## Appendix 6.E Single-nucleon transfer for pedestrians

In this Appendix we discuss some aspects of threlation existing between nuclear structure and one–particle transfer cross sections. To do so, we repeat some of the steps carried out in the text but this time in the most simple and straightforward way, ignoring the complications associated with the spin carried out by the particles, the spin–orbit dependence of the optical model potential, the recoil effect, etc. We consider the case of A(d, p)A + 1 reaction, namely of neutron stripping. The intrinsic wave functions  $\psi_{\alpha}$  and  $\psi_{\beta}$ , where  $\alpha = (A, d)$  and  $\beta = ((A + 1), p)$ .

$$\psi_{\alpha} = \psi_{M_{\Lambda}}^{I_{\Lambda}}(\xi_{\Lambda})\phi_{d}(\vec{r}_{np}), \tag{6.E.1a}$$

$$\psi_{\beta} = \psi_{M_{A+1}}^{I_{A+1}}(\xi_{A+1})$$

$$= \sum_{l,l',} (I'_A; l| J_{A+1}) [\psi^{I'_A}(\xi_A) \phi^l(\vec{r}_n)]_{M_{A+1}-M_A}^{I_{A+1}},$$
(6.E.1b)

where  $(I'_A; l|)I_{A+1})$  is a generalized fractional parentage coefficient. It is of notice that this fractional parentage expansion is not well defined. In fact, as a rule,

 $(I'_A; I|)I_{A+1})\phi'(\vec{r}_n)_{M_{A+1}-M_A}$  is an involved, dressed quasiparticle state containing only a fraction of the "pure" single particle strength (cf.  $\mathcal{B}$ ). For simplicity we assume the expansion is operative. To further simplify the derivation we assume we are dealing with spinless particles. The variable  $\vec{r}_{np}$  is the relative coordinate of the proton and the neutron (see Fig.  $\mathcal{B}$ ).

The transition matrix element can now be written as

$$T_{d,p} = \langle \psi_{M_{A+1}}^{I_{A+1}}(\xi_{A+1})\chi_{p}^{(-)}(k_{p},\vec{r}_{p}), V_{\beta}^{\prime}\psi_{M_{A}}^{I_{A}}(\xi_{A})\chi_{d}^{(+)}(k_{d},\vec{r}_{d})\rangle \not\stackrel{H}{=}$$

$$= \sum_{l,l'_{A}} (I'_{A};l|\{I_{A+1})(I'_{A}M'_{A}lM_{A+1} - M'_{A}|I_{A+1}M_{A+1})$$

$$= \sum_{l,l'_{A}} (I'_{A};l|\{I_{A+1})(I'_{A}M'_{A}lM_{A+1} - M'_{A}|I_{A+1}M_{A+1})$$

$$\times \int d\vec{r}_{n}d\vec{r}_{p}\chi_{p}^{*(-)}(k_{p},\vec{r}_{p})\phi_{M_{A+1}-M'_{A}}^{*l}(\vec{r}_{n})(\psi_{M_{A}}^{I_{A}}(\xi_{A}), V'_{\beta}\psi_{M'_{A}}^{l'_{A}}(\xi_{A}))$$

$$\times \phi_{d}(\vec{r}_{np})\chi_{d}^{(+)}(k_{d},\vec{r}_{d}) \delta_{l'_{A},I_{A}}\delta_{M'_{A},M_{A}}.$$

$$(6.E.2)$$

In the stripping approximation

$$V'_{\beta} = V_{\beta}(\xi, \vec{r}_{\beta}) - \bar{U}_{\beta}(r_{\beta})$$

$$= V_{\beta}(\xi_{A}, \vec{r}_{pA}) + V_{\beta}(\vec{r}_{pn}) - \bar{U}_{\beta}(r_{pA})$$
(6.E.3)

Then

$$(\psi_{M_A}^{I_A}(\xi_A), V_{\beta}' \psi_{M_A}^{I_A}(\xi_A)) = (\psi_{M_A}^{I_A}(\xi_A), V_{\beta}(\xi_A, \vec{r}_{pA}) \psi_{M_A}^{I_A}(\xi_A)) + (\psi_{M_A}^{I_A}(\xi_A), V_{\beta}(\vec{r}_{pn}) \psi_{M_A}^{I_A}(\xi_A)) - \bar{U}_{\beta}(r_{pA}).$$
(6.E.4)

We assume

$$U_{\beta}(r_{pA}) = (\psi_{M_A}^{I_A}(\xi_A), V_{\beta}(\xi_A, \vec{r}_{pA})\psi_{M_A}^{I_A}(\xi_A)). \tag{6.E.5}$$

Then

$$(\psi_{M_A}^{l_A}(\xi_A), V_{\beta}' \psi_{M_A}^{l_A}(\xi_A)) = V_{np}(\vec{r}_{pn}) \ \ \rho \tag{6.E.6}$$

Inserting eq. (6.E.6) into eq. (6.E.2) we obtain

$$T_{d,p} = \sum_{l} (I_{A}; l| I_{A+1}) (I_{A} M_{A} l M_{A+1} - M_{A} | I_{A+1} M_{A+1})$$

$$\times \int d\vec{r}_{n} d\vec{r}_{p} \chi_{p}^{*(-)}(k_{p}, \vec{r}_{p}) \phi_{M_{A+1}-M_{A}}^{*l}(\vec{r}_{n}) V(\vec{r}_{pn}) \phi_{d}(\vec{r}_{np}) \chi_{d}^{(+)}(k_{d}, \vec{r}_{d})$$
(6.E.7)

[Appenduer] 6 A and 6 B

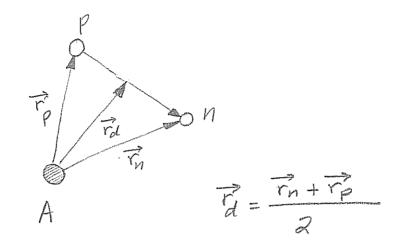


Fig. 6, E. 1 Gordenate used in the description of the A(d,p)(A+1) stripping

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The differential cross section is then equal to

$$\frac{d\sigma}{d\Omega} = \frac{2}{3} \frac{\mu_p \mu_d}{(2\pi\hbar^2)^2} \frac{(2I_{A+1} + 1)}{(2I_A + 1)} \frac{k_p}{k_d} \sum_{l,m_l} \frac{(I_A; l||I_{A+1})^2}{2l + 1} |B_{m_l}^l|^2, \tag{6.E.8}$$

where

$$B_{m_l}^l(\theta) = \int d\vec{r}_n d\vec{r}_p \chi_p^{*(-)}(k_p, \vec{r}_p) Y_m^{*l}(\hat{r}_n) u_{nl}(r_n) V(\vec{r}_{pn}) \phi_d(\vec{r}_{np}) \chi_d^{(+)}(k_d, \vec{r}_d)$$
(6.E.9)

and

The relation

$$\phi_m^l(\vec{r}_n) = u_{nl}(r_n)Y_m^l(\hat{r}_n)$$
, (6.E.10)

is the single-particle wave function of a neutron moving in the core A. For simplicity, the radial wave function  $u_{nl}(r_n)$  can be assumed to be a solution of a Saxon-Woods potential of parameters  $V_0 \approx 50$  MeV, a = 0.65 fm and  $r_0 = 1.25$  fm.

Equation (6.E.8) gives the cross section for the stripping from the projectile of a neutron that would correspond to the  $n^{th}$  valence neutron in the nucleus (A + 1). If we now want the cross section for stripping any of the valence nutrons of the final nucleus from the projectile, we must multiply eq. (6.E.8) by n. A more careful treatment of the antisymmetry with respect to the neutrons shoes this to be the correct answer.

Finally we get

$$\frac{d\sigma}{d\Omega} = \frac{(2I_{A+1} + 1)}{(2I_A + 1)} \sum_{l} S_l \sigma_l(\theta)$$
 (6.E.11)

where

$$S_l = n(I_A; l||I_{A+1})^2$$
 (6.E.12)

and

$$\sigma_l(\theta) = \frac{2}{3} \frac{\mu_p \mu_d}{(2\pi\hbar^2)^2} \frac{k_p}{k_d} \frac{1}{2l+1} \sum_m |B_m^l|^2$$
 (6.E.13)

The distorted wave programs numerically evaluate the quantity  $B_{m_l}^l(\theta)$ , using for the wave functions  $\chi^{(-)}$  and  $\chi^{(+)}$  the solution of the optical potentials that fit the elastic scattering, i.e.

$$(-\nabla^2 + \bar{U} - k^2)\chi = 0$$
 (6.E.14)

(see eq.  $(6.\dot{\mathbf{R}})$ 15)). Note that if the target nucleus is even,  $I_A = 0$ ,  $I = I_{A+1}$ . That is, only one I value contributes in eq.  $(6.\dot{\mathbf{E}}.8)$ , and the angular distribution is uniquely given by  $\sum_m |B_m^l|^2$ . The I-dependence of the angular distributions helps to identify  $I = I_{A+1}$ . The factor  $S_I$  needed to normalize the calculated function to the data yields (assuming a good fit to the angular distribution), is known in the literature as the spectroscopic factor. It was assumed not only that it could be defined, but also that it contained all the nuclear structure information (aside from that associated with the angular distribution) which could be extracted from single-particle transfer. In other words, that it was the bridge directly connecting theory with experiment.—Because-nucleons are never bare, but are dressed by the coupling to collective modes (cf.  $(\mathbf{R})$ ), the spectroscopic factor approximation is at best a helpful tool to get order of magnitude information from one particle transfer data. There is a fundamental problem which makes the handling of integrals like that of  $(6.\dot{\mathbf{E}}.9)$  difficult to handle, if not numerically at least conceptually. This difficulty is connected with the so called recoil effect  $^2$ , namely the fact that the

<sup>2</sup>While this effect could be treated in a cavalier fashion in the case of light ion reactions  $(m_a/m_A \ll 1)$ , this was not possible in the case of heavy ion reactions, as the change in momenta involved were always sizeable (cf. Breglia and Winther, 1991 and refs. therein). was

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center of mass of the two interacting particles in entrance  $(\mathbf{r}_{\alpha}: \alpha = a + A)$  and exit  $(\mathbf{r}_B : \beta = b + B)$  channels is different. This is at variance with what one is accustomed to deal with in nuclear structure calculations, in which the Hartree potential depends on a single coordinate, as well as in the case of elastic and inelastic reactions, situations in which  $\mathbf{r}_{\alpha} = \mathbf{r}_{\beta}$ . When  $\mathbf{r}_{\alpha} \neq \mathbf{r}_{\beta}$  we enter a rather more complex many-body problem, in particular if continuum states are to be considered, than nuclear structure practitioners were accustomed to.

Of notice that similar difficulties have been faced in connection with the non-local k (exchange) potential. As a rule, the corresponding (HF) man factor for the corresponding to the corresponding t Fock (exchange) potential. As a rule, the corresponding (HF) mean field equations are rendered local making use of the k-mass approximation or within the framework of Local Density Functional Theory (DFT), in particular with the help of the Kohn-Sham equations (see e.g. C. Mahaux et al. (1985), Broglia et al. (2004)). Although much of the work in this field is connected with the correlation potential (interweaving of single-particle and collective motion), an important fraction is connected with the exchange potential.

In any case, and returning to the subject of the present appendix, it is always useful to be able to introduce approximations which can help the physics which is at the basis of the phenomenon under discussion (single-particle motion) emerge in a natural way, if not to compare in detail with the experimental data. Within this context, to reduce the integral (6.E.9) it is customary to assume that the proton-neutron interaction  $V_{np}$  has zero-range, i.e.

$$V_{np}(\vec{r}_{np})\phi_d(\vec{r}_{np}) = D_0\delta(\vec{r}_{np})$$
 (6.E.15)

so that  $B_m^l$  becomes equal to

$$B_{m_l}^l(\theta) = D_0 \int d\vec{r} \chi_p^{*(-)}(k_p, \vec{r}) Y_{m_l}^{*l}(\hat{r}) u_l(r) \chi_d^{(+)}(k_d, \vec{r}), \tag{6.E.16}$$

which is a three dimensional integral, but in fact essentially a one-dimensional integral, as the integration over the angles is simple to carry out.

Plane-wave limit

If in eq. (6.E.14) we set  $\bar{U} = 0$ , the distorted waves become plane waves i.e.

$$\chi_d^{(+)}(k_d, \vec{r}) = e^{i\vec{k}_d \cdot \vec{r}},$$
 (6.E.17a)

$$\chi_d^{*(-)}(k_p, \vec{r}) = e^{-i\vec{k}_p \cdot \vec{r}}.$$
 (6.E.17b)

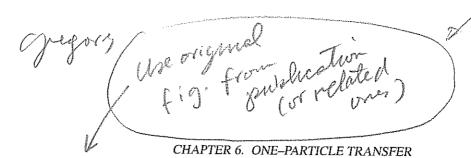
Equation (6.E.16) can now be written as

$$B_{m}^{l} = D_{0} \int d\vec{r} e^{i(\vec{k}_{d} - \vec{k}_{p}) \cdot \vec{r}} Y_{m}^{*l}(\hat{r}) u_{l}(r). \tag{6.E.18}$$

The linear momentum transferred to the nucleus is  $\vec{k}_d - \vec{k}_p = \vec{q}$ . Let us expand  $e^{i\vec{q}\cdot\vec{r}}$  in spherical harmonics, i.e.

$$e^{i\vec{q}\cdot\vec{r}} = \sum_{l} i^{l} j_{l}(qr)(2l+1) P_{l}(\hat{q}\cdot\hat{r})$$

$$= 4\pi \sum_{l} i^{l} j_{l}(qr) \sum_{m} Y_{m}^{*l}(\hat{q}) Y_{m}^{l}(\hat{r}),$$
(6.E.19)



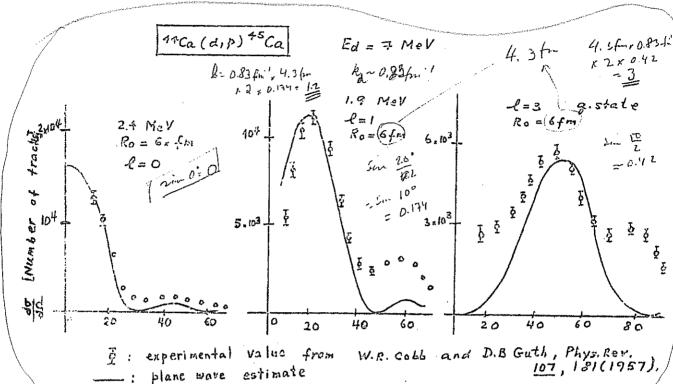


Figure 6.E.1:

so

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$$\int d\hat{r}e^{i\vec{q}\cdot\vec{r}}Y_{m}^{l}(\hat{r}) = 4\pi i^{l}j_{l}(qr)Y_{m}^{*l}(\hat{q}). \tag{6.E.20}$$

Then

$$\sum_{m} |B_{m}^{l}|^{2} = \sum_{m} |Y_{m}^{l}(\hat{q})|^{2} D_{0}^{2} 16\pi^{2} \times$$

$$\left| \int_{0}^{\infty} r^{2} dr j_{l}(qr) u_{l}(r) \right|^{2} =$$

$$\frac{2l+1}{4\pi} D_{0}^{2} 16\pi^{2} \left| \int_{0}^{\infty} r^{2} dr j_{l}(qr) u_{l}(r) \right|^{2}.$$

$$O^{\infty \ell}$$

Thus, the angular distribution is given by the integral  $\left|\int r^2 dr j_l(qr)u_l(r)\right|_{+}^{2}$ . If we assume 5 that the process takes place mostly on the surface, the angular distribution will be given by  $\left|j_l(qR_0)\right|_{+}^{2}$ , where  $R_0$  is the nuclear radius.

We then have

$$q^{2} = k_{d}^{2} + k_{p}^{2} - 2k_{d}k_{p}\cos(\theta)$$

$$= (k_{d}^{2} + k_{p}^{2} - 2k_{d}k_{p}) + 2k_{d}k_{p}(1 - \cos(\theta))$$

$$= (k_{d} - k_{p})^{2} + 4k_{d}k_{p}(\sin(\theta/2))^{2}$$

$$\approx 4k_{d}k_{p}(\sin(\theta/2))^{2}$$
(6.E.22)

Plane-wave approximation analysis of three

44 Ca (d,p) 45 Ca differential cross section leading
to the ground state (l=3), to the 1,9 MeV (l=1)

and lead 2,4 MeV (l=0) excited states, i.e f3/2, 19/2 and
51/2 states (Cobbon 16,11,11,1957)

While the derivation presented below is quite general, special emphasis is set to one-particle knochout snockers.

6.F. ONE-PARTICLE KNOCKOUT WITHIN DWBA

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since  $k_d \approx k_p$  for stripping reactions at typical energies. Thus the angular distribution has a diffraction-like structure given by

$$|j_l(qR_0)|^2 = j_l^2 (2R_0 \sqrt{k_d k_p} \sin(\theta/2)).$$
 (6.E.23)

The function  $j_l(x)$  has its first maximum at x = l, i.e. where

$$\sin(\theta/2) = \frac{l}{2R_0k}, \qquad (k_p \approx k_d = k), \tag{6.E.24}$$

Examples of the above relation are provided in Fig. 2 6.E.1

# Appendix 6.F One-particle knockout within DWBA

## 6.F.1 Spinless particles

We are going to consider the reaction  $A + a \rightarrow a + b + c$ , in which the cluster b is knocked out from the nucleus A(=c+b). Cluster b is thus initially bounded, while the final states of a, b and the initial state of a are all in the continuum, and can be described with distorted waves defined as scattering solutions of a (as a rule, complex) suitable optical potential. A schematic depiction of the situation is shown in Fig. 6.F.1. We will begin by considering the simplified case in which the clusters a, b, c are spinless.

#### Transition amplitude

We consider optical potentials  $U(r_{aA})$ ,  $U(r_{cb})$ ,  $U(r_{ac})$  which will be central potentials without a spin-orbit term. In addition, the interaction  $v(r_{ab})$  between a and b is taken to be an arbitrary function of the distance  $r_{ab}$ . Then, the transition amplitude which is at the basis of the evaluation of the multi-differential cross section is the 6-dimensional integral

$$T_{m_b} = \int d\mathbf{r}_{aA} d\mathbf{r}_{bc} \chi^{(-)*}(\mathbf{r}_{ac}) \chi^{(-)*}(\mathbf{r}_{bc}) v(r_{ab}) \chi^{(+)}(\mathbf{r}_{aA}) u_{l_b}(r_{bc}) Y_{m_b}^{l_b}(\hat{\mathbf{r}}_{bc}). \tag{6.F.1}$$

#### Coordinates

The vectors  $\mathbf{r}_{ab}$ ,  $\mathbf{r}_{ac}$  can easily be written in function of the integration variables  $\mathbf{r}_{aA}$ ,  $\mathbf{r}_{bc}$  (see Fig. 6.F.1), namely

$$\mathbf{r}_{ac} = \mathbf{r}_{aA} + \frac{b}{A}\mathbf{r}_{bc},$$

$$\mathbf{r}_{ab} = \mathbf{r}_{aA} - \frac{c}{A}\mathbf{r}_{bc},$$
(6.F.2)

where b, c, A stand for the number of nucleons of the species b, c and A respectively.

## Distorted waves in the continuum

A standard way to reduce the dimensionality of the integral (6.F.1) consists in expanding the continuum wave functions  $\chi^{(+)}(\mathbf{r}_{aA}), \chi^{(-)*}(\mathbf{r}_{ac}), \chi^{(-)*}(\mathbf{r}_{bc})$  in a basis of eigenstates of

ecuaciones siengras la parentesi the angular momentum operator (partial waves). Then we can exploit the transformation properties of these eigenstates under rotations to perform the angular integrations. With time–reversed phase convention, that is

$$Y_m^l(\theta,\phi) = i^l \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\phi},$$
 (6.F.3)

the general form of these expansions is

$$\chi^{(+)}(\mathbf{k}, \mathbf{r}) = \sum_{l} \frac{4\pi}{kr} t^{l} \sqrt{2l+1} e^{i\sigma^{l}} F_{l}(r) \left[ Y^{l}(\hat{\mathbf{r}}) Y^{l}(\hat{\mathbf{k}}) \right]_{0}^{0}, \tag{6.F.4}$$

$$\chi^{(-)*}(\mathbf{k}, \mathbf{r}) = \sum_{l} \frac{4\pi}{kr} i^{-l} \sqrt{2l+1} e^{i\sigma^{l}} F_{l}(r) \left[ Y^{l}(\hat{\mathbf{r}}) Y^{l}(\hat{\mathbf{k}}) \right]_{0}^{0}, \tag{6.F.5}$$

where  $\sigma_l$  is the Coulomb phase shift. The radial functions  $F_l(r)$  are regular (finite at r=0) solutions of the one-dimensional Schrödinger equation with an effective potential  $U(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2}$  and suitable asymptotic behaviour at  $r \to \infty$  as boundary conditions. So the distorted waves appearing in (6.F.1) are

$$\chi^{(+)}(\mathbf{k}_{\mathbf{a}}, \mathbf{r}_{aA}) = \sum_{l_a} \frac{4\pi}{k_a r_{aA}} i^{l_a} \sqrt{2l_a + 1} e^{i\sigma^{l_a}} F_{l_a}(r_{aA}) \left[ Y^{l_a}(\hat{\mathbf{r}}_{aA}) Y^{l_a}(\hat{\mathbf{k}}_a) \right]_0^0, \tag{6.F.6}$$

(initial relative motion between A and a, defined from the complex optical potential  $U(r_{Aa})$ )

$$\chi^{(-)*}(\mathbf{k}'_{a}, \mathbf{r}_{ac}) = \sum_{l'_{a}} \frac{4\pi}{k'_{a}r_{ac}} i^{-l'_{a}} \sqrt{2l'_{a} + 1} e^{i\alpha l'_{a}} F_{l'_{a}}(r_{ac}) \left[ Y^{l'_{a}}(\hat{\mathbf{k}}_{ac}) Y^{l'_{a}}(\hat{\mathbf{k}}'_{a}) \right]_{0}^{0}, \tag{6.F.7}$$

(final relative motion between c and a, defined from the complex optical potential  $U(r_{ac})$ )

$$\chi^{(-)*}(\mathbf{k}_{b}', \mathbf{r}_{bc}) = \sum_{l_{b}'} \frac{4\pi}{k_{b}' r_{bc}} i^{-l_{b}'} \sqrt{2l_{b}' + 1} e^{i\sigma_{b}'} F_{l_{b}'}(r_{bc}) \left[ Y^{l_{b}'}(\hat{\mathbf{r}}_{bc}) Y^{l_{b}'}(\hat{\mathbf{k}}_{b}') \right]_{0}^{0}, \tag{6.F.8}$$

(final relative motion between b and c, defined from the complex optical potential  $U(r_{bc})$ ).

### Recoupling of angular momenta

We thus need to evaluate the 6-dimensional integral

$$\frac{64\pi^{3}}{k_{a}k'_{a}k'_{b}} \int d\mathbf{r}_{aA}d\mathbf{r}_{bc}u_{l_{b}}(r_{cb})v(r_{ab}) \sum_{l_{a},l'_{a},l'_{b}} \sqrt{(2l_{a}+1)(2l'_{a}+1)(2l'_{b}+1)} \\
\times e^{i(\sigma^{l_{a}}+\sigma^{l'_{a}}+\sigma^{l'_{b}})} \frac{F_{l_{a}}(r_{aA})F_{l'_{a}}(r_{ac})F_{l'_{b}}(r_{bc})}{r_{ac}r_{aA}r_{bc}} \\
\times \left[Y^{l_{a}}(\hat{\mathbf{r}}_{aA})Y^{l_{a}}(\hat{\mathbf{k}}_{a})\right]_{0}^{0} \left[Y^{l'_{a}}(\hat{\mathbf{r}}_{ac})Y^{l'_{a}}(\hat{\mathbf{k}}'_{a})\right]_{0}^{0} \left[Y^{l'_{b}}(\hat{\mathbf{r}}_{bc})Y^{l'_{b}}(\hat{\mathbf{k}}'_{b})\right]_{0}^{0} Y^{l_{b}}_{m_{b}}(\hat{\mathbf{r}}_{bc}).$$
(6.F.9)

Note that this expression depends explicitly on the asymptotic kinetic energies  $(k_a, k'_a, k'_b)$  and scattering angles  $(\hat{\mathbf{k}}_a, \hat{\mathbf{k}}'_a, \hat{\mathbf{k}}'_b)$  of a, b. Now we will take advantage of the partial

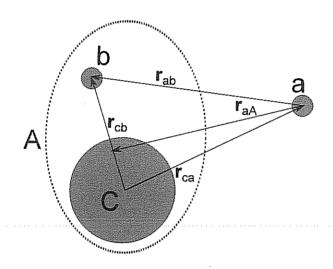


Figure 6.F.1: Sketch of the system considered to describe the reaction  $A+a \rightarrow a+b+c$ . The nucleus A is viewed as an inert cluster b bounded to an inert core c.

wave expansion to reduce the dimensions of the integral from 6 to 3. A possible strategy to deal with (6.F.9)s to recouple together all the terms that depend on the integration variables to a global angular momentum and retain only the term coupled to 0 as the only one surviving the integration. Let us couple separately the terms corresponding to particle a and particle b. For particle a

$$\begin{split} \left[ Y^{l_{a}}(\hat{\mathbf{r}}_{aA}) Y^{l_{a}}(\hat{\mathbf{k}}_{a}) \right]_{0}^{0} \left[ Y^{l'_{a}}(\hat{\mathbf{r}}_{ac}) Y^{l'_{a}}(\hat{\mathbf{k}}'_{a}) \right]_{0}^{0} &= \sum_{K} ((l_{a}l_{a})_{0} (l'_{a}l'_{a})_{0} | (l_{a}l'_{a})_{K} (l_{a}l'_{a})_{K})_{0} \\ &\times \left\{ \left[ Y^{l_{a}}(\hat{\mathbf{r}}_{aA}) Y^{l'_{a}}(\hat{\mathbf{r}}_{ac}) \right]^{K} \left[ Y^{l_{a}}(\hat{\mathbf{k}}_{a}) Y^{l'_{a}}(\hat{\mathbf{k}}'_{a}) \right]^{K} \right\}_{0}^{0}. \end{split}$$
(6.F.10)

We can evaluate the 9 i symbol,

$$((l_a l_a)_0 (l'_a l'_a)_0 | (l_a l'_a)_K (l_a l'_a)_K)_0 = \sqrt{\frac{2K+1}{(2l'_a+1)(2l_a+1)}},$$
(6.F.11)

and expand the coupling,

$$\begin{aligned}
& \left\{ \left[ Y^{l_{a}}(\hat{\mathbf{r}}_{aA}) Y^{l'_{a}}(\hat{\mathbf{r}}_{ac}) \right]^{K} \left[ Y^{l_{a}}(\hat{\mathbf{k}}_{a}) Y^{l'_{a}}(\hat{\mathbf{k}}'_{a}) \right]^{K} \right\}_{0}^{0} = \sum_{M} \langle K | K | M - M | 0 | 0 \rangle \\
& \times \left[ Y^{l_{a}}(\hat{\mathbf{r}}_{aA}) Y^{l'_{a}}(\hat{\mathbf{r}}_{ac}) \right]_{M}^{K} \left[ Y^{l_{a}}(\hat{\mathbf{k}}_{a}) Y^{l'_{a}}(\hat{\mathbf{k}}'_{a}) \right]_{-M}^{K} = \sum_{M} \frac{(-1)^{K+M}}{\sqrt{2K+1}} \\
& \times \left[ Y^{l_{a}}(\hat{\mathbf{r}}_{aA}) Y^{l'_{a}}(\hat{\mathbf{r}}_{ac}) \right]_{M}^{K} \left[ Y^{l_{a}}(\hat{\mathbf{k}}_{a}) Y^{l'_{a}}(\hat{\mathbf{k}}'_{a}) \right]_{-M}^{K}.
\end{aligned} (6.F.12)$$

Thus.

$$\left[Y^{l_{a}}(\hat{\mathbf{r}}_{aA})Y^{l_{a}}(\hat{\mathbf{k}}_{a})\right]_{0}^{0} \left[Y^{l'_{a}}(\hat{\mathbf{r}}_{ac})Y^{l'_{a}}(\hat{\mathbf{k}}'_{a})\right]_{0}^{0} = \sqrt{\frac{1}{(2l'_{a}+1)(2l_{a}+1)}} \times \sum_{KM} (-1)^{K+M} \left[Y^{l_{a}}(\hat{\mathbf{r}}_{aA})Y^{l'_{a}}(\hat{\mathbf{r}}_{ac})\right]_{M}^{K} \left[Y^{l_{a}}(\hat{\mathbf{k}}_{a})Y^{l'_{a}}(\hat{\mathbf{k}}'_{a})\right]_{-M}^{K}.$$
(6.F.13)

We can further simplify the above expression if we take the direction of the initial momentum to be parallel to the z axis, so  $Y_m^{l_n}(\hat{\mathbf{k}}_n) = Y_m^{l_n}(\hat{\mathbf{z}}) = \sqrt{\frac{2l_n+1}{4\pi}} \delta_{m,0}$ . Then,

$$\left[Y^{l_a}(\hat{\mathbf{r}}_{aA})Y^{l_a}(\hat{\mathbf{k}}_a)\right]_0^0 \left[Y^{l'_a}(\hat{\mathbf{r}}_{ac})Y^{l'_a}(\hat{\mathbf{k}}'_a)\right]_0^0 = \sqrt{\frac{1}{4\pi(2l'_a+1)}} \sum_{KM} (-1)^{K+M} \\
\times \langle l_a \ 0 \ l'_a \ -M|K \ -M \rangle \left[Y^{l_a}(\hat{\mathbf{r}}_{aA})Y^{l'_a}(\hat{\mathbf{r}}_{ac})\right]_M^K Y^{l'_a}_{-M}(\hat{\mathbf{k}}'_a).$$
(6.F.14)

For the particle b we have

$$Y_{m_b}^{l_b}(\hat{\mathbf{r}}_{bc}) \left[ Y_{m_b}^{l_b}(\hat{\mathbf{r}}_{bc}) Y_{bc}^{l_b}(\hat{\mathbf{k}}_b') \right]_0^0 = Y_{m_b}^{l_b}(\hat{\mathbf{r}}_{cb}) \sum_m \frac{(-1)^{l_b'+m}}{\sqrt{2l_b'+1}} Y_m^{l_b'}(\hat{\mathbf{r}}_{bc}) Y_{-m}^{l_b'}(\hat{\mathbf{k}}_b'), \tag{6.F.15}$$

but we can write

$$Y_{m_b}^{l_b}(\hat{\mathbf{r}}_{bc})Y_m^{l_b}(\hat{\mathbf{r}}_{bc}) = \sum_{K'} \langle l_b \ m_b \ l_b' \ m|K' \ m_b + m \rangle \left[ Y^{l_b}(\hat{\mathbf{r}}_{bc})Y_b^{l_b'}(\hat{\mathbf{r}}_{bc}) \right]_{m_b+m}^{K'}. \tag{6.F.16}$$

In order to couple to 0 angular momentum with 6.F.14 we must only keep the term with K' = K,  $m = -M - m_b$  so

$$Y_{m_b}^{l_b}(\hat{\mathbf{r}}_{bc}) \left[ Y_{m_b}^{l'_b}(\hat{\mathbf{r}}_{bc}) Y_{b}^{l'_b}(\hat{\mathbf{k}}_b') \right]_0^0 = \frac{(-1)^{l'_b - M - m_b}}{\sqrt{2l'_b + 1}} \langle l_b \ m_b \ l'_b - M - m_b | K - M \rangle \times \left[ Y_{bc}^{l_b}(\hat{\mathbf{r}}_{bc}) Y_{bc}^{l'_b}(\hat{\mathbf{r}}_{bc}) \right]_{-M}^K Y_{-M - m_b}^{l_b}(\hat{\mathbf{k}}_b'),$$
(6.F.17)

and 6.F.9 becomes

$$\frac{32\pi^{2}}{k_{a}k'_{a}k'_{b}} \sum_{KM} (-1)^{K+l'_{b}-m_{b}} \langle l_{a} \ 0 \ l'_{a} - M|K - M\rangle \langle l_{b} \ m_{b} \ l'_{b} - M - m_{b}|K - M\rangle 
\times \sum_{l_{a},l'_{a},l'_{b}} \sqrt{(2l_{a}+1)} e^{i(\sigma^{l_{a}}+\sigma^{l'_{a}}+\sigma^{l'_{b}})} Y_{-M-m_{b}}^{l'_{b}}(\hat{\mathbf{k}}'_{b}) Y_{-M}^{l'_{a}}(\hat{\mathbf{k}}'_{a}) \int d\mathbf{r}_{aA} d\mathbf{r}_{bc} u_{l_{b}}(r_{bc}) v(r_{ab}) 
\times \frac{F_{l_{a}}(r_{aA})F_{l'_{a}}(r_{ac})F_{l'_{b}}(r_{bc})}{r_{ac}r_{aA}r_{bc}} \left[ Y^{l_{a}}(\hat{\mathbf{r}}_{aA})Y^{l'_{a}}(\hat{\mathbf{r}}_{ac}) \right]_{M}^{K} \left[ Y^{l_{b}}(\hat{\mathbf{r}}_{bc})Y^{l'_{b}}(\hat{\mathbf{r}}_{bc}) \right]_{-M}^{K}.$$
(6.F.18)

Note that

$$\begin{split} \left[ Y^{l_{a}}(\hat{\mathbf{r}}_{aA}) Y^{l'_{a}}(\hat{\mathbf{r}}_{ac}) \right]_{M}^{K} \left[ Y^{l_{b}}(\hat{\mathbf{r}}_{bc}) Y^{l'_{b}}(\hat{\mathbf{r}}_{bc}) \right]_{-M}^{K} &= \sum_{P} \langle K \ M \ K \ - M | P \ 0 \rangle \\ &\times \left\{ \left[ Y^{l_{a}}(\hat{\mathbf{r}}_{aA}) Y^{l'_{a}}(\hat{\mathbf{r}}_{ac}) \right]^{K} \left[ Y^{l_{b}}(\hat{\mathbf{r}}_{bc}) Y^{l'_{b}}(\hat{\mathbf{r}}_{bc}) \right]^{K} \right\}_{0}^{P}, \end{split}$$
(6.F.19)

and that to survive the integration the rotational tensors must be coupled to P = 0. Keeping only this term in the sum over P, we get

$$\left[Y^{l_{a}}(\hat{\mathbf{r}}_{aA})Y^{l'_{a}}(\hat{\mathbf{r}}_{ac})\right]_{M}^{K} \left[Y^{l_{b}}(\hat{\mathbf{r}}_{bc})Y^{l'_{b}}(\hat{\mathbf{r}}_{bc})\right]_{-M}^{K} = \frac{(-1)^{K+M}}{\sqrt{2K+1}} \left\{ \left[Y^{l_{a}}(\hat{\mathbf{r}}_{aA})Y^{l'_{a}}(\hat{\mathbf{r}}_{ac})\right]^{K} \left[Y^{l_{b}}(\hat{\mathbf{r}}_{bc})Y^{l'_{b}}(\hat{\mathbf{r}}_{bc})\right]^{K}\right\}_{0}^{0}.$$
(6.F.20)

The coordinate-dependent part of the latter expression is a rotationally invariant scalar, so it can be evaluated in any conventional "standard" configuration such as the one depicted in Fig. 6.F.2. It must then be multiplied by a factor resulting of the integration of the remaining angular variables, which accounts for the rigid rotations needed to connect any arbitrary configuration to one of this type. This factor turns out to be  $8\pi^2$  (a  $4\pi$  factor for all possible orientations of, say,  $\mathbf{r}_{aA}$  and a  $2\pi$  factor for a complete rotation around its direction). According to Fig. 6.F.2,

$$\mathbf{r}_{bc} = r_{bc} \left( \sin \theta \, \hat{x} + \cos \theta \, \hat{z} \right),$$

$$\mathbf{r}_{aA} = -r_{aA} \, \hat{z},$$

$$\mathbf{r}_{ac} = \frac{b}{A} r_{bc} \sin \theta \, \hat{x} + \left( \frac{b}{A} r_{bc} \cos \theta - r_{aA} \right) \hat{z}.$$
(6.F.21)

As  $\mathbf{r}_{aA}$  lies parallel to the z axis,  $Y_{M_K}^{l_a}(\hat{\mathbf{r}}_{aA}) = \sqrt{\frac{2l_a+1}{4\pi}}\delta_{M_K,0}$  and

$$\begin{split} \left[ Y^{l_a}(\hat{\mathbf{r}}_{aA}) \ Y^{l'_a}(\hat{\mathbf{r}}_{ac}) \right]_{M_K}^K &= \sum_m \langle l_a \ m \ l'_a \ M_K - m | K \ M_K \rangle Y^{l_a}_m(\hat{\mathbf{r}}_{aA}) Y^{l'_a}_{M_K - m}(\hat{\mathbf{r}}_{ac}) = \\ \sqrt{\frac{2l_a + 1}{4\pi}} \langle l_a \ 0 \ l'_a \ M_K | K \ M_K \rangle Y^{l'_a}_{M_K}(\hat{\mathbf{r}}_{ac}). \end{split} \tag{6.F.22}$$