon of all the other nucleons. The spins and magnetic moments of the protons and the neutrons were assumed to pair off, respectively. In such a model the nuclei are composed of shells of nucleons, each shell consisting of a number of closely spaced levels. Between two major shells there is a sizable energy gap. A nucleus with all its shells filled has a magic mass number. Because of the pairing effect and the gap between shells a magic number nucleus is quite stable and a nucleus with one or two nucleons outside a closed shell has properties mainly due to the last unpaired loose nucleons. This is especially true when the "core" of the nucleus is doubly closed, that is, both the proton and the neutron numbers of the nucleus are magic numbers; for example, the nucleus F^{18} has one proton and one neutron outside a doubly closed core, the O^{16} nucleus.

If the existence of two extra nucleons does not change the structure of the core radically, then the potential in the Hamiltonian of the two-nucleon system is effectively the average single particle potential plus the residual interaction between the two nucleons. From the spectra of core plus one nucleon one can extract the needed information on the single particle potential. One is then interested in finding out what the residual interaction is.

In this respect one can do mainly two things. One can either do a phenomenological fit to the known nuclear data and thus determine the effective residual interaction, such as done by Elliot and Flowers[3], or one can use a realistic residual interaction. By realistic we mean the interaction is derived from free nucleon-nucleon interaction data. The latter of the two approaches is certainly more interesting in that it gives a unified picture of nuclear interaction whereas the effective interaction determined by the first method generally varies from nucleus to nucleus.

Dawson, Talmi, and Walecka[4], Kahana and Tomusiak[5], and more recently Kuo and Brown[6] used realistic interactions to calculate energy levels of nuclei with core plus two nucleons and the results were encouraging.

The purpose of this work is to investigate the validity of using the free nucleon reaction matrix as the residual interaction, in the cases of F^{18} and Sc^{42}.

The Hamiltonian of the core plus two-nucleon system is derived in Chapter 2 by means of exploring the properties of the one-particle and two-particl Green's functions. The nuclear reaction matrix K is then defined and its relation to the Hamiltonian established. In Chapter 3 the free nucleon reaction matrix K_F is defined and determined from two nucleon scattering data. It is then shown that K_F is a first order approximation of K, and one expects correction terms to be small. In Chapter 4 the single particle energies and the spectra of F^{18} and Sc^{42} are extracted from experimental data. Using K_F as the residual interaction in Chapter 5, the calculation of the energy levels of F^{18} and Sc^{42} are discussed and the results presented. The results are discussed in Chapter 6. In Chapter 7 our work is concluded.

CHAPTER 2

THE NUCLEAR REACTION MATRIX AND THE RELEVANT SCHROEDINGER EQUATION

2.1 The Derivation of the Schroedinger Equation

Our object is to calculate the zero isotopic spin, positive parity energy levels of F^{18} and Sc^{42}, both of which have two nucleons, a neutron and a proton, outside a doubly closed shell. To do this we have to solve the appropriate Schroedinger equation, which we derive by introducing the one- and two-particle Green's functions:

$$G_{\rho\sigma}(t_\rho - t_\sigma) = -i\langle N|T[a_\rho(t_\rho)\, a_\sigma^+(t_\sigma)]\,|N\rangle \tag{2-1}$$

$$G_{\rho\sigma,\mu\gamma}(t_\rho t_\sigma, t_\mu t_\gamma) = (-i)^2\langle N|T\,[a_\rho(t_\rho)\, a_\sigma(t_\sigma)\, a_\gamma^+(t_\gamma) a_\mu^+(t_\mu)]\,|N\rangle \tag{2-2}$$

Where $a_\sigma(t_\sigma)$ and $a_\sigma^+(t_\sigma)$ are the time dependent creation and annihilation operators respectively, for particles in states $(\sigma) \equiv n_\sigma, \ell_\sigma, m_\sigma, s_\sigma$ etc. $|N\rangle$ is the ground state of a doubly closed shell nucleus. T is the time ordering operator[7]. We shall assume that the one particle Green's function is well approximated by the single particle Green's function which describes the motion of particle in an effective one particle potential used in the Hartree-Fock* calculation to obtain the ground state $|N\rangle$. We denote the energy of a HF single particle state by ϵ_σ. Thus we have from (2-1)

*Hereafter abbreviated by HF

$$G_{\rho\sigma}(t_\rho - t_\sigma) \sim G^{(o)}_{\rho\sigma}(t_\rho - t_\sigma)$$

$$= -i \sum_{\alpha,\alpha'} \Big\{ \theta(t_\rho - t_\sigma) \langle N | a^{(o)}_\rho (t_\rho) | N+1,\alpha \rangle \langle N+1,\alpha | a^{(o)+}_\sigma (t_\sigma) | N \rangle$$

$$-\theta(t_\sigma - t_\rho) \langle N | a^{(o)+}_\sigma (t_\sigma) | N-1,\alpha' \rangle \langle N-1,\alpha' | a^{(o)}_\rho (t_\rho) | N \rangle \Big\} \qquad (2\text{-}3)$$

Where $$a^{(o)}_\rho (t_\rho) = e^{iH_o t_\rho} a_\rho e^{-iH_o t_\rho} \qquad (2\text{-}4)$$

and H_o is an effective single particle Hartree-Fock Hamiltonian,

$$H_o | N \rangle = E^o_N | N \rangle$$

$\theta(t)$ is the time step function,

$$\begin{aligned} \theta(t) &= 1, \quad t > 0 \\ &= 0, \quad t < 0 \end{aligned} \qquad (2\text{-}5)$$

a_ρ and a_ρ^+ are the time independent creation and annihilation operators, respectively, and have the following anticommutation relations,

$$[a_\rho , a_\sigma^+]_+ = \delta_{\rho\sigma}$$

$$[a_\rho^+ , a_\sigma^+]_+ = [a_\rho , a_\sigma]_+ = 0$$

The states $| N+1,\alpha \rangle$ and $| N-1,\alpha \rangle$ form complete sets of eigenstates of H_o with $N+1$ and $N-1$ particles, which we shall call the HF single-particle and single-hole states, respectively. Equation (2-3) now becomes

$$G_{\rho\sigma}(t) = -i\,\delta_{\rho\sigma}\left[(1-f_\rho)\theta(t)-f_\rho\,\theta(-t)\right]e^{-i\epsilon_\rho t} \tag{2-6}$$

where

$$f_\rho = 0, \quad \text{if } \rho \text{ is a particle state,}$$
$$= 1, \quad \text{if } \rho \text{ is a hole state.}$$

For the two-particle Green's function, since we are not going to consider any particle-hole states, the two creation operators and the two annihilation operators will always have the same time. So it is sufficient to consider only

$$G_{\rho\sigma,\mu\gamma}(t,t,0,0) \equiv G_{\rho\sigma,\mu\gamma}(t) \tag{2-7}$$

Making use of the relation

$$a_\rho(t)\,a_\sigma(t) = e^{iHt}\,a_\rho\,a_\sigma\,e^{-iHt}$$

and introducing a set of "two-particle" states $|N+2,\alpha\rangle$ and "two-hole" states $|N-2,\alpha\rangle$ into (2-2) we get

$$G_{\rho\sigma,\mu\gamma}(t) = (-i)^2 \sum_{\alpha,\alpha'} \Big\{ \theta(t)\,\langle N|\,a_\rho a_\sigma\,|N+2,\alpha\rangle\langle N+2,\alpha|\,a_\gamma^+ a_\mu^+\,|N\rangle$$
$$\times\; e^{-i(E^{\alpha}_{N+2} - E^{o}_{N})t} + \theta(-t)\,\langle N|\,a_\gamma^+\;a_\mu^+\,|N-2,\alpha'\rangle$$
$$\times\;\langle N-2,\alpha'|\,a_\rho a_\sigma\,|N\rangle\; e^{i(E^{\alpha'}_{N-2} - E^{o}_{N})t}\Big\}$$
$$\equiv\; \theta(t)\,G^{(+)}_{\rho\sigma,\mu\gamma}(t) + \theta(-t)\,G^{(-)}_{\rho\sigma,\mu\gamma}(t) \tag{2-8}$$

We have separated the Green's function into $G^{(+)}$, which propagates forward in time, and $G^{(-)}$, which propagates backward in time.

Now define the Fourier transformation

$$G(\omega) \equiv i \int d\, t\, e^{i\omega t}\, G(t) \tag{2-9}$$

and obtain

$$G_{\rho\sigma,\mu\gamma}(\omega) = \left[G^{(+)}_{\rho\sigma,\mu\gamma}(\omega) + G^{(-)}_{\rho\sigma,\mu\gamma}(\omega) \right] \tag{2-10}$$

where

$$G^{(+)}_{\rho\sigma,\mu\gamma}(\omega) = \sum_{\alpha} \frac{\langle N | a_\rho a_\sigma | N+2,\alpha \rangle \langle N+2,\alpha | a_\gamma^{+} a_\mu^{+} | N \rangle}{\omega - (E^{\alpha}_{N+2} - E^{o}_{N}) + i\epsilon} \tag{2-11a}$$

and

$$G^{(-)}_{\rho\sigma,\mu\gamma}(\omega) = \sum_{\alpha} \frac{\langle N | a_\gamma^{+} a_\mu^{+} | N-2,\alpha \rangle \langle N-2,\alpha | a_\rho a_\sigma | N \rangle}{\omega + (E^{\alpha}_{N-2} - E^{o}_{N}) - i\epsilon} \tag{2-11b}$$

The term $\epsilon = 0^{+}$ in the denominator is inserted to insure that $G^{(\pm)}(\omega)$ have the appropriate boundary conditions. As a result we see that $G^{(+)}_{\rho\sigma,\mu\gamma}(\omega)$ is analytic in the upper half ω-plane and has poles on the positive real axis which correspond to the differences $E^{\alpha}_{N+2} - E^{o}_{N}$, while $G^{(-)}_{\rho\sigma,\mu\gamma}(\omega)$ is analytic in the lower half ω-plane and has poles on the real axis corresponding to $E^{o}_{N} - E^{\alpha}_{N-2}$. We have now reduced the problem of calculating the energy levels of the $|N+2\rangle$ and $|N-2\rangle$

nucleon states to that of locating the poles of $G^{(+)}_{\rho\sigma,\mu\gamma}(\omega)$ and $G^{(-)}_{\rho\sigma,\mu\gamma}(\omega)$ respectively.

The two-particle Green's function we are interested in can be shown to satisfy an equation of the form

$$G_{\rho\sigma,\mu\gamma}(tt;00) = G_{\rho\mu}(t)\, G_{\sigma\gamma}(t) - G_{\rho\gamma}(t)\, G_{\sigma\mu}(t)$$

$$+ \sum_{\substack{\rho_1\sigma_1\\ \rho_2\sigma_2}} i \int dt_1 dt_2, dt_1' dt_2' \; G_{\rho\rho_1}(t-t_1)\, G_{\sigma\sigma_1}(t-t_1) I_{\rho_1\sigma_1,\rho_2\sigma_2}(t_1t_1',t_2t_2')$$

$$\times\; G_{\rho_2\sigma_2,\mu\gamma}(t_2t_2',00) \qquad (2\text{-}12)$$

Where $I_{\rho_1\sigma_1,\rho_2\sigma_2}(t_1t_1',t_2t_2')$ is an interaction operator, for which we shall make the simplifying assumption:

$$I_{\rho_1\sigma_1,\rho_2\sigma_2}(t_1t_1',t_2t_2') = v_{\rho_1\sigma_1,\rho_2\sigma_2}\delta(t_1-t_1')\,\delta(t_1-t_2)\,\delta(t_1-t_2') \qquad (2\text{-}13)$$

where $v\,(1,2)$ is a two-particle potential and

$$v_{\rho_1\sigma_1,\rho_2\sigma_2} = \langle \rho_1(1)\sigma_1(2) |\; v\,(1,2) |\; \rho_2(1)\,\sigma_2(2) \rangle$$

The numbers 1 and 2 in the brackets denote the spatial positions.

Substituting (2-13) into (2-12) we get

$$G_{\rho\sigma,\mu\gamma}(tt,00) = G_{\rho\sigma,\mu\gamma}(t)$$

$$= G_{\rho\mu}(t)\, G_{\sigma\gamma}(t) - G_{\rho\gamma}(t)\, G_{\sigma\mu}(t)$$

$$+ \sum_{\substack{\rho_1\sigma_1\\ \rho_2\sigma_2}} i \int dt'\, G_{\rho\rho_1}(t-t')\, G_{\sigma\sigma_1}(t-t')\, v_{\rho_1\sigma_1,\rho_2\sigma_2}\, G_{\rho_2\sigma_2,\mu\gamma}(t') \qquad (2\text{-}14)$$

If we again try to separate the forward going and backward going Green's function in time, we encounter some complication in dealing with the integral term. Consider the contribution from this integral to $G^{(+)}_{\rho\sigma,\mu\gamma}(t)$. We have two terms,

$$i\, v_{\rho_1\sigma_1,\rho_2\sigma_2} \int_0^t dt\, \theta(t-t')\delta_{\rho\rho_1}\delta_{\sigma\sigma_1}(1-f_\rho)(1-f_\sigma)\, e^{-i(\epsilon_\rho+\epsilon_\sigma)(t-t')}\, G^{(+)}_{\rho_2\sigma_2,\mu\gamma}(t') \tag{2-15a}$$

for $t' > 0$ and

$$i\, v_{\rho_1\sigma_1,\rho_2\sigma_2} \int_{-\infty}^{0} dt\, \theta(t-t')\delta_{\rho\rho_1}\delta_{\sigma\sigma_1}(1-f_\rho)(1-f_\sigma)\, e^{-i(\epsilon_\rho+\epsilon_\sigma)(t-t')}\, G^{(-)}_{\rho_2\sigma_2,\mu\gamma}(t') \tag{2-15b}$$

for $t' < 0$. A third term vanishes when the Fourier transformation is taken, so we shall drop it here.

It is obvious the Fourier transformation of (2-15a) is

$$\sum_{\rho_1\sigma_1} \frac{(1-f_\rho)(1-f_\sigma)}{\omega-\epsilon_\rho-\epsilon_\sigma+i\epsilon}\, v_{\rho\sigma,\rho_1\sigma_1}\, G^{(+)}_{\rho_1\sigma_1,\mu\gamma}(\omega) \tag{2-16}$$

The Fourier transformation of (2-15b)has, however, a different form as we can see by considering the boundary condition. It is not very hard to see that the Fourier transformation of (2-15b), to the first order approximation, is

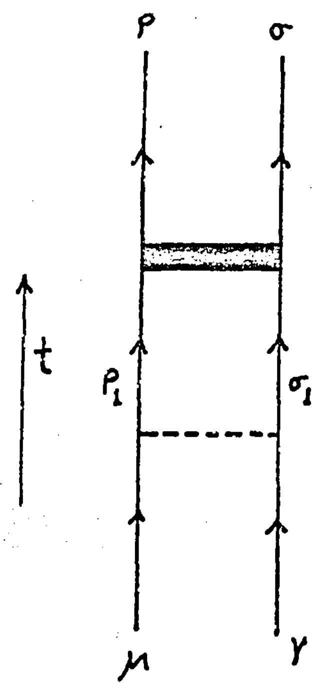

Fig. 2-1. Schematic diagram representing (2-16). Two particles μ and γ interact once and go into particle states ρ_1 and σ_1. These two particles interact any number of times and then go into final states ρ and σ. The dotted line represents an interaction $V_{\rho_1\sigma_1,\mu\gamma}$. The thick solid line with legs represents the two-particle Green's function $G^{(+)}_{\rho\sigma,\rho_1\sigma_1}(t)$.

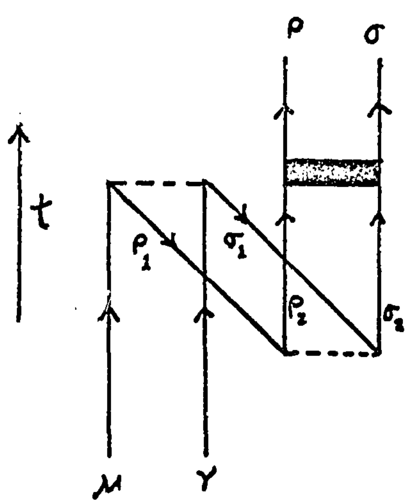

Fig. 2-2. Two particle-hole pairs $\rho_2\rho_1$ and $\sigma_2\sigma_1$ are created simultaneously. The two holes ρ_1 and σ_1 are then annihilated by the two particles μ and γ. The two particles ρ_2 and σ_2 continue to propagate forward in time, interact any number of times and finally go into two particle states ρ and σ. The exchange diagrams are not shown.

$$\sum_{\substack{\rho_1\sigma_1,\\ \rho_2\sigma_2}} \frac{(1-f_\rho)(1-f_\sigma)}{\omega-\epsilon_\rho-\epsilon_\sigma+i\epsilon}\, v_{\rho\sigma,\rho_1\sigma_1} \frac{f_{\rho_1} f_{\sigma_1}}{\omega-\epsilon_{\rho_1}-\epsilon_{\sigma_1}}$$

$$\times\; v_{\rho_1\sigma_1,\rho_2\sigma_2}\, G^{(+)}_{\rho_2\sigma_2,\mu\gamma}(\omega) \qquad (2\text{-}17)$$

Graphically (2-16) and (2-17) are represented by Figs. 2-1 and 2-2, respectively.

In our calculation the term in (2-17) will be ignored. The Fourier transformation of the forward going part of (2-14) then becomes

$$G^{(+)}_{\rho\sigma,\mu\gamma}(\omega) = \frac{(1-f_\rho)(1-f_\sigma)}{\omega-\epsilon_\rho-\epsilon_\sigma+i\epsilon}\Bigg(\delta_{\rho\mu}\,\delta_{\sigma\gamma} - \delta_{\rho\gamma}\,\delta_{\sigma\mu}$$

$$+ \sum_{\rho_1\sigma_1} v_{\rho\sigma,\rho_1\sigma_1}\, G^{(+)}_{\rho_1\sigma_1,\mu\gamma}(\omega)\Bigg) \qquad (2\text{-}18)$$

Graphically we have

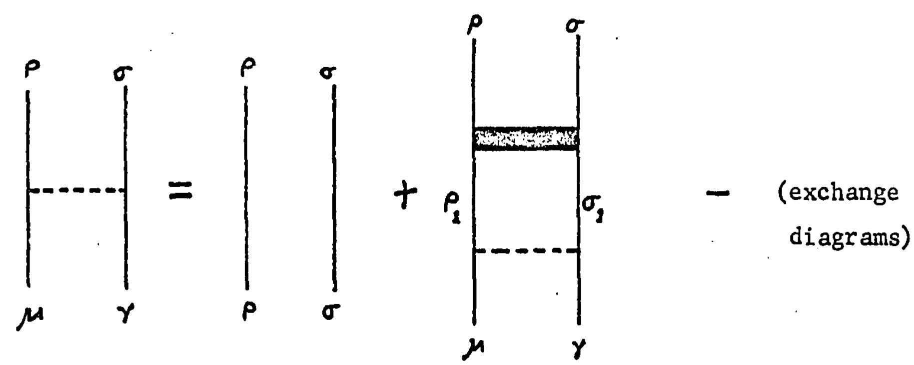

Fig. 2-3

In the approximation (2-18) the two-particle Green's function is the sum of all the so-called ladder-diagrams. It is also obvious in (2-18) that all subscripts have to denote particle states. The factor $(1-f_\rho)(1-f_\sigma)$ can thus be dropped.

Let us adopt the matrix notation,

$$\langle \rho\sigma | G^{(+)}(\omega) | \mu\gamma \rangle \equiv G^{(+)}_{\rho\sigma,\mu\gamma}(\omega) \tag{2-19}$$

$$\langle \rho\sigma | \mathbb{1} | \mu\gamma \rangle \equiv \delta_{\rho\mu}\,\delta_{\sigma\gamma} - \delta_{\rho\gamma}\,\delta_{\sigma\mu}$$

where $|\rho\sigma\rangle$ is the HF two-nucleon state, i.e.

$$H_o |\rho\sigma\rangle = (\epsilon_\rho + \epsilon_\sigma)|\rho\sigma\rangle \equiv \epsilon_{\rho\sigma}|\rho\sigma\rangle \tag{2-20}$$

Equation (2-18) can then be written as

$$G^{(+)}(\omega) = -i\left(\frac{1}{\omega - H_o - v}\right) \tag{2-21}$$

Suppose $|\alpha\rangle$ form a set of two-nucleon state in which H_o+v is diagonal, and are related with $|\rho\sigma\rangle$ by

$$|\rho\sigma\rangle = \sum_\alpha \chi_{\rho\sigma,\alpha} |\alpha\rangle \tag{2-22}$$

Then

$$\langle \rho\sigma | G^{(+)}(\omega) | \mu\gamma \rangle$$

$$= -i \sum_{\substack{\rho_1\sigma_1 \\ \alpha}} \langle \rho\sigma | \mathbb{1} | \rho_1\sigma_1 \rangle\, \chi^*_{\rho_1\sigma_1,\alpha}\, \chi_{\mu\gamma,\alpha} \langle \alpha | \frac{1}{\omega - H_o - v} | \alpha \rangle \tag{2-23}$$

The poles of $G^{(+)}(\omega)$ are at

$$\omega^{\alpha} = \langle \alpha | H_o + v | \alpha \rangle \qquad (2\text{-}24)$$

Where $|\alpha\rangle$ are the appropriate two-particle wave functions. Thus, the problem of locating the poles of $G^{(+)}(\omega)$ is further reduced to that of the diagonalization of $H_o + v$. We can also identify the state $|\alpha\rangle$ with $|N+2, \alpha\rangle$. Our object is now clear: to solve the Schroedinger equation

$$(H_o + v)|\alpha\rangle = \omega^{\alpha}|\alpha\rangle = (E^{\alpha}_{N+2} - E^{o}_{N})|\alpha\rangle \qquad (2\text{-}25)$$

with the eigenstates and eigenvalues of H_o known.

If the two-particle interaction v is well behaved, i.e., the matrix elements of v between the unperturbed two particle wave functions are small, then one can diagonalize $H_o + v$ in a finite dimensional subspace of unperturbed two-particle states with low unperturbed energies, since the high energy unperturbed states will not be affected by v. On the other hand, if the matrix elements of v are always comparable to the unperturbed energies, $H_o + v$ must then be diagonalized in the complete space of unperturbed wave functions. The matrix $H_o + v$ which enters the calculation then becomes infinite dimensional and cannot be diagonalized in practice.

Unfortunately, the realistic two-nucleon interaction is not well behaved. As we know two nucleons repel each other very strongly when they are at very close distances. In fact v must either have a hard core or be momentum dependent to fit the N-N free scattering data. In either case, the matrix elements of v will not be small compared to the unperturbed energies $\epsilon_{\rho\sigma}$. It is thus clear that one cannot diagonalize $H_o + v$ in a finite subspace, and we have to proceed otherwise to solve (2-25).

2.2 The Nuclear Reaction Matrix

Let us make the following two observations. (a) Since two nucleons interact strongly at short distances once they are sufficiently close to each other they will interact many times before they separate. (b) The total effect of this multiple-interaction is finite. It then follows that instead of using v we should use something which describes the multiple-scattering between two nucleons in our calculation. For this purpose let us define the nuclear reaction matrix K.

$$K(\omega) = v + v \frac{Q_M}{\omega - H_o} K(\omega) \tag{2-26}$$

Where Q_M is an operator which excludes from the two-nucleon intermediate states all occupied states and those states included in a subspace M, which we shall choose at our convenience. Graphically (2-26) describes the following processes.

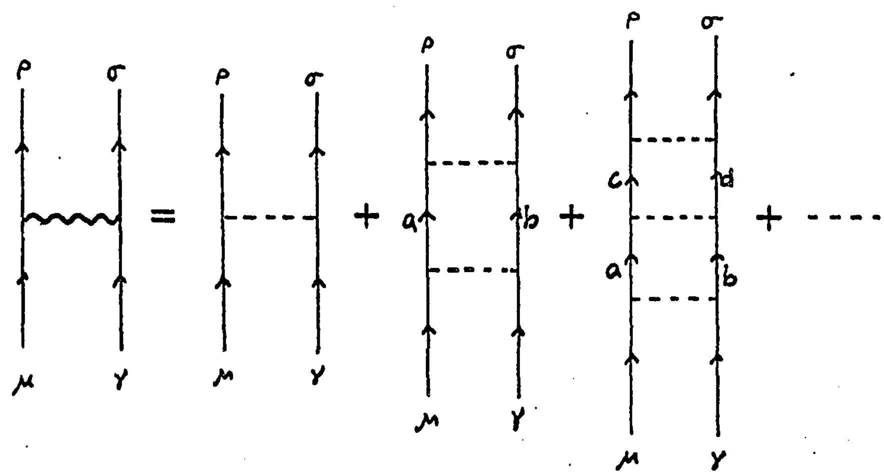

Fig. 2-4

Where the wavy line represents a K-interaction and the dotted line a v-interaction. ab and cd are two-particle intermediate states allowed by the operator Q_M. We have in the present formalism omitted all core excitations.

Let us also define the wave operator Ω_M and the model wave function $|\alpha, M\rangle$:

$$\Omega_M \equiv 1 + \frac{Q_M}{\omega - H_o} v \Omega_M \tag{2-27}$$

$$|\alpha\rangle \equiv \Omega_M |\alpha, M\rangle$$

$$= |\alpha, M\rangle + \frac{Q_M}{\omega - H_o} v |\alpha\rangle \tag{2-28}$$

Where $|\alpha\rangle$ is the actual two-particle wave function, i.e., the eigenfunction of (2-25).

From (2-26), (2-27) and (2-28), we have

$$K\ (\omega) \;=\; v\ \Omega_M \tag{2-29}$$

and

$$K\ (\omega)\ |\alpha, M\rangle \;=\; v\,|\alpha\rangle \tag{2-30}$$

In the following we shall show that the eigenvalues of $H_o + v$ when diagonalized in the complete space is the same as the eigenvalues of $H_o + K(\omega)$ when diagonalized in the subspace M. Let $x_{\rho\sigma}$ be the amplitude of $|\alpha\rangle$ in the unperturbed two particle state $|\rho\sigma\rangle$, then

$$|\alpha\rangle \;=\; \sum_{\rho\sigma}^{\infty} x_{\rho\sigma}\,|\rho\sigma\rangle \tag{2-31}$$

From (2-28) since Q_M excludes all states in M we can write

$$|\alpha\rangle \;=\; |\alpha, M\rangle \;+\; |\chi\rangle \tag{2-32}$$

where

$$|\alpha, M\rangle \;=\; \sum_{\rho\sigma\in M} x_{\rho\sigma}\,|\rho\sigma\rangle \tag{2-32a}$$

$$|\chi\rangle \;=\; \sum_{\rho\sigma\notin M} x_{\rho\sigma}\,|\rho\sigma\rangle \tag{2-32b}$$

$|\alpha, M\rangle$ and $|\chi\rangle$ are orthogonal to each other.

Equation (2-25) now becomes

$$(H_o - \omega)\,|\alpha, M\rangle \;+\; K(\omega)\,|\alpha, M\rangle \;+\; (H_o - \omega)\,|\chi\rangle = 0 \tag{2-33}$$

Looking for the component $|\rho\sigma\rangle$ we get

$$\sum_{\mu\gamma} (\epsilon_{\rho\sigma} - \omega)\, \chi_{\rho\sigma} + \langle \rho\sigma | K(\omega) | \mu\gamma \rangle\, \chi_{\mu\gamma} = 0, \quad \rho\sigma, \mu\gamma \in M \tag{2-34}$$

$$\sum_{\mu\gamma} (\epsilon_{\rho'\sigma'} - \omega)\, \chi_{\rho'\sigma'} + \langle \rho'\sigma' | K(\omega) | \mu\gamma \rangle\, \chi_{\mu\gamma} = 0, \quad \rho'\sigma' \notin M, \quad \mu\gamma \in M \tag{2-35}$$

Equation (2-34) shows that ω is obtained by diagonalizing $H_o + K(\omega)$ in M. Our effective Schroedinger equation can now be written as

$$(H_o + K(\omega))|\alpha, M\rangle = \omega|\alpha, M\rangle \tag{2-36}$$

The eigenfunction of (2-34) is not the actual wave function $|\alpha\rangle$ but the model wave function $|\alpha, M\rangle$. The components of $|\alpha\rangle$ not in M, i.e., the components of $|\chi\rangle$, can be calculated using (2-35), which is just another way of writing (2-32b). It should be pointed out that if one were to do an exact calculation of $K(\omega)$ using (2-26) the subspace M one chooses is irrelevant to the final solution of (2-36). But in the actual calculation,which will be described below, it is necessary that we choose M to be those with low unperturbed energies. This will be discussed in more detail later.

Now we have to calculate $K(\omega)$. This is non-trivial because $K(\omega)$ depends explicitly on ω. In fact $K(\omega)$ cannot be calculated exactly. Moszkowski and Scott[8] developed a method to calculate $K(\omega)$ approximately. They first assumed that the behaviour of nucleons in the low density region of nuclei is not very different from free nucleons with low energies. Then they separated the two-nucleon potential, derived by fitting two-nucleon scattering data, into a short range potential v_s and a long range potential v_ℓ. The cut was made such that v_s, which includes the strongly repulsive core and part of the attractive force, produces no phase shift for low energy free nucleon scattering. In this way they can assume the matrix elements of the short range free nucleon reaction matrix to be zero, and make the approximation

$$K(\omega) \approx v_\ell$$

Our approach, developed by Kahana and Tomusiak[5], is to expand $K(\omega)$ directly in terms of the free nucleon reaction matrix, K_F*. This method has the advantage that no separation distance has to be determined. Moreover, the separation distance in the Moszkowski and Scott method is usually state dependent, and is capable of causing some ambiguity when it is taken state independently. In our calculation we shall actually use the approximation

$$K(\omega) = K_F \tag{2-37}$$

It is the purpose of this work to test this approximation in the case of F^{18} and Sc^{42}. We mention here that (2-37) also has some ambiguity of its own. This ambiguity stems from the fact that $K(\omega)$ should be evaluated at the total energy, ω, of the two-particle system in the nucleus, while K_F is a function of the relative kinetic energy, E, of the free two-particle system, and in the right-hand side of (2-37) one is not certain at what value of E to take K_F. This point will be discussed in detail in Chapter 5.

*See next chapter.

CHAPTER 3

THE FREE REACTION MATRIX

3.1 The Free Reaction Matrix

The reaction matrix describing the multiple-scattering of two free nucleons is the free reaction matrix $K_F(E)$

$$K_F(E) = v + v \frac{P}{E - t} K_F(E) \tag{3-1}$$

where t is the energy of an intermediate nucleon pair.

Here unlike the problem of finite nuclei we are not interested in diagonalizing the Hamiltonian so the operator P excludes only the initial state and actually becomes the principal value operator in the integral equation (3-1). The free nucleons have definite momenta so the unperturbed Hamiltonian is just the relative kinetic energy of the two nucleons.

The total Hamiltonian is

$$H = t + v \tag{3-2}$$

with the wave function ψ satisfying the Schroedinger equation:

$$H \psi = (t + v)\psi = E\psi \tag{3-3}$$

The model wave function now is just the plane wave $\emptyset$ itself and analogous to (2-29) and (2-31)

$$= \emptyset + \frac{P}{E - t} v \psi \tag{3-4}$$

and

$$K_F(E)\, \emptyset = v \psi \tag{3-5}$$

In the center of mass frame t is the relative kinetic energy of the two free nucleons in the intermediate states and E is the relative kinetic energy of the scattering nucleons.

For a central interaction, $v(\underline{r}) = v(r)$, the scattered wave ψ will be taken to satisfy the boundary condition that it behaves asymtotically as a sum of spherical standing waves,

$$\psi_{\underline{k}} \longrightarrow \sum_{\ell=0}^{\infty} \sqrt{4\pi(2\ell+1)}\ \frac{i^{\ell}}{kr}\, C_{\ell} \sin(kr - \frac{\ell\pi}{2} + \delta_{\ell})\, Y_{\ell 0}\ (\underline{k}, \underline{r}) \tag{3-6}$$

where δ_{ℓ} is the phase shift of the partial wave with angular momentum ℓ and

$$C_{\ell} = \frac{1}{(2\pi)^{3/2} \cos \delta_{\ell}}$$

It is shown in Appendix A that the on-the-energy-shell matrix element of K_F is related to the tangent of the phase shift δ_{ℓ} by

$$\left\langle \underline{k}' \right| K_F(E = \frac{k^2\hbar^2}{M}) \left| \underline{k} \right\rangle \Big|_{|\underline{k}'| = |\underline{k}|}$$

$$= - \frac{\hbar^2}{2\pi^2 kM} \sum_{\ell=0}^{\infty} \sqrt{4\pi(2\ell+1)}\ \tan \delta_{\ell}\, Y_{\ell 0}\, (\underline{k}', \underline{k}) \tag{3-7}$$

where $|\underline{k}\rangle$ is the plane wave $\emptyset$ with relative momentum $\underline{k}$.

The matrix elements on the left-hand side of (3-7) can be numerically evaluated when the phase shifts are measured experimentally.

3.2 The Free Reaction Matrix as an Approximation to the Nuclear Reaction Matrix

The nuclear reaction matrix $K(\omega)$ is related to the free reaction matrix $K_F(E)$ by the following equation,

$$K(\omega) = K_F(E) + K_F(E)\left(\frac{Q_M}{\omega - H_o} - \frac{P}{E-t}\right) K(\omega) \tag{3-8}$$

This equation is simply obtained by solving (3-1) for v and substituting into (2-26).

As mentioned in the last chapter, we actually used in our calculation the approximation

$$K(\omega) = K_F(E) \tag{3-9}$$

One would think that K and K_F actually would differ considerably since bound nucleons behave differently from free nucleons. The reason the approximation is worth making is because the two nucleons we are considering are outside a doubly closed shell and are quite loosely bound. As a result they spend appreciably more time in regions of low density than the core nucleons. Furthermore, the two-particle intermediate states included in Q_M in (3-8) are either more loosely bound or are free states and a large part of this contribution is cancelled by the terms included in P. In any case (3-9) is the first step one has to do in our calculation and corrections to (3-9) can always be added if they need be. These corrections include the second term in (3-8) and those caused by the excitation of nucleons in the nucleus core.

We mentioned in the last chapter that were $K(\omega)$ calculated exactly the solution of (2-36) would have been independent of the model space M. Since we are using approximation (3-9) instead, it is clear that our solution will depend on M. Naturally we then want to choose M such that the second term in (3-8) will contribute the least. We thus choose M to be a set of unperturbed two-particle states which have the lowest energies. The states outside M, i.e., those included in Q_M will be practically free and will mostly cancel with the corresponding states in P in (3-8).

3.3 The Determination of $K_F(E)$

We shall write the K_F-matrix element in the relative coordinates of the scattering nucleons. So in (3-7) the denominator is E-t, where E is the relative energy parameter, and t the relative kinetic energy operator. In (3-9) the matrix element of K_F in the momentum space can be transformed into coordinate space representation,

$$\langle \underline{k}'|K_F(E)|\underline{k}\rangle = \iint d^3r\, d^3r' \langle \underline{k}'|\underline{r}'\rangle \cdot \langle \underline{r}'|K_F(E)|\underline{r}\rangle \cdot \langle \underline{r}|\underline{k}\rangle \tag{3-10}$$

where

$$\langle \underline{k} | \underline{r} \rangle = \frac{1}{(2\pi)^{3/2}} e^{-i \underline{k} \cdot \underline{r}} \tag{3-11}$$

In our work we are interested in the determination of the isotopic singlet K_F. The isotopic triplet K_F was already described by Kahana and Tomusiak[5]. We shall find a K_F which reproduces the relative S-wave phase shift. It is known that nuclear force has very short range, hence the S-wave interaction dominates at low energies. Other relative waves may contribute significantly but we will ignore them in this work. In this case there can be no spin-orbit force. In calculating the K_F-matrix we shall also neglect the purely tensor component. As is know from calculations concerning the deuteron ground state, which consists of a proton and a neutron with total spin equal to 1 and isotopic spin equal to 0, the tensor force is probably as strong as the central force. Thus using a pure central force in our calculation is not completely justifiable except that it makes the calculation much more transparent. On the other hand a first order central K matrix includes contributions from a tensor component in the potential.

As a consequence of the simplifications made above, we shall not expect our calculation to agree with the experimental data in any detailed manner.

With only a central K_F being taken into account the spin triplet S-wave K_F-matrix, ${}^3K_{Fo}$, elements can be written as

$$\langle \underline{r}' | \, ^3K_{Fo} (E) | \underline{r} \rangle = \sqrt{\frac{1}{4\pi}} \; ^3K_o (\underline{r}', \underline{r}; E) \; Y_{00} \; (\underline{r}', \underline{r}) \qquad (3\text{-}12)$$

Comparing (3-10) and (3-12) we get

$$-\frac{\hbar^2}{M\,k} \tan \delta\, (^3S_1) = \int_0^{\infty} (r'r)^2 \; ^3K_o \; (\underline{r}', \underline{r}; E) \; d^3r \; d^3r' \qquad (3\text{-}13)$$

where $\delta\,(^3S_1)$ is the spin triplet S-wave phase shift.

It was pointed out by Kahana[9] that components of relative kinetic energy up to 100 MeV in free nucleon scattering could also enter into the interaction between two nucleons outside the closed shell of a finite nucleus. Thus contrary to earlier authors who calculated effective forces by only considering the very low energy phase shifts, we shall also take phase shifts of energies up to 100 MeV into account.

The numerical calculation of $^3K_{Fo}$ was done by Kahana, Lee and Scott[10]. It was found to be necessary to use an energy dependent form. The result is:

$$^3K_{Fo}(E) = -8\pi\,(12{,}677.0)\,\lambda_p^3\,\frac{1}{2} \left\{ \left[\delta(\underline{r}_{12}) \frac{1}{E/E_o - 1} + \frac{1}{E/E_o - 1} \delta(\underline{r}_{12}) \right] \right.$$

$$\left. - \, 5.9355 \left[\delta(\underline{r}_{12}) \frac{E/MC^2}{E/E_o - 1} + \frac{E/MC^2}{E/E_o - 1} \delta(\underline{r}_{12}) \right] \right\} \text{ MeV} \qquad (3\text{-}14)$$

In (3-14) λ_p is the proton Compton wave length in fermis,

$$\lambda_p = .2103 \text{ (f)}$$

In determining (3-14), E was taken as the relative kinetic energy explicitly.

The relative coordinates are denoted explicitly by the subscript 12,

$$\underline{r}_{12} = \underline{r}_1 - \underline{r}_2$$

$$\underline{p}_{12} = \frac{1}{2}\frac{\hbar}{i}\left(\frac{\partial}{\partial \underline{r}_1} - \frac{\partial}{\partial \underline{r}_2}\right) = \frac{1}{2}\left(\underline{p}_1 - \underline{p}_2\right) \tag{3-15}$$

p_{12}, when taken as an operator, on the right-hand side of $\delta(\underline{r}_{12})$ operates only on the states to its right; likewise when it is on the left of $\delta(\underline{r}_{12})$. The denominator $(E/E_o - 1)^{-1}$ in (3-14) is introduced to account for the infinity which occurs in tan $\delta(^3S_1)$. It is known that if the reaction matrix has a pole at a negative E, which in this case corresponds to the deuteron bound state in the $^3S_1$ channel, it will also have a pole at some positive value of E. In the phase shifts determined by Hamada and Johnston[11] tan $\delta(^3S_1)$ has a pole, i.e. $\delta(^3S_1) = \pi/2$, at 8.6 MeV. So we set E_o at this value. The second term in the curly bracket in (3-14) accounts for the vanishing of the phase shift at about 150 MeV and reflects the existence of a hard core.

CHAPTER 4

THE SINGLE PARTICLE ENERGIES AND THE EXPERIMENTAL SPECTRA OF F^{18} AND Sc^{42}

In this work we calculated the energy levels of F^{18} and Sc^{42}. The calculations are similar for both nuclei. In the following we shall discuss the determination of single particle energies and the experiment spectrum of F^{18} only. Data for Sc^{42} are included in Tables 4-4 and 4-5 at the end of this chapter.

4.1 Data for F^{18}

For F^{18} we choose the 2s-1d shell to be the model space M. The single particle energies of these shells are taken from the experimental spectra of O^{17} and F^{17} (12). In Fig. 4-1 are shown the relevant spectra.

Notice there is a difference of 2.762 MeV between the ground states of O^{17} and F^{17}. This is presumably caused by the Coulomb force. Also the energy differences between the $s_{1/2}$ level and the $d_{3/2}$ level and the $d_{3/2}$ and the $d_{5/2}$ ones, differ by 0.4 and 0.3 MeV, respectively, in the two nuclei.

For the eigenvalues of our secular equation (2-36), we take arbitrarily the scale correspond to

$$\epsilon_{5/2,5/2} = \epsilon^{p}_{5/2} + \epsilon^{n}_{5/2} = 0$$

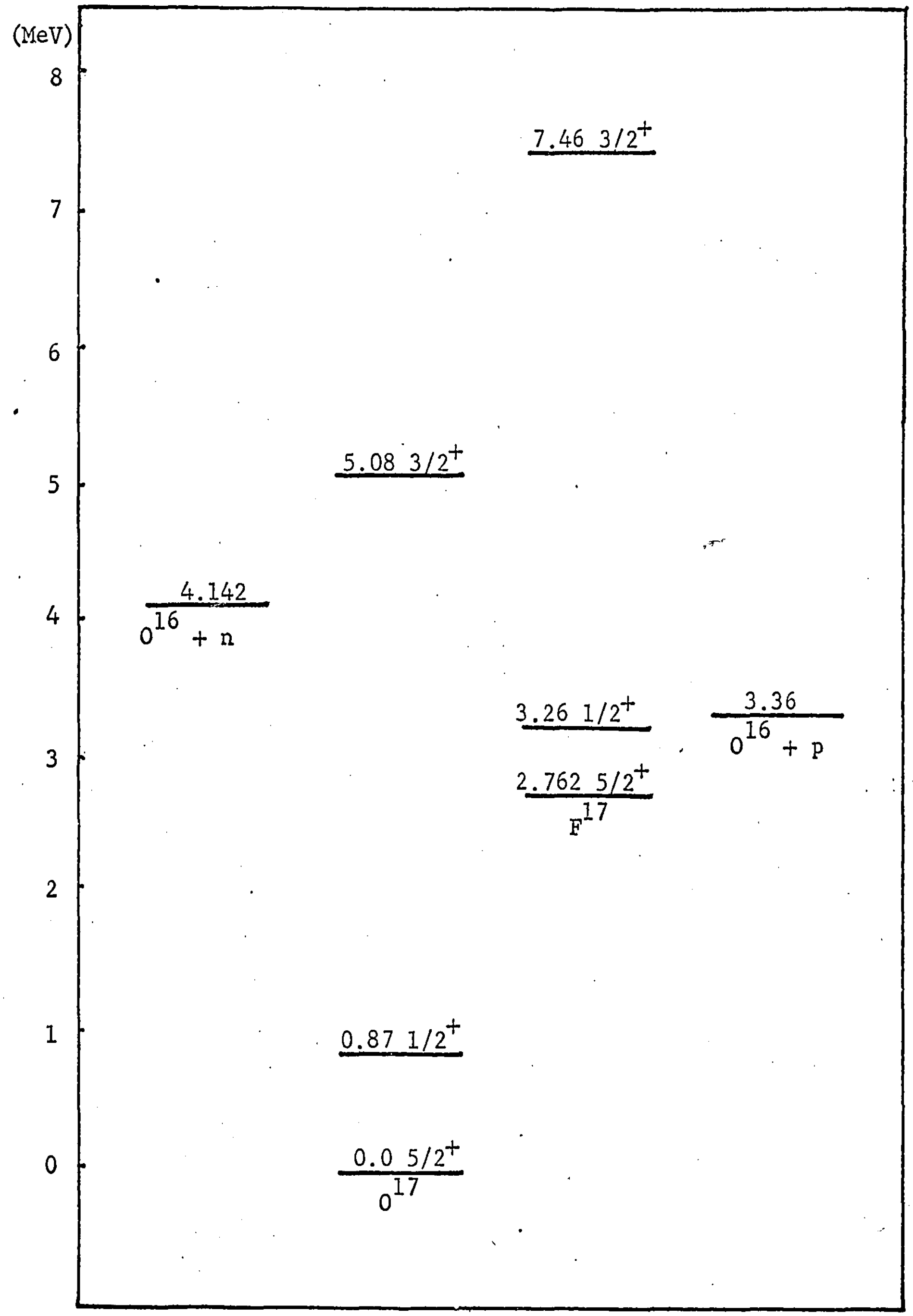

Fig. 4-1

Spectra of O^{17} and F^{17}

Physically the eigenvalues of (2-36) correspond then to the pairing energies between the proton and neutron. The experimental values can be extracted from the relevant spectra by subtracting the binding energies of F^{17} and O^{17} from the binding energy of F^{18}. The relevant spectra are shown in Figs. 4-1 and 4-2.

The binding energy of deuteron is known to be -2.226 MeV, so the binding energy of the ground state of F^{18} is

$$-7.514 - 2.226 = -9.74 \text{ (MeV)} \tag{4-1}$$

The ground state energy of F^{18} is at

$$-9.74 + 0.598 + 4.142 = -5.00 \text{ (MeV)}$$

In Table 4-1 are listed all low lying experimental levels of F^{18}.(13)

If we extract in the same manner the ground state $(J^{\pi}; T = 0^{+}; 1)$ of O^{18} from Figs. 4-1 and 4-2, we get

$$\omega^{0^{+};1} = -3.92 \text{ MeV}$$

Comparing this to the lowest $0^{+}; 1$ level of F^{18}, there is only a small discrepancy of 0.03 MeV. We thus have good evidence for the charge independence of the nuclear force. We shall here concern ourselves with the $T = 0$ states, the $T = 1$ states being essentially those of O^{18}. The lowest two-particle state with negative parity has an unperturbed energy at about 12 MeV, and so we do not expect the actual state to be lower than 7 MeV.

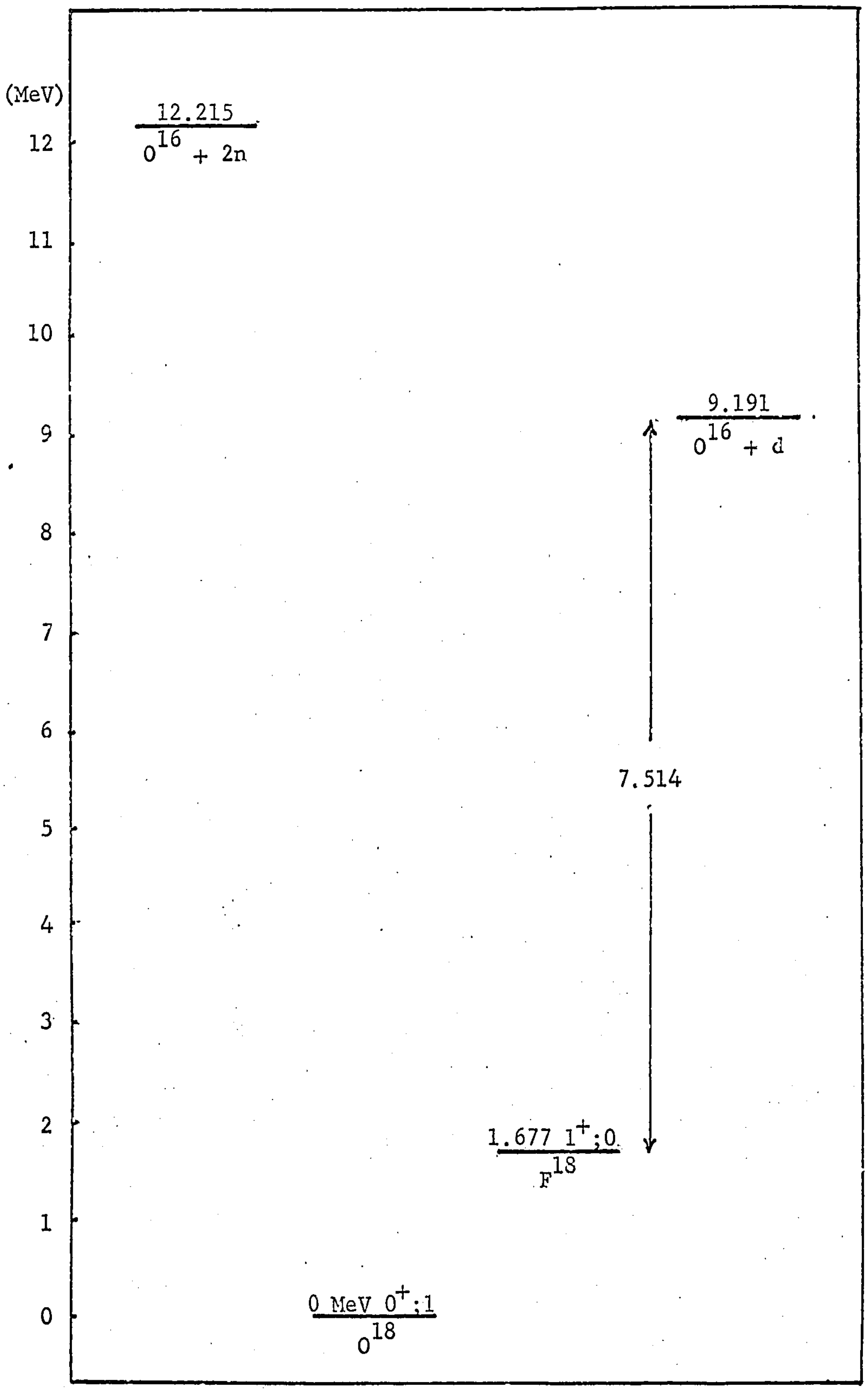

Fig. 4-2

Ground States of O^{18} and F^{18}

TABLE 4-1

Experimental energy levels of F^{18}.

Quantum numbers not specified are not yet known, those in brackets are unconfirmed.

Energy (MeV)	J^{π}; T	Energy (MeV)	J^{π}; T
-5.00	1^+; 0	-1.94	2^+; 1
-4.06	3^+; 0	-1.87	1; 0
-3.95	0^+; 1	-1.65	(2); 0
-3.92	0^-; 0	+1.16	(3^+,4^+,5^+)
-3.87	5^+; 0	+1.28	(2; 1)
-3.30	1^+; 0	+2.18	(4^+)
-2.90	2^-; 0	+3.09	(1^+)
-2.48	2^+		

In any case as mentioned before, solving the secular equation (2-36) only in the 2s-1d shell will not give us any negative parity states.

Because of the crude nature of our calculation, we shall compare our result only with the lower five $T=0$ positive parity levels in Table 4-1, which we list again below.

TABLE 4-2

Energy	$J^{\pi};T$
-5.00	$1^{+};0$
-4.06	$3^{+};0$
-3.87	$5^{+};0$
-3.30	$1^{+};0$
-2.48	$2^{+};0$

A more subtle point concerns with the difference between the spectra of F^{17} and O^{17}. Consider a HF state with two particles in the $2s_{1/2}$ shell, then the unperturbed energy is

$$0.87 + 0.50 = 1.37 \text{ MeV}$$

If, however, one of the particles is in the $1d_{5/2}$ shell and the other one in the $2s_{1/2}$ shell, then there is the problem of choosing for the unperturbed energy to be

$$\epsilon_{d_{5/2}, s_{1/2}} = 0.00 + 0.87 = 0.87 \text{ MeV}$$

or

$$= 0.00 + 0.5 = 0.50 \text{ MeV}$$

that is, taking the particle in the $2s_{1/2}$ shell to be a proton or a neutron.

To treat this problem properly we should take into account o the difference between single particle energy of a proton and a neutron by writing the HF energy

$$\epsilon_{\rho\sigma} = \epsilon_\rho^p \left(\frac{1}{2} + \tau_{\rho 3}\right) + \epsilon_\rho^n \left(\frac{1}{2} - \tau_{\rho 3}\right) + \epsilon_\sigma^p \left(1 + \tau_{\sigma 3}\right) + \epsilon_\sigma^n \left(\frac{1}{2} - \tau_{\sigma 3}\right)$$

where τ_3 is the third component of the isotopic spin operator. The superscripts p and n denote the single particle energy taken from F^{17} and O^{17}, respectively. This formalism, however, breaks the symmetry of the isotopic spin (charge independence), as can be seen by realizing that $\tau_{\rho 3}$ does not commute with

$$\underline{T} = \underline{\tau}_\rho + \underline{\tau}_\sigma$$

i.e.,

$$\left[\tau_{\rho_3}, \underline{T}\right] \neq 0$$

In this case the perturbed states should not have T as a good quantum number and everything becomes quite a bit more complicated.

We feel reluctant to accept this complication just because of a difference of 0.3 MeV, when previously we made approximations which were at least as important.

Still we have to decide to use the O^{17} or the F^{17} spectra. Now the proton in F^{17} is very loosely bound by only 0.1 MeV. This presumably is because of the Coulomb repulsion exerted on the proton by the core. In our calculation the Coulomb force is entirely ignored. So it is most reasonable to think that if we had done a proper HF calculation, the O^{17} and F^{17} spectra would resemble the real O^{17} spectrum more closely. So, if the two particles are in different shells, we shall take the single particle energy from the O^{17} spectrum. In Table 4-3 are listed the unperturbed energies of the two particle states. A proper treatment of the Coulomb force was done by Gillet.[14]

TABLE 4-3

Unperturbed two-particle energies of F^{18}

State	Energy	State	Energy
$(d_{5/2})^2$	0.0	$d_{5/2}d_{3/2}$	5.08
$d_{5/2}s_{1/2}$	0.87	$s_{1/2}d_{3/2}$	5.95
$(s_{1/2})^2$	1.37	$(d_{3/2})^2$	9.78

4.2 The Single Particle Wave Function

For the single particle wave functions we take the harmonic oscillator wave functions. This is the usual practice in the literature. The reason is the harmonic wave functions can be transformed into wave functions in terms of relative and center of mass coordinates readily.* We should, however, mention that the harmonic oscillator wave functions as approximations to the real wave functions are at their worst for the outmost nucleons in the nucleus. This is because the effective one particle potential decreases towards zero as the distance from the center of the nucleus increases, while the harmonic oscillator potential increases quadratically. The wave functions relevant to our calculation will be given in the next chapter.

4.3 Data for Sc^{42}

Experiemntal data for Sc^{42} relevant to this work are listed in Tables 4-4 and 4-5.

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*See Chapter 5, section 5.1.

TABLE 4-4

Unperturbed two-particle energies of Sc^{42} (15)

State	Energy (MeV)
$f_{1/2}^{2}$	0.0
$f_{1/2}p_{3/2}$	2.08
$p_{3/2}^{2}$	4.16

TABLE 4-5

Experimental low lying levels (T=0, positive parity) of Sc^{42} (16)

J^{π}	Energy	J^{π}	Energy
1^{+}	-2.57	3^{+}	-1.68
7^{+}	-2.48	?	-0.19
5^{+}	-1.85	?	0.33

CHAPTER 5

METHODS AND RESULTS OF CALCULATION

5.1 The Calculation of the Matrix Elements

The secular equation (2-36) can be written as

$$\sum_{\mu\gamma}\left[\epsilon_{\rho\sigma}\delta_{\rho\mu}\delta_{\sigma\gamma} + K_{F_{\rho\sigma,\mu\gamma}}\right]\chi_{\mu\gamma,\alpha} = \omega^{\alpha}\chi_{\rho\sigma,\alpha}$$

where $\chi_{\rho\sigma,\alpha}$ are the components of the model wave function $|\alpha, M\rangle$ and ρ denotes the set of quantum numbers which label the harmonic oscillator wave functions

$$\rho = (n_{\rho}\ell_{\rho}\ j_{\rho})$$

To solve we have to calculate the matrix elements

$$K_{F_{\rho\sigma,\mu\gamma}} = \langle\rho\sigma|K_F(E)|\ \mu\gamma\rangle \tag{5-1}$$

and diagonalize the matrix

$$\epsilon_{\rho\sigma}\delta_{\rho\mu}\delta_{\sigma\gamma} + K_{F_{\rho\sigma,\mu\gamma}} \tag{5-2}$$

The eigenvalues ω^{α} are to be compared with those listed in Tables 4-1 and 4-5. The eigenvectors $\chi_{\rho\sigma,\alpha}$ give the configuration mixing. To calculate the matrix elements, we couple the two particles to a state of good total spin J and isotopic spin T, using the j-j coupling scheme. Since the particles are in the 2s-1d shell (for F^{18}), all states have positive parity. The unperturbed states in the j-j coupling scheme are

$$|\rho\sigma;JT\rangle = \sum_{\substack{m_\rho, m_\sigma\\ \tau_\rho, \tau_\sigma}} \langle J0 | (n_\rho \ell_\rho)\, j_\rho m_\rho\, (n_\sigma \ell_\sigma)\, j_\sigma m_\sigma \rangle$$

$$\times \langle T0 | \tfrac{1}{2}\tau_\rho \tfrac{1}{2}\tau_\sigma \rangle\, |(j_\rho j_\sigma);\, J0\rangle\, |(\tfrac{1}{2}\tfrac{1}{2});\, T0\rangle \qquad (5\text{-}3)$$

Our K_F-matrix is local and central, and spin independent. To evaluate the radial integrals we have to transform the j-j coupling to L-S coupling

$$|(j_\rho j_\sigma);\, JM\rangle = \sum_{\substack{L,\ S\\ m_L, m_S}} \langle (\ell_\rho \ell_\sigma)L,\, (\tfrac{1}{2}\tfrac{1}{2})\, S;\, J | (j_\rho j_\sigma);\, J\rangle$$

$$\times \langle L\, M_L S M_S | JM\rangle\, |(n_\rho \ell_\rho n_\sigma \ell_\sigma);\, LM_L\rangle\, |(\tfrac{1}{2}\tfrac{1}{2});\, SM_S\rangle$$

$$(5\text{-}4)$$

The j-j L-S transformation coefficients are related to the X-coefficients[17] by

$$\langle (\ell_\rho \ell_\sigma)\, L,\, (s_\rho s_\sigma)\, S;\, J | (\ell_\rho s_\rho)\, j_\rho\, (\ell_\sigma s_\sigma)\, j_\sigma\, ;\, J\rangle$$

$$= \left[(2L+1)(2S+1)(2j+1)(2j+1)\right]^{1/2}\, X\begin{pmatrix} \ell_\rho & \ell_\sigma & L\\ s_\rho & s_\sigma & S\\ j & j & J\end{pmatrix} \qquad (5\text{-}5)$$

These coefficients are tabulated by Kennedy and Cliff.[18]

The K_F-matrix is expressed in terms of relative coordinates of the two nucleons, so we have to transform the harmonic wave functions to wave functions in terms of relative and center of mass coordinates of the two particles.

$$\left|(n_\rho \ell_\rho \, n_\sigma \ell_\sigma);\, LM_L\right\rangle = \sum_{n,\ell,N,L} \langle n\ell N\mathcal{L};L \,|\, n_\rho \ell_\rho n_\sigma \ell_\sigma;\, L\rangle$$

$$\times \,\left|(n\ell N\mathcal{L});\, LM_L\right\rangle \tag{5-6}$$

Where $|n\,\ell\rangle$ and $|N\mathcal{L}\rangle$ are harmonic oscillator wave functions in terms of relative and center of mass coordinates, respectively.[19] The transformation brackets

$$\langle n\ell N\mathcal{L};\, L\,|\, n_\rho \ell_\rho \;\; n_\sigma \ell_\sigma \;;\, L\rangle$$

are tabulated by Brody and Moshinsky.[20]

All transformations involved are straightforward and the result is

$$\langle \rho\sigma\, ;\, J'T' |\; K\, |\, \mu\gamma;\, JT\rangle$$

$$= \sum_{\substack{L,L',S,N,\mathcal{L}\\ \ell,\ell',n,n',\mathcal{J}}} \langle(\ell_\rho \ell_\sigma)\; L',\; (\tfrac{1}{2}\,\tfrac{1}{2})S;\; J' \,|\, (j_\rho\; j_\sigma\;)\;\; J'\rangle$$

$$\times \;\langle(\ell_\mu \ell_\gamma)\; L,\; (\tfrac{1}{2}\,\tfrac{1}{2})\; S;\; J\,|\,(j_\mu j_\gamma)\; J\rangle$$

$$\times \;\langle n_\rho \ell_\rho n_\sigma \ell_\sigma\, ;\; L' \,|\; n'\ell' N\mathcal{L};\; L'\rangle$$

$$\times \;\langle n_\mu \ell_\mu \;\, n_\gamma \ell_\gamma;\; L\,|\, n\,\ell N\mathcal{L}\,;\; L\rangle$$

$$\times \;\; U\,(\mathcal{L}\,\ell' JS;\; L'\mathcal{J}\,)\;\;\; U\,(\mathcal{L}\ell JS;\; L\mathcal{J})\;\, (-)^{\ell+\ell'-L-L'}$$

$$\times \;\langle n'\ell' S;\mathcal{J}\, T\,|\, K\,|\, n\ell\, S;\mathcal{J}\, T\rangle \;\;\; \delta_{TT'}\; \delta_{JJ'} \tag{5-7}$$

$\mathcal{J}$ is the relative total angular momentum. U is the U- coefficient, related to the Racah coefficient[21] W by

$$U(a\ b\ c\ d;\ e\ f) = (2e+1)^{1/2}\ (2f+1)^{1/2}\ W(a\ b\ c\ d;\ e\ f)$$

Since we are considering only S-wave interaction ℓ and ℓ' in (5-7) are always equal to zero. In this case the U-coefficients in (5-7) are equal to one and also

$$L' = L = \mathcal{L}$$

Because we are dealing with two fermion states, the state vectors have to be antisymmetrized. This can be done by multiplying $|\rho\sigma;\ JT\rangle$ by a factor of

$$\frac{1-(-1)^{S+T+\ell}}{2} \times \begin{cases} 1 & \text{if } (n_\rho \ell_\rho j_\rho) = (n_\sigma \ell_\sigma j_\sigma) \\ \sqrt{2} & \text{otherwise} \end{cases}$$

In our work this factor reduces to

$$\begin{matrix} 1 & \text{if} \quad (n_\rho \ell_\rho j_\rho) = (n_\sigma \ell_\sigma j_\sigma) \\ \sqrt{2} & \text{otherwise} \end{matrix} \qquad (5\text{-}8)$$

Another remark we have to make is that the relative coordinate used in determining the Moshinsky transformation brackets is different from the $\underline{r}_{12}$ used in our K_F.[19] The two are related by

$$\underline{r}_M = \frac{1}{\sqrt{2}}(\underline{r}_1 - \underline{r}_2) = \frac{1}{\sqrt{2}}\ \underline{r}_{12}$$

Hence,

$$\underline{r}_{12} = \sqrt{2}\ \underline{r}_M , \qquad \underline{p}_{12} = \frac{1}{\sqrt{2}}\ \underline{p}_M \tag{5-9}$$

Henceforth, $\underline{r}$ and $\underline{p}$ with no subscripts will denote the Moshinsky coordinates.

As mentioned at the end of Chapter 2, we would like to point out that there is a possible ambiguity in our treatment of the free reaction matrix. Essentially, we will be using the form given in (3-14), i.e. we use

$$\begin{aligned} {}^3K_{Fo} = {} & -8\pi(12,677)\lambda_p^3\ \frac{1}{2}\Bigg\{\left[\delta(\underline{r}_{12})\ \frac{1}{E/E_o - 1} + \frac{1}{E/E_o - 1}\ \delta(\underline{r}_{12})\right] \\ & -5.9355\left[\frac{(p/MC)^2}{E/E_o - 1}\ \delta(\underline{r}_{12}) + \delta(\underline{r}_{12})\ \frac{(p/MC)^2}{E/E_o - 1}\right]\Bigg\} \end{aligned} \tag{3-14}$$

The ambiguity then arises because we can treat E as a free parameter as equation (3-7) would seem to indicate or else we can set $E = \frac{p_{12}^2}{M}$, the relative kinetic energy operator. The physics contained in this ambiguity is that we are uncertain at what energy E to compare the nuclear reaction matrix $K(\omega)$ to the free reaction matrix $K_F(E)$ in equation (3-9). For two nucleons in the shell model potential one might be inclined to take some average relative kinetic energy determined by the depth of the well, or one might allow the relative kinetic energy to be an operator and in effect permit the shell model wave functions to perform an average over this operator. Another possibility is to take the E in the factor $(E/E_o - 1)^{-1}$, which results from the existence of the deuteron bound state, as a parameter, while taking the relative kinetic energy in the repulsion term, which accounts for the repulsive nature between two nucleons at high energies, to be an operator. This is to weight the repulsive force more for states with high relative kinetic energies than those with low energies. That we should treat E differently at two places is subject to some criticism. But we know that E is equal to the relative kinetic energy only when both of the nucleons are on the energy shell, on the other hand nucleons in a nucleus are most of the time off the energy shell. So we believe our treatment of E is not inconsistent but is part of the ambiguity. We will in fact follow all of these prescriptions and compare the results. Since the calculations are essentially similar, the preliminary discussion immediately below applies to all. Concerning the evaluation of the radial integrals we do the term $\langle n'o |\, \delta(\underline{r}_{12})\; f(\underline{p}_{12}) \,| no\rangle$ explicitly.

$$\langle n'o |\, \delta(\underline{r}_{12})\; f(\underline{p}_{12}) \,| no\rangle = \frac{1}{4\pi\sqrt{8}} \langle n'o |\, \frac{\delta(r)}{r^2}\; f(\frac{\hbar k}{\sqrt{2}}) \,| no\rangle \tag{5-10}$$

The function $f(\underline{p}_{12}) = f(\frac{\hbar k}{\sqrt{2}})$ can be taken as a constant, or as a function of the relative momentum appropriate to our interpretation of E as a constant or as an operator. The factor $1/4$ in (5-10) comes from the normalization of the δ-function,

$$\int \delta\,(\underline{r}_{12})\; d^3\, \underline{r}_{12} = 1$$

and the factors $1/\sqrt{8}$ and $1/\sqrt{2}$ from using (5-9).

When E is taken as a constant then (5-10) simply becomes

$$\langle n'0 | \delta(\underline{r}_{12})\ f(\underline{p}_{12}) | n0 \rangle = f(M\sqrt{E})\ \frac{1}{4\pi\sqrt{8}}\ R_{n'o}(0)\ R_{no}(0) \tag{5-11}$$

Where R_{n0} is a harmonic oscillator radial wave function.*

When E is taken as an operator (5-10) becomes

$$\frac{1}{4\pi\sqrt{8}} \int d^3r'd^3r''d^3k'd^3k'' \langle n'0 | \underline{r}' \rangle \langle \underline{r}' | \frac{\delta(r)}{r^2} | \underline{r}'' \rangle$$

$$x \cdot \langle \underline{r}'' | \underline{k}' \rangle \langle \underline{k}' | f(\frac{\hbar k}{\sqrt{2}}) | k'' \rangle \langle \underline{k}'' | n0 \rangle \tag{5-12}$$

where

$$\langle \underline{r}' | n0 \rangle = Y_{oo}(\Omega_{\underline{r}})\ R_{n0}(\beta r)^* \tag{5-13a}$$

$$\langle \underline{k}' | n0 \rangle = Y_{oo}(\Omega_{\underline{k}})\ \beta^{-3}\ R_{n0}(k/\beta) \tag{5-13b}$$

$$\langle \underline{k} | \underline{r} \rangle = \frac{1}{\sqrt{8\pi^3}}\ e^{-i\underline{k}\cdot\underline{r}} \tag{5-13c}$$

$$= \frac{4\pi}{\sqrt{8\pi^3}} \sum_{\ell,m} (-i)^\ell\ j_\ell(kr)\ Y_{\ell m}(\Omega_{\underline{r}})\ Y^*_{\ell m}(\Omega_{\underline{k}})$$

---

*The harmonic oscillator radial wave functions $R_{n\ell}(r)$ are defined as

$$R_{n\ell}(r) = \beta^{3/2}\left[2(n!)/\Gamma(n+\ell+3/2)\right]^{1/2} (\beta r)^\ell \exp(-\beta^2 r^2/2) L_n^{\ell+1/2}(\beta^2 r^2)$$

where $L_n^a(z)$ are the Laguerre polynomials generated by

$$\frac{e^{-zt/(1-t)}}{(1-t)^{a+1}} = \sum_{n=0}^{\infty} t^n L_n^a(z) .$$

Following we give the R_{n0}'s relevant to our calculation,

$$R_{00}(\beta r) = \beta^{3/2} \sqrt{\frac{2}{\Gamma(3/2)}} \quad e^{-\frac{1}{2}\beta^2 r^2}$$

$$R_{10}(\beta r) = \beta^{3/2} \sqrt{\frac{2}{\Gamma(5/2)}} \quad (3/2 - \beta^2 r^2) \quad e^{-\frac{1}{2}\beta^2 r^2}$$

$$R_{20}(\beta r) = \beta^{3/2} \sqrt{\frac{4}{\Gamma(7/2)}} \quad (\frac{15}{8} - \frac{5}{2}\beta^2 r^2 + \frac{1}{2}\beta^4 r^4) \; e^{-\frac{1}{2}\beta^2 r^2}$$

$$R_{30}(\beta r) = \beta^{3/2} \sqrt{12/\Gamma(9/2)} \quad (\frac{35}{16} - \frac{35}{8}\beta^2 r^2 + \frac{7}{4}\beta^4 r^4 - \frac{1}{6}\beta^6 r^6)$$

β is related to the harmonic oscillator parameter ω by

$$\beta^2 = \frac{M\omega}{\hbar} = 0.024115\ \omega\hbar\ (f^{-2})$$

For the value of $\omega\hbar$, we take the one used by Kahana and Tomusiak in their calculation of the energy levels of O^{18}[5]:

$$\omega\hbar = 14.4\ (\text{MeV}) \quad .$$

We will be discussing explicitly the nucleus F^{18}. The calculation for Sc^{42} is similar and only the result need be presented.

Putting (5-12) into (5-11) we get

$$\langle n'0|\delta(\underline{r}_{12})\; f(\underline{p}_{12})|\; n0\rangle = \frac{1}{(4\pi)^{3/2}\beta^3} \quad R_{n'0}(0) \int_0^\infty f(\frac{\hbar k}{\sqrt{2}}) \; R_{n0}(k/\beta)k^2 dk \tag{5-15}$$

The function $f(z)$ in (5-15) has the form

$$P \frac{h(z)}{z^2 - a^2}$$

where $h(z)$ is a second order polynomial in z and p the principal value operator. So essentially we have to perform the integration

$$P \int_0^\infty \frac{1}{z^2 - a^2} \quad g\,(z)\,.d\,z \tag{5-16}$$

where in our case $g(z)$ and $g'(z)$ are analytic in the range $(0, \infty)$ and vanish exponentially as $z \longrightarrow \infty$ and are equal to zero at $z = 0$. The pole in the integrand is extracted by means of the principal value operator and the result is*

$$P \int_0^\infty \frac{1}{z^2 - a^2} \; g(z)\; dz \; = \; -\frac{1}{2a} \int_0^\infty \frac{g(z)}{z + a} \; dz$$

$$+ \; \frac{1}{2a} \int_0^\infty \Big[(z - a)\, \ell n\, (z - a) - (z - a) \Big] \; g''(z)\; dz \tag{5-17}$$

The calculation of the other radial integrals is straightforward.

In the following we shall outline the results obtained from treating E by the three aforementioned different prescriptions separately.

---

*See Appendix B.

We shall call the case when E is a constant method A and the case when E is an operator method B. The prescription in which $\bar{E}$ in $(E/E_0 - 1)^{-1}$ is taken as a constant and p^2/M in the repulsive term is taken as an operator will be called method C. We find in fact it is better to set E equal to some average value of the relative kinetic energy and we shall outline these results first.

5.2 Results for F^{18}

5.2.1 Method A

In $^3K_{F_0}$ E is the relative kinetic energy of the two nucleons. In this section E will be taken as a constant representing the average relative kinetic energy of the neutron and the proton in the nucleus.

Before doing the calculation, we will see what is a reasonable value for E. The depth of the average potential in the shell model is about 50 MeV. The two particles outside a doubly closed shell are loosely bound. This means the total energy of each particle in the 2s-1d shell of a harmonic oscillator appropriate to F^{18} is about 50 MeV. Its average kinetic energy is about half this value, since in a harmonic oscillator the average kinetic energy is half the total energy. Thus the total kinetic energy of the two particles can be from zero to 100 MeV and has an average value around 50 MeV. Then the relative kinetic energy should vary in the range, 0-50 MeV.

In the actual calculation we varied E from 30 MeV to 60 MeV in steps of 0.5 MeV and diagonalize $H_o + K_F$ for each value of E in the 2s-1d shell. Fig. 5-1 shows the eigenvalues corresponding to the two lowest 1^+ levels, the lowest 3^+, 5^+ and 2^+ levels, as a function of E. At $E = 64$ MeV we have the following energies for method A.

TABLE 5-1

F^{18} result using method A.

Energy (MeV)	$J^{\pi}(T = 0)$
-5.55	1^+
-2.42	3^+
-2.12	5^+
-1.41	1^+
-0.31	2^+

$E = 64$ MeV is the optimum value of the parameter. The fit to experiment is clearly only qualitative at this point in our calculation.

A more complete discussion will be presented in the next chapter.

5.2.2 Method B

If we treat E as an operator we will have no parameters in our calculation. The low lying levels are shown in Table 5-5.

TABLE 5-5

F^{18} result using method B.

Energy (MeV)	J^{π} (T = 0)
-17.32	1^+
-7.76	3^+
-2.27	5^+
-3.71	1^+
-4.39	2^+

Clearly it is not appropriate to take $\dot{E}$ as an operator and let the harmonic oscillator wave functions perform the averaging of the relative kinetic energy.

5.2.3 Method C

In this method E in the denominator is treated as a constant and E in the numerator in the repulsive term is treated as an operator. The low lying levels are listed in Table 5-6 for E = 46 MeV.

The results of method A and method C are quite similar but the latter is definitely an improvement over the former. Also we see E in this method has a value more reasonable than that of method A, where it is somewhat large. The calculated model wave functions using this method are in Table 5-7.

TABLE 5-6

F^{18} result using method C.

Energy (MeV)	J (T = 0)
-5.59	1^+
-3.11	3^+
-2.86	5^+
-1.49	1^+
-0.86	2^+

5.3 Results for Sc^{42}

The nucleus Sc^{42} is treated as a proton and a neutron outside the Ca^{40} core, which consists of a doubly closed shell. The Hamiltonian $H_o + K_F(\mathcal{E})$ is diagonalized in the $1f_{7/2}$ and $2p_{3/2}$ shell. Method C is used. The optimum value of $\mathcal{E}$ is 34 MeV. Only the T = 0 levels are calculated. The T = 1 levels are the same as those of Ca^{42}, which were calculated by Kahana and Tomusiak.[5] The experiment and calculated levels and the model wave functions are listed in Table 5-8.

The reduced matrix elements of K_F for F^{18} and Sc^{42} are listed in Table 5-9. The matrix elements are given in Tables 5-10 and 5-11. The calculated levels of F^{18} and Sc^{42} versus $\mathcal{E}$ using method C are plotted in Figs. 5-1 and 5-2, respectively.

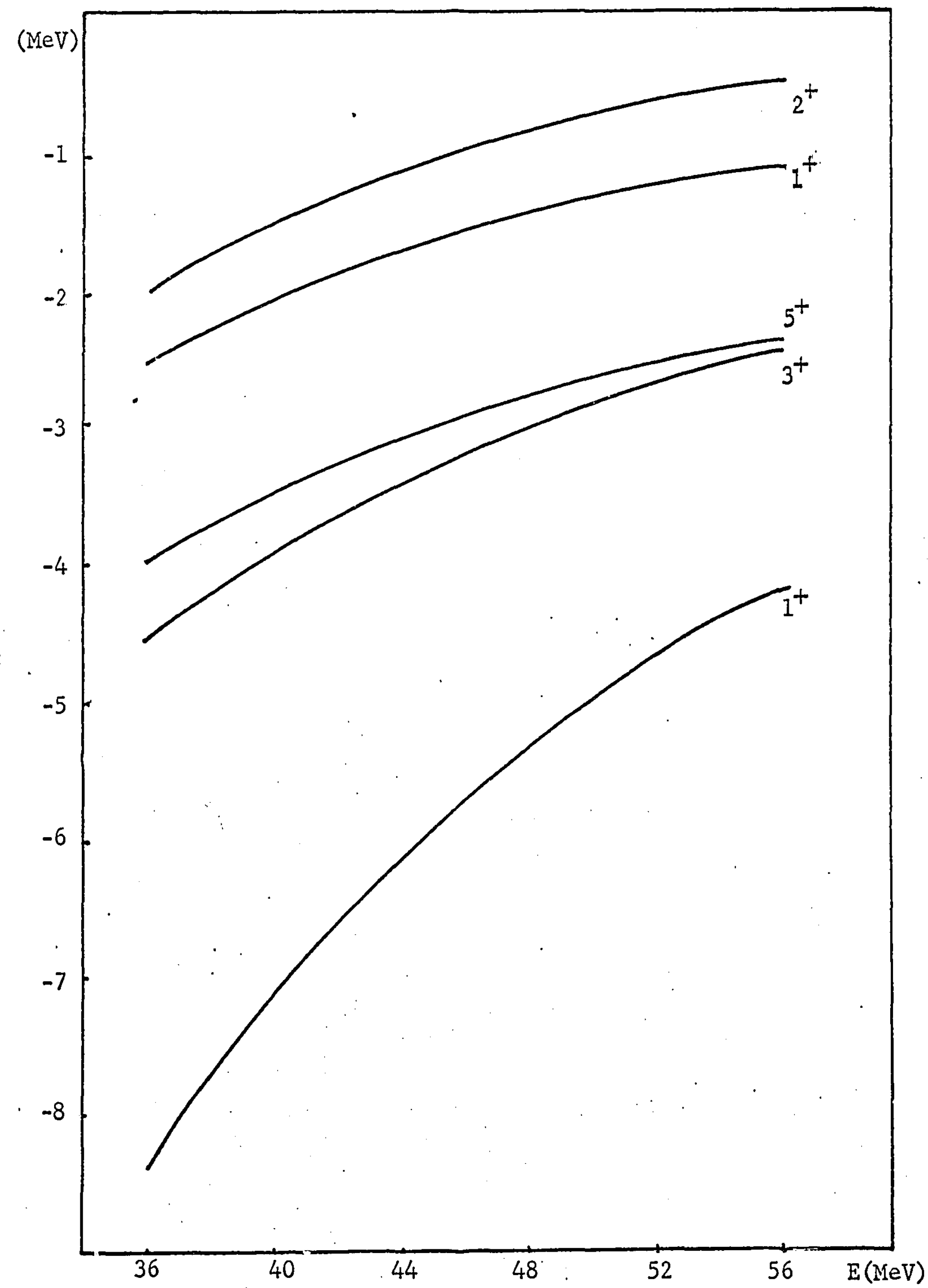

Fig. 5-1 Levels of F^{18} vs E

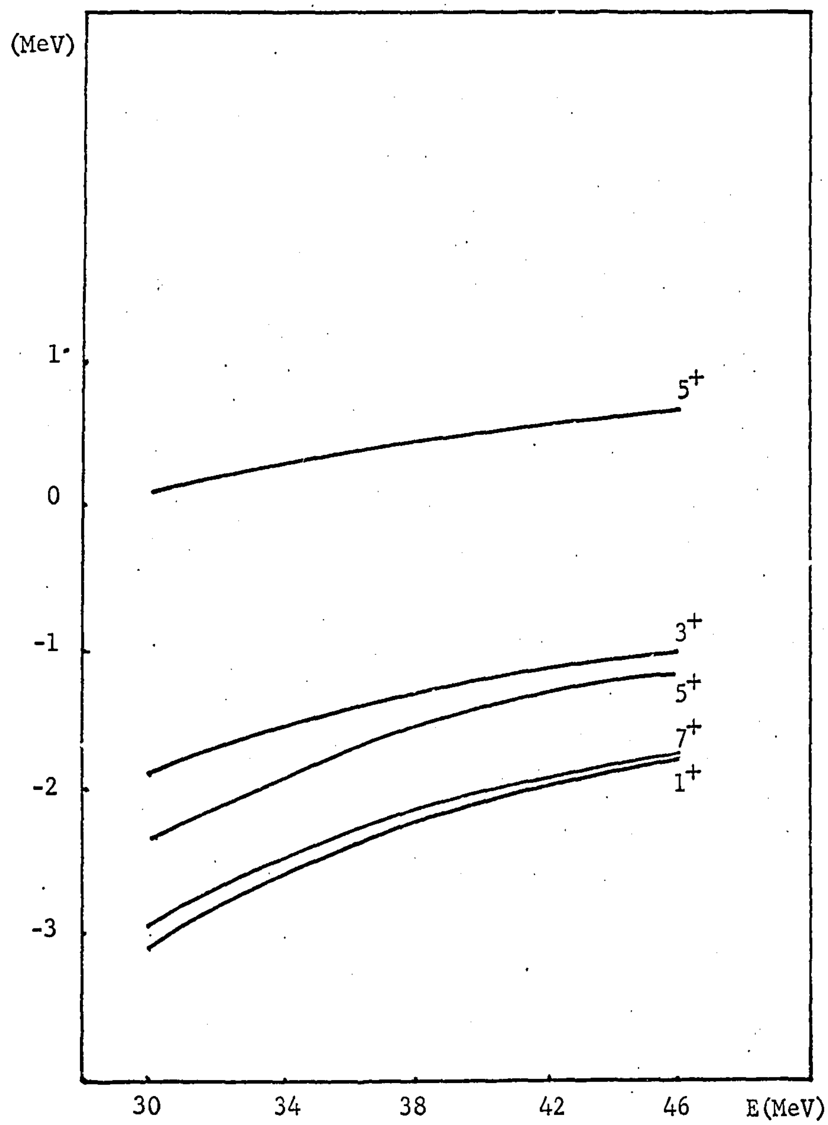

Fig. 5-2 Levels of Sc^{42} vs E

TABLE 5-7

Eigenvalues and (model) eigenfunctions of F^{18*} (T=0)

J^{π}	Energy Exp	(MeV) Cal	$d_{5/2}^2$	$d_{5/2}S_{1/2}$	$S_{1/2}^2$	$d_{5/2}d_{3/2}$	$S_{1/2}d_{3/2}$	$d_{3/2}^2$
1^+	-5.00	-5.59	.706	0	.450	-.526	.021	-.148
3^+	-4.06	-3.11	.702	.684	0	-.193	0	-.041
5^+	-3.874	-2.86	1.0	0	0	0	0	0
1^+	-1.87	-1.49	-.490	0	.864	.061	-.069	.064
2^+	-1.65	-0.86	0	.890	0	.363	.276	.0

$^{*}\omega\hbar$ = 14.4 MeV, E = 46 MeV. The third lowest 1^+ and the second lowest 2^+ experiment levels are listed.

TABLE 5-8

Eigenvalues and (model) eigenfunctions of Sc^{42*}

J^{π}	Energy Exp	(MeV) Cal	$f_{7/2}^2$	$f_{7/2}p_{3/2}$	$p_{3/2}^2$
1^+	-2.57	-2.58	.982	0	.189
7^+	-2.48	-2.49	7	0	0
5^+	-1.85	-1.83	.858	.514	0
3^+	-1.68	-1.57	.931	.302	.204
5^+	0.33	0.39	-.514	.858	0

$^*\omega\hbar$ = 11.2 MeV, E = 34 MeV

TABLE 5-9

Reduced matrix element of K_F for F^{18} and Sc^{42}.

	$\omega\hbar$	E		$\langle n0 \mid K_F(E) \mid n0 \rangle$			
				n = 0	n = 1	n = 2	n = 3
F^{18}	14.4	46	A	-5.652	-8.478	-10.600	
			B	-6.044	-37.727	24.385	
			C	-7.634	-9.012	-8.217	
Sc^{42}	11.2	34	C	-7.984	-10.060	-10.179	-9.080

TABLE 5-10

Matrix elements of F^{18} (T = 0)

J = 1	$d_{5/2}^2$	$s_{1/2}^2$	$d_{5/2}\,d_{3/2}$	$s_{1/2}d_{3/2}$	$d_{3/2}^2$
$d_{5/2}^2$	-2.524	-0.970	2.732	-0.663	1.860
$s_{1/2}$		-3.553	1.467	0	0.519
$d_{5/2}d_{3/2}$			-5.562	0.877	-0.785
$s_{1/2}d_{3/2}$				-2.350	1.241
$d_{3/2}^2$					-1.940

J = 2	$d_{5/2}s_{1/2}$	$d_{5/2}d_{3/2}$	$s_{1/2}d_{3/2}$
$d_{5/2}s_{1/2}$	-0.940	-1.049	-1.152
$d_{5/2}d_{3/2}$		-2.388	-1.284
$s_{1/2}d_{3/2}$			-1.411

J = 3	$d_{5/2}^2$	$d_{5/2}s_{1/2}$	$d_{5/2}d_{3/2}$	$d_{3/2}^2$
$d_{5/2}^2$	-1.539	-1.303	0.965	0.638
$d_{5/2}s_{1/2}$		-2.351	1.003	0.217
$d_{5/2}d_{3/2}$			-1.315	0.831
$d_{3/2}^2$				-2.396

J = 4	$d_{5/2}d_{3/2}$
	-2.863

J = 5	$d_{5/2}^2$
	-2.863

TABLE 5-11

Matrix elements of Sc^{42} (T=0)

J = 2

	$f_{7/2}^2$	$p_{1/2}^2$
$f_{7/2}^2$	-2.397	-0.938
$p_{1/2}^2$		-1.859

J = 3

	$f_{7/2}^2$	$f_{7/2}p_{3/2}$	$p_{3/2}^2$
$f_{7/2}^2$	-1.187	-0.735	-0.657
$f_{7/2}p_{3/2}$		-1.172	-0.304
$p_{3/2}^2$			-2.273

J = 5

	$f_{7/2}^2$	$f_{7/2}p_{3/2}$
$f_{7/2}^2$	-1.245	-0.979
$f_{7/2}p_{3/2}$		-1.881

J = 7

$f_{7/2}^2$
-2.495

CHAPTER 6

DISCUSSION

6.1 Discussion of the F^{18} Result

We shall concentrate our discussion on the result calculated using method C. It is seen the result agrees with the experiment only qualitatively. The splittings between the excited states and the ground state are about 1 to 2 MeV too large. Since we have made more than one assumption or approximation, it is not easy to say which is mainly responsible for the discrepancy between the calculated and the empirical levels. It is possible that they are equally responsible. For the purpose of separating the sources of these discrepancies, let us recall the important assumptions and approximations we have made.

(a) We assumed the O^{16} core of F^{18} was inert.

(b) We approximated $K(\omega)$ by $K_F(E)$, thus neglecting all corrections due to the second term in (3-8).

(c) We included only triplet S-wave interaction in the calculation of K_F. We shall discuss these effects separately.

6.1.1 Let us start by comparing our result with the work done by Kuo and Brown[6] * on F^{18}. Essentially they used the Hamada-Johnston potential and did a Scott-Moszkowski type calculation, including core

*Hereafter referred to as KB.

polarization. We want to compare with their calculated spectrum before the core polarization is included, which is shown in Fig. 6-1. The two are quite similar. But the 3^+ , 5^+ and 2^+ levels in ours are higher than theirs. After a careful comparison between the matrix elements of the two calculations, it is found that the singlet force, which we ignored completely, contributed most significantly to the 1^+ levels in KB. The 2^+ and 3^+ levels are much less affected, the 5^+ level not at all. Thus it seems possible that had we added the triplet D-wave and the singlet P-wave interactions, which are mainly repulsive, the 1^+ levels would have been pushed up relative to the other levels. By using a smaller E value the whole spectrum can be pulled down such that it matches the KB result.

6.1.2 It is certainly not satisfactory that our result should depend on the free parameter E so sensitively that the spectrum can be shifted up and down at will. This dependence on E probably comes entirely from neglecting the second term in (3-8) since $K(\omega)$ itself does not depend on E at all. One realizes after a closer look at the correction terms that the most important part of them come from the term

$$- K_F(E) \frac{P}{E - t} K_F(E)$$

with only two-particle intermediate states in the 2s-1d shell included. This is because Q_M did not include these states. Other higher states included in both P and Q_M are practically free so the denominators of the two terms become essentially the same and the two terms cancel.

Now consider

$$K_F(E) + K_F(E) \frac{P^{sd}}{t - E} K_F(E) \tag{6-1}$$

where P^{sd} limits states to the 2s-1d shell.

When E is small $K_F(E)$ is large and negative but the second term is positive. When E is large $K_F(E)$ is small and negative and the second is also negative. So adding the second term in (6-1) to $K_F(E)$ already reduces the sensitivity of our force on E. Naturally only a detailed calculation will reveal to what extent the sensitivity is reduced.

6.1.3 We expect the core polarization effect in our calculation to be much the same as that in KB. It is interesting to know that our S-wave calculation involves only three reduced matrix elements. Treating these as parameters one can fit any three of the levels and predict the remaining ones. We fitted the three lowest and the resulting spectrum is shown in Table 6-1.

The phenomenological spectrum is strikingly similar to the final KB result including core polarization.

6.2 Discussion of the Sc^{42} Result

It is perhaps accidental that our Sc^{42} result agrees so well with the experiment. Probably this is because we ignored the repulsive forces on the one hand, while also throwing away the $p_{1/2}$ and $f_{5/2}$ shells on the other hand. Some matrix elements between states (like $f_{7/2}\ f_{5/2}$) coupled to spin 1 are known to be large and will depress the lowest state while the repulsive forces we neglected will compensate this depression.

TABLE 6-1

J^{π} (T=0)	Exp	Phenomenological fit with S-wave force	Result of KB
1^+	-5.00	-5.00	-4.83
3^+	-4.06	-4.04	-4.04
5^+	-3.87	-3.84	-3.69
1^+	-1.87	-1.37	-1.23
2^+	-1.65	-1.65	-1.59

CHAPTER 7

CONCLUSIONS

In this work we used the triplet S-wave free reaction matrix as the nuclear reaction matrix to calculate the $T=0$ spectra of F^{18} and Sc^{42}. The O^{16} and Ca^{40} cores were assumed to be inert. In the case of F^{18} the agreement was qualitative. But for Sc^{42} the predicted spectrum more closely resembled the experimental one. The splitting between the F^{18} ground state and the excited states was generally too large, and the spectrum as a whole was somewhat sensitive to the parameter E in the free reaction matrix. We argued that the sensitivity of the spectra on E can be reduced by including in our K-matrix the most important correction term in (3-8), and the calculated results can be brought into a closer agreement with experiment when high relative orbital wave interactions and core excitations such as the core polarizations are taken into account.

We are thus led to the conclusion that if one wants to obtain a detailed agreement between calculation and experiment, the free reaction matrix cannot literally be used as the two-particle nuclear reaction matrix, since correction terms had to be added. But the approximation (3-9) is certainly a good starting point. The terms not included in (3-9) can be added later. Calculation along these lines are much needed in the future for the understanding of nuclear structure.

APPENDIX A

We had from equation (3-4)

$$|\psi_{\underline{k}}\rangle = |\underline{k}\rangle + \frac{P}{E - t} v |\psi_{\underline{k}}\rangle \tag{A-1}$$

where E is the relative kinetic energy of the scattering particles and t the relative kinetic energy of the intermediate state.

In the coordinate representation, (A-1) becomes

$$\langle \underline{r} | \psi_{\underline{k}}\rangle = \langle \underline{r} | \underline{k}\rangle + \iiint d^3k'' \, d^3k' \, d^3r \, \langle \underline{r} | \underline{k}''\rangle$$

$$\times \quad \langle \underline{k}'' | \frac{P}{E - t} | \underline{k}'\rangle \quad \langle \underline{k}' | \underline{r}'\rangle \, \langle \underline{r}' | v | \psi_{\underline{k}}\rangle \tag{A-2a}$$

or

$$\psi_{\underline{k}}(\underline{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\underline{k}\cdot\underline{r}}$$

$$+ \frac{2M}{\hbar^2} \frac{1}{8\pi^2} P \int d^3k' \int d^3r \; e^{i\underline{k}'\cdot(\underline{r}-\underline{r}')} \frac{1}{k^2 - k'^2} v(\underline{r}') \psi_{\underline{k}}(\underline{r}') \tag{A-2b}$$

Now define

$$I \equiv P \int d^3k' \, e^{i\underline{k}'\cdot(\underline{r}-\underline{r}')} \frac{1}{k^2 - k'^2}$$

$$= \frac{2}{i|\underline{r}-\underline{r}'|} \quad P \int_{-\infty}^{+\infty} e^{ik'|\underline{r}-\underline{r}'|} \frac{1}{k^2 - k'^2} k' \, dk'$$

$$= - \frac{2\pi}{i|\underline{r}-\underline{r}'|} \int_C \frac{e^{ik'|\underline{r}-\underline{r}'|}}{k'^2 - k^2} k' \, dk'$$

The path C is shown in Fig. A-1. Noticing that the integrand vanishes in the upper-half k'-plane for very large k', we have

$$I = -\frac{2\pi}{i|\underline{r} - \underline{r}'|} \oint_{C'} \frac{e^{ik'|\underline{r}-\underline{r}'|}}{k^2 - k'^2}\, k'\, dk'$$

$$- (i\pi)\, \frac{2\pi}{i|\underline{r} - \underline{r}'|} \sum_{k'=\pm k} \mathrm{Res}\left(\frac{e^{ik'|\underline{r}-\underline{r}'|}}{k^2 - k'^2}\, k \right) \qquad \text{(A-3)}$$

The contour C' is shown in Fig. A-2. The first term on the right-hand side of (A-3) vanishes from Cauchy's theorem, so

$$I = -\frac{2\pi^2}{|\underline{r} - \underline{r}'|} \cos (k\, |\underline{r} - \underline{r}'|) \qquad \text{(A-4)}$$

Substituting (A-4) into (A-2b) we have

$$\psi_{\underline{k}}(\underline{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\underline{k}\cdot\underline{r}} - \frac{M}{4\pi\hbar^2} \int d^3r' \frac{\cos(k|\underline{r}-\underline{r}'|)}{|\underline{r} - \underline{r}'|}\, v(\underline{r}')\ {}_{\underline{k}}(\underline{r}') \qquad \text{(A-5)}$$

To see the asymtotic behavior of $\psi_{\underline{k}}(\underline{r})$ we note

$$\lim_{r\to\infty} |\underline{r} - \underline{r}'| = \lim_{r\to\infty} (r^2 + r^2 - 2\underline{r}\cdot\underline{r}')^{1/2}$$

$$= \lim_{r\to\infty} \left(r - \frac{\underline{r}\cdot\underline{r}'}{r} \right) \qquad \text{(A-6)}$$

Thus for large r (A-5) becomes

$$\psi_{\underline{k}}(\underline{r}) \longrightarrow \frac{1}{(2\pi)^{3/2}} e^{i\underline{k}\cdot\underline{r}} - \frac{e^{ikr}}{r} \Lambda(\underline{k}_1,\underline{k}) - \frac{e^{-ikr}}{r} \Lambda(-\underline{k}_1,\underline{k}) \tag{A-7}$$

where $\underline{k}_1 \equiv \frac{k}{r}\, \underline{r}$

and

$$\Lambda(\underline{k}_1,\underline{k}) \equiv \frac{M}{8\pi\hbar^2} \int d^3r' \; e^{i\underline{k}_1\cdot\underline{r}'} \; v(\underline{r}') \; \psi_{\underline{k}}(\underline{r}') \tag{A-8}$$

Since $v(\underline{r}) = v(r)$ is central $\Lambda(\underline{k}_1,\underline{k})$ depends only on the angle between $\underline{k}_1$ and $\underline{k}$, i.e., between $\underline{r}$ and $\underline{k}$, we can expand $\Lambda(\underline{k}_1,\underline{k})$ in the following manner.

$$\Lambda(\underline{k}_1,\underline{k}) = \frac{1}{(2\pi)^{3/2}} \sum_{\ell=0}^{\infty} \sqrt{4\pi(2\ell+1)} \; \lambda_\ell(k) \; Y_{\ell o}(\underline{k},\underline{r}) \tag{A-9a}$$

Also

$$\Lambda(-\underline{k}_1,\underline{k}) = \frac{1}{(2\pi)^{3/2}} \sum_{\ell=0}^{\infty} (-1)^\ell \sqrt{4\pi(2\ell+1)} \; \lambda_\ell(k) \; Y_{\ell o}(\underline{k},\underline{r}) \tag{A-9b}$$

Using the relations

$$e^{i\underline{k}\cdot\underline{r}} = \sum_{\ell=0}^{\infty} \sqrt{4\pi(2\ell+1)} \; i^\ell \cdot j_\ell(kr) \; Y_{\ell o}(\underline{k},\underline{r})$$

and

$$\lim_{Z\to\infty} j_\ell(Z) = \frac{1}{Z} \sin\left(Z - \frac{\ell\pi}{2}\right)$$

and together with (A-9,a) and (A-9b), (A-7) becomes

$$\psi_{\underline{k}}(\underline{r}) \longrightarrow \frac{1}{(2\pi)^{3/2}} \sum_{\ell=0}^{\infty} \frac{\sqrt{4\pi(2\ell+1)}}{kr} \; i^{\ell} \left[\sin\left(kr - \frac{\ell\pi}{2}\right) \right.$$

$$\left. - 2\lambda_{\ell}(k)\, k \cos\left(kr - \frac{\ell\pi}{2}\right)\right] Y_{\ell o}(\underline{k},\underline{r}) \tag{A-10}$$

The phase shift δ_ℓ is defined as follows:

$$\psi_{\underline{k}}(\underline{r}) \longrightarrow \sum_{\ell=0}^{\infty} \sqrt{4\pi(2\ell+1)} \; \frac{i^{\ell}}{kr} \; C_\ell \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right) Y_{\ell o}(\underline{k}\cdot\underline{r}) \tag{A-11}$$

where

$$C_\ell = (2\pi)^{-3/2} (\cos\delta_\ell)^{-1}$$

Comparing (A-10) and (A-11) we have

$$\tan\delta_\ell = -2k\lambda_\ell(k) \tag{A-12}$$

Now define the free reaction matrix K_F

$$K_F(E) \equiv v + v \frac{P}{E - t} K_F(E) \tag{A-13}$$

K_F operated on the free wave state vector $|\underline{k}\rangle$ gives us

$$K_F |\underline{k}\rangle = v |\psi_{\underline{k}}\rangle \tag{A-14}$$

In obtaining (A-14), (A-1) has been used.

Combining (A-8), (A-9), (A-12) and (A-14), we finally have the on-the-energy-shell relation

$$\langle \underline{k}' | \, K_F \left(E = \frac{k^2 \;\; {}^2}{2M}\right) | \, \underline{k} \rangle$$

$$= - \frac{\hbar^2}{2\pi^2 kM} \sum_{\ell=0}^{\infty} \sqrt{4\pi(2 \;+1)} \;\; \tan \delta_\ell \; Y_{\ell o} \, (\underline{k}', \underline{k}) \qquad \text{(A-15)}$$

where

$$|\underline{k}'| = |\underline{k}|$$

Q.E.D.

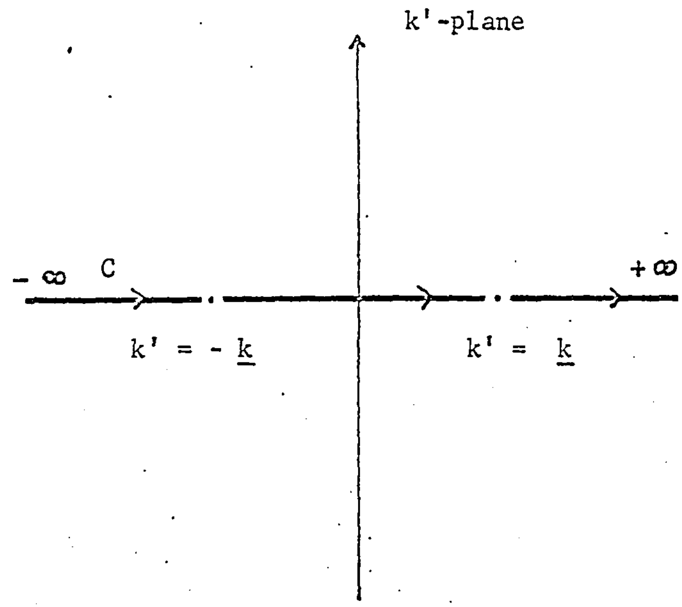

Fig. A-1

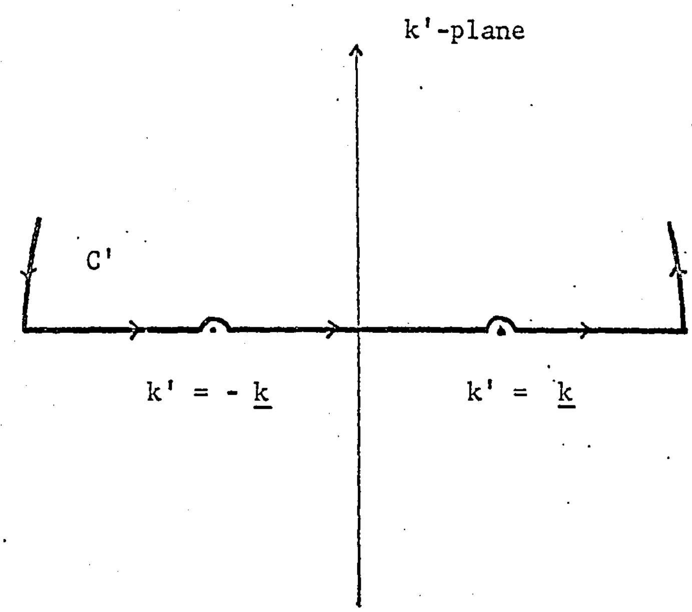

Fig. A-2

APPENDIX B

We had in section 2.2

$$I = P \int_0^\infty \frac{1}{x^2 - a^2} \, g(x) \, dx \qquad \text{(B-1)}$$

where $g(x)$ is analytic in (o, ∞) and $g(x)$ and $g'(x)$ vanish as $x \longrightarrow \infty$ and at $x = 0$.

Integrating by parts, we get from (B-1)

$$I = \frac{1}{2a} P \int_0^\infty \left(\frac{1}{x-a} - \frac{1}{x+a} \right) g(x) \, dx$$

$$= - \frac{1}{2a} \int_0^\infty \frac{g(x)}{x+a} \, dx - \frac{1}{2a} P \int_0^\infty \ln|x-a| \, g'(x) \, dx$$

$$+ \frac{1}{2a} \left\{ \lim_{\epsilon \to 0^+} \left[\left(\ln|x-a| \, g(x) \right) \Big|_{a+\epsilon}^{\infty} + \left(\ln|x-a| \, g(x) \right) \Big|_{0}^{a-\epsilon} \right] \right\} \qquad \text{(B-2)}$$

The terms in the curly bracket in (B-2) vanish at infinity and at $x = 0$. The remaining terms in the bracket vanish as well, since

$$\lim_{\epsilon \to 0^+} \left[-g(a+\epsilon) \ln \epsilon + g(a-\epsilon) \ln \epsilon \right]$$

$$= \lim_{\epsilon \to 0^+} \left[-2\epsilon \, g'(a) \ln \epsilon \right] = 0$$

The second term on the right-hand side of (B-2) is

$$- \frac{1}{2a} \; P \int_0^{\infty} \ln|x-a| g'(x) \, dx$$

$$= \lim_{\epsilon \to 0^+} \left(- \frac{1}{2a} \right) \left[\int_{a+\epsilon}^{\infty} \ln (x-a) \, g'(x) \, dx + \int_0^{a-\epsilon} \ln(a-x) \, g'(x) \, dx \right]$$

$$= - \lim_{\epsilon \to 0^+} \frac{1}{2a} \left\{ \left[(x-a) \ln (x-a) - (x-a) \right] g'(x) \Big|_{a+\epsilon}^{\infty} + \left[(x-a) \ln (a-x) - (x-a) \right] g'(x) \Big|_0^{a-\epsilon} \right\}$$

$$+ \frac{1}{2a} \int_0^{\infty} \left[(x-a) \ln |x-a| - (x-a) \right] g''(x) \, dx \qquad \text{(B-3)}$$

The terms in the bracket vanish. So finally we have

$$I = -\frac{1}{2a} \int_0^{\infty} \frac{g(x)}{x+a} \, dx + \frac{1}{2a} \int_0^{\infty} (x-a) \; (\ln(x-a)-1) \; g''(x) \, dx$$

Q.E.D.

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