Nuclear Reaction Theory: concepts and applications – Part I

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100 years of nuclei – scattering was critical

[669]

LXXIX. The Scattering of α and β Particles by Matter and the Structure of the Atom. By Professor E. RUTHERFORD, F.R.S., University of Manchester *.

§ 1. IT is well known that the α and β particles suffer deflexions from their rectilinear paths by encounters with atoms of matter. This scattering is far more marked for the β than for the α particle on account of the much

smaller momentum and energy of the form There seems to be no doubt that such swiftly ticles pass through the atoms in their path, a deflexions observed are due to the strong e traversed within the atomic system. It has ge

Philosophical Magazine, volume **21** (1911), pages 669-688



There are several good reaction theory texts: e.g.

<u>Direct nuclear reaction theories</u> (Wiley, Interscience monographs and texts in physics and astronomy, v. 25) <u>Norman Austern</u>

<u>Direct Nuclear Reactions</u> (Oxford University Press, International Series of Monographs on Physics, 856 pages) <u>G R Satchler</u>

Introduction to the Quantum Theory of Scattering (Academic, Pure and Applied Physics, Vol 26, 398 pages) <u>L S Rodberg</u>, <u>R M Thaler</u>

Direct Nuclear Reactions (World Scientific Publishing, 396 pages) Norman K. Glendenning

Introduction to Nuclear Reactions (Taylor & Francis, Graduate Student Series in Physics, 515 pages) <u>C A Bertulani, P Danielewicz</u>

<u>Theoretical Nuclear Physics: Nuclear Reactions</u> (Wiley Classics Library, 1938 pages) <u>Herman Feshbach</u>

Introduction to Nuclear Reactions (Oxford University Press, 332 pages) <u>G R Satchler</u>

<u>Nuclear Reactions for Astrophysics</u> (Cambridge University Press, 2010) <u>Ian Thompson and Filomena Nunes</u>

Some other notes/resources available at:

http://www.nucleartheory.net/DTP_material Please let me know if there are problems.

EBSS 2011 at NSCL: Ian Thompson Lawrence Livermore National Laboratory Nuclear Reactions (Theory) http://www.nscl.msu.edu/~zegers/ebss2011/thompson.pdf

Read introduction to Thompson lectures 2011 ...

... for a discussion of the characteristics of direct (fast) and compound (massive energy sharing) nuclear reactions.

<u>Direct reactions</u>: Reactions in which nuclei make glancing contact and then separate immediately. Projectile may exchange some energy and / or angular momentum, or have one or more nucleons <u>transferred to</u> it or <u>removed from</u> it.

<u>Direct reactions:</u> take place at/near the nuclear surface and at larger impact parameters

<u>Direct reaction</u> products tend to be strongly forward peaked as projectile continues to move in general forward direction

<u>Direct reactions</u> take place on a short timescale (we will quantify) – a timescale that reduces with increasing energy of the projectile beam (and that allows extra approximations)

<u>Direct reaction</u> clock has ticks in units of $\sim 10^{-22}$ s – timescale for a nucleon's motion across in a typical nucleus

Single-particle aspects of structure from reactions

S



Reaction timescales – surface grazing collisions

For say 10 and 100 MeV/u incident energy:

$$\gamma = 1.01, v/c = 0.14, \gamma = 1.1, v/c = 0.42,$$

 $\Delta t = 2.4 \times d \times 10^{-23} s, \Delta t = 7.9 \times d \times 10^{-24} s$



d<nuclear diameter (a few fm) – unless strong Coulomb effects are an important factor in the collisions of interest

To discuss: 1. solutions of the Schrodinger equation for states of **two** bodies with specific quantum numbers over a wide range of energies – the need for bound, resonant, continuum (and continuum bin) states.

2. The form of these two-body problem solutions at large separations and their relationships to nuclear structure, absorption, reaction and scattering observables.

3. Stress constraints on two-body potentials and their parameters. Parameter conventions. The need to cross reference to known nuclear structures, resonances, nuclear sizes and experiment whenever possible in constraining parameter choices for calculations.

Underpinnings of direct reaction methods

<u>Solutions of Schrodinger's equation</u> for (pairs of) nuclei interacting via a potential energy function of the form*

$$U(r) = \underbrace{V_C(r)}_{\mathsf{Coulomb}} + \underbrace{V(r) + V_{so}(r)\vec{\ell} \cdot \vec{s}}_{\mathsf{Nuclear}}$$

$$\ell$$
 $\phi_{\ell j}^{m}(\vec{r})$
 $\phi_{\ell j}^{m}(\vec{r})$
 $\phi_{\ell j}^{m}(\vec{r})$

Need descriptions of wave functions of:

- (1) <u>Bound states</u> of nucleons or clusters (valence particles) to a core (that is assumed for now to have spin zero).
- (2) <u>Unbound</u> scattering or resonant states at <u>low energy</u>
- (3) <u>Distorted waves</u> for such bodies in complex potentials

$$U(r) = V_C(r) + V(r) + iW(r) + V_{so}(r)\vec{\ell}\cdot\vec{s}$$

*Additional, e.g. tensor terms, when s=1 or greater neglected

Direct reactions – types and characteristics





Direct reactions – types and characteristics



Direct reactions – requirements (1)

Description of wave functions of **bound** systems (both nucleons or clusters) – (a) can take from structure theory, if available or, (b) more usually, use a <u>real potential</u> model to bind system with the required experimental separation energy. Refer to <u>core and valence particles</u>

$$U(r) = V_C(r) + V(r) + V_{so}(r)\vec{\ell}\cdot\vec{s}$$

$$\phi_{n\ell j}^m(\vec{r}) = \sum_{\lambda\sigma} (\ell\lambda s\sigma|jm) \frac{u_{n\ell j}(r)}{r} Y_\ell^\lambda(\hat{r})\chi_s^\sigma, \quad \int_0^\infty [u_{n\ell j}(r)]^2 dr = 1$$

Usually just one or a few such states are needed. Separation energies/Q-values: many sites, e.g. http://ie.lbl.gov/toi2003/MassSearch.asp

Bound states - real potentials



Bound states potential parameters - nucleons

$$U(r) = V_C(r) + V(r) + V_{so}(r)\vec{\ell} \cdot \vec{s}$$

$$V(r) = -\frac{V_R}{[1 + \exp(X_R)]}, \qquad X_i = \frac{r - R_i}{a_i}$$

$$V_{so}(r) = -\frac{4 V_{so}}{r a_{so}} \frac{\exp(X_{so})}{[1 + \exp(X_{so})]^2},$$

$$R_i = r_i A_c^{1/3}$$

$$r_R = r_C = r_{so} \approx 1.25 \text{fm}$$

 $a_R = a_{so} \approx 0.7 \text{fm} \quad V_{so} = 6 \text{MeV}$

Bound states – single particle quantum numbers



Bound states – for nucleons - conventions



Conventions

 $\phi^m_{n\ell i}(\vec{r})$

With this potential, and using <u>sensible</u> parameters, we will obtain the independent-particle shell model level orderings, shell closures with spin-orbit splitting.

NB: In diagram $2d_{5/2}$ means the <u>second</u> $d_{5/2}$ state. Defined this way, n>0 and <u>n-1 is the number</u> of nodes in the radial wave function. Reaction codes can ask for n, or n-1 (the actual number of nodes). Care is needed.

Bound states – can also use mean field information

	*		*					
INPUT VALUES	* IA,]	[Z =	24 8 *					
	*		*					
	*****	*******	*******					
Neu	tron bound	state	results					
knl j	e IE	OCC						
$1 \ 1 \ s \ 1/2$	-26.757 1	2.00	36.70	35.28				
2 1 p 3/2	-16.883 1	4.00	36.70	35.80				
31p1/2	-12.396 1	2.00	36.70	36.04				
4 1 d 5/2	-6.166 1	6.00	36.70	36.37				
51d3/2	-0.109 1	0.00	36.70	36.69				
6.2 s 1/2	-3.360 1	2.00	36.70	36.52				

-0.200 3

-0.200 3

-0.200 3

7 1 f 7/2

8 1 f 5/2

92p3/2

But must make small corrections as HF is a fixed centre calculation

 $\langle r^2 \rangle = \frac{A}{A-1} \langle r^2 \rangle_{HF}$

----- Neutron single-particle radii -----

0.00

0.00

0.00

R(2) rho(8.9) rho(9.9) rho(10.9) R(4) OCC

46.01

60.55

48.09

$1 \ 1 \ s \ 1/2$	2.274	2.575	2.000	0.848E-09	0.706E-10	0.600E-11
2 1 p 3/2	2.863	3.133	4.000	0.188E-07	0.244E-08	0.325E-09
3 1 p 1/2	2.954	3.268	2.000	0.727E-07	0.122E-07	0.210E-08
41d5/2	3.434	3.757	6.000	0.524E-06	0.129E-06	0.327E-07
51d3/2	4.662	6.063	0.000	0.131E-04	0.675E-05	0.371E-05
62s1/2	4.172	4.895	2.000	0.769E-05	0.278E-05	0.102E-05
7 1 f 7/2	3.865	4.440	0.000	0.324E-05	0.134E-05	0.600E-06
8 1 f 5/2	3.890	4.477	0.000	0.341E-05	0.141E-05	0.631E-06
92p3/2	6.815	8.635	0.000	0.451E-04	0.270E-04	0.167E-04

46.02

60.56

48.10



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Direct reactions – requirements (2)

Description of wave functions for unbound (often light) systems (nucleons or clusters) with low relative energy: Usually have <u>low nuclear level density</u> of isolated resonances. Use the same real potential model as binds the system \rightarrow scattering wave functions in this potential. (Also 'bin' wave functions)



Completeness and orthogonality - technical piont

Given a fixed two-body Hamiltonian

$$H = T + U(r) = T + V_C(r) + V(r) + V_{so}(r)\vec{\ell}\cdot\vec{s}$$

the set of all of the bound and unbound wave functions $\{\phi_{n\ell j}^{m}(\vec{r}), \phi_{k\ell j}^{m}(\vec{r})\}$

form a complete and orthogonal set, and specifically

$$\left\langle \phi_{n\ell j}^m(\vec{r}) \right| \phi_{k\ell j}^m(\vec{r}) \right\rangle = 0$$

When including both bound to unbound states it is essential to use a <u>fixed</u> Hamiltonian for both the bound and unbound states (in each l j channel) else we lose the orthogonality and the states will couple even without any perturbation or interactions with a reaction target.

Direct reactions – requirements (3)

Description of wave functions for scattering of nucleons or clusters from a heavier target and/or at higher energies: (a) high nuclear level density and broad overlapping resonances, (b) many open reaction channels, inelasticity and absorption. Use a complex (absorptive) optical model potential – from theory or 'simply' fitted to a body of elastic scattering data for a system and energy near that of interest.

Distorted waves:



Optical potentials – the role of the imaginary part



$$\bar{k}^2 = \frac{2\mu}{\hbar^2} (E + V_0 + iW_0) = \frac{2\mu}{\hbar^2} (E + V_0) \left[1 + \frac{iW_0}{E + V_0} \right]$$
$$\bar{k} = k \left[1 + \frac{iW_0}{E + V_0} \right]^{1/2} \approx k \left[1 + \frac{iW_0}{2(E + V_0)} \right], \quad W_0 \ll E, V_0$$

So, for $W_0 > 0$, $\bar{k} = k + ik_i/2$, $k_i = kW_0/(E + V_0) > 0$,

$$\bar{\psi}(x) = e^{i\bar{k}x} = e^{ikx}e^{-\frac{1}{2}k_ix}, \quad |\bar{\psi}(x)|^2 = e^{-k_ix}$$

The Schrodinger equation (1)

The Schrodinger equation (2)



Large r: The Asymptotic Normalisation Coefficient



outside of the range of the nuclear potential – only

requirement if a reaction probes only these radii

 $C_{\ell j}$

Large r: The phase shift and partial wave S-matrix

$$\frac{\text{Scattering states}}{\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2\mu}{\hbar^2}U_{\ell j}(r) + k^2\right)u_{k\ell j}(r) = 0}$$

and beyond the range of the nuclear forces, then

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2\eta k}{r} + k^2\right) u_{k\ell j}(r) = 0, \quad \eta = \frac{\mu Z_c Z_v e^2}{\hbar k}$$

 $F_{\ell}(\eta, kr), \ G_{\ell}(\eta, kr)$ regular and irregular Coulomb functions

$$u_{k\ell j}(r) \rightarrow e^{i\delta_{\ell j}} [\cos \delta_{\ell j} F_{\ell}(\eta, kr) + \sin \delta_{\ell j} G_{\ell}(\eta, kr)]$$

$$\rightarrow (i/2) [H_{\ell}^{(-)}(\eta, kr) - S_{\ell j} H_{\ell}^{(+)}(\eta, kr)]$$

$$H_{\ell}^{(\pm)}(\eta, kr) = G_{\ell}(\eta, kr) \pm iF_{\ell}(\eta, kr)$$

Phase shift and partial wave S-matrix

$$u_{k\ell j}(r) \rightarrow e^{i\delta_{\ell j}} [\cos \delta_{\ell j} F_{\ell}(\eta, kr) + \sin \delta_{\ell j} G_{\ell}(\eta, kr)]$$

If $U(r)$ is real, the phase shifts $\delta_{\ell j}$ are real, and [...] also

$$\begin{array}{rccc} u_{k\ell j}(r) & \to & (i/2)[H_{\ell}^{(-)}(\eta,kr) - S_{\ell j}H_{\ell}^{(+)}(\eta,kr)] \\ & & & \\ S_{\ell j} = e^{2i\delta_{\ell j}} & & & \\ & &$$

Having calculate the phase shifts and the partial wave S-matrix elements we can then compute all scattering observables for this energy and potential (but later).

S-matrix with absorption



$$u_{k\ell j}(r) \to (i/2)[H_{\ell}^{(-)} - S_{\ell j}H_{\ell}^{(+)}]$$



Phase shifts and S-matrix: Resonant behaviour

In real potentials, at low energies, the combination of an attractive nuclear, repulsive Coulomb and centrifugal terms can lead to potential <u>pockets</u> and resonant behaviour – the system being able to trapped in the pocket for some (life)time τ .

$$\frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} + U_{\ell j}(r)$$



Phase shifts and S-matrix: Resonant behaviour

Potential pockets can lead to resonant behaviour – the system being able to trapped in the pocket for some (life)time τ .

A signal is the rise of the phase shift through 90 degrees.





Potential parameters should describe any known resonances

Bound states – spectroscopic factors

In a potential model it is natural to define <u>normalised</u> bound state wave functions. $^{A}Y(J^{\pi}_{i})$

$$\phi_{n\ell j}^{m}(\vec{r}) = \sum_{\lambda\sigma} (\ell\lambda s\sigma|jm) \frac{u_{n\ell j}(r)}{r} Y_{\ell}^{\lambda}(\hat{r}) \chi_{s}^{\sigma},$$

$$\int_{0}^{\infty} [u_{n\ell j}(r)]^{2} dr = 1$$

$$n\ell_{j} = 1$$

The potential model wave function approximates the <u>overlap function</u> of the A and A–1 body wave functions (A and A–n in the case of an n-body cluster) i.e. the overlap

$$\langle \ell j, \vec{r}, ^{A-1} \operatorname{X}(J_f^{\pi}) | ^A \operatorname{Y}(J_i^{\pi}) \rangle \to I_{\ell j}(r), \quad \int_0^\infty [I_{\ell j}(r)]^2 dr = S(J_i, J_f \ell j)$$

S(...) is the <u>spectroscopic factor</u> \leftarrow a structure calculation

Bound states – microscopic overlaps





Microscopic overlap from Argonne 9- and 8-body wave functions (*Bob Wiringa et al.*) Available for a few cases

Normalised bound state in Woods-Saxon potential well x (0.23)^{1/2} Spectroscopic factor $r_V = r_{so} = \text{fitted}, \ a_V = a_{so} = \text{fitted}, \ V_{so} = 6.0$

Bound states – shell model overlaps

$$\langle \vec{r}, ^{25} \operatorname{Ne}(5/2^+, E^*) |^{26} \operatorname{Ne}(0^+, \text{g.s.}) \rangle$$

USDA sd-shell model overlap from e.g. OXBASH (*Alex Brown et al.*). Provides <u>spectroscopic factors</u> but <u>not</u> the bound state radial wave function.





Optical potentials - parameter conventions

$$R_i = r_i A_2^{1/3}$$
 or $R_i = r_i \left[A_1^{1/3} + A_2^{1/3} \right]$

Ingoing and outgoing waves amplitudes

 $u_{k\ell j}(r) \to (i/2) [\mathbf{1} H_{\ell}^{(-)} - \mathbf{S}_{\ell j} H_{\ell}^{(+)}]$



Barrier passing models of fusion



Gives basis also for simple (barrier passing) models of nucleus-nucleus fusion reactions

an imaginary part in U(r), at short distances, can be included to absorb all flux that passes over or through the barrier – assumed to result in fusion

$$\begin{array}{c} U(r) & T_{\ell}(E) & E_{cm} \\ t & & & \\ n & & & \\ R_{i} R_{b} R_{o} & r \end{array} \right)$$

$$\sigma(E) = \sum_{\ell=0}^{\infty} \sigma_{\ell}(E) = \frac{\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1)(1-|S_{\ell}|^2)$$

End of Part I: to be continued

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Neither bound nor scattering – continuum bins

Scattering states

$$u_{k\ell j}(r) \rightarrow e^{i\delta_{\ell j}} [\cos \delta_{\ell j} F_{\ell}(\eta, kr) + \sin \delta_{\ell j} G_{\ell}(\eta, kr)]$$

$$\int_{0}^{\infty} dr \, u_{k\ell j}(r) \, u_{k'\ell j}^{*}(r) = \frac{\pi}{2} \delta(k - k')$$

$$\hat{u}_{\alpha\ell j}(r) = \sqrt{\frac{2}{\pi N_{\alpha}}} \int_{\Delta k_{\alpha}} dk \, g(k) \, u_{k\ell j}(r)$$

$$N_{\alpha} = \int_{\Delta k_{\alpha}} dk \, [g(k)]^{2} \quad \underset{\text{function}}{\text{weight}}$$

$$0 \quad \text{orthonormal} \quad \int_{0}^{\infty} dr \, \hat{u}_{\alpha\ell j}^{*}(r) \, \hat{u}_{\beta\ell j}(r) = \delta_{\alpha\beta}$$

$$g(k) = 1 \quad g(k) = \sin \delta_{\ell j}$$

Bound states – for clusters – conventions (1)

How many nodes for cluster states ?

 $\phi^m_{n\ell j}(ec r)$

Usually guided by what the 3D harmonic oscillator potential requires - so as not to violate the Pauli Principle.

⁷Li (α +t) $[2(n-1) + \ell]\hbar\omega \begin{cases} excitation due to a nucleon each level \end{cases}$



Bound states – for clusters - conventions (2)

