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Breakup Reactions at Intermediate Energy

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Abstract

Breakup reactions may be considered by a quasi-three-body model in which the two-body subsystems interact through optical model potentials with imaginary parts describing the excitation of unobserved channels. The distorted wave off-shell impulse approximation neglects only gradients of the optical model potentials. At sufficiently high energies it factorizes into a quantity describing the elementary two-body collision and a distorted wave transform of the bound-state wavefunction, which gives a distorted orbital momentum profile. Examples showing the validity of the approximation are given.

Introduction

A breakup reaction is one in which two particles are detected in coincidence emerging from the reaction region. Modern breakup experiments are kinematically complete, in that the momenta of the incident particle $\boldsymbol{k}_0$ and each outgoing particle $\boldsymbol{k}_A$ and $\boldsymbol{k}_B$ are determined. Of course the energy transferred to the remainder of the system is determined by the same measurement, so it is possible to resolve reactions in which the remainder of the system is left in a particular bound state, or at least one of a set of states with trivial degeneracy such as magnetic substates. If the excitation energy of the remaining system is so large that it can decay, then an energy–momentum spectral function defining the cross section as a function of energy and momentum can be determined.

We are most interested in breakup experiments in which the residual system is left in a bound or just unbound state. Then the cross section for resolved final states is measured as a function of $\boldsymbol{k}_0$, $\boldsymbol{k}_A$ and $\boldsymbol{k}_B$. Since many kinematic variables are involved, it is usual to hold most of them constant and vary one. Normally we are interested in the angular correlation for fixed energies, and two geometries are of primary interest:

coplanar symmetric geometry

$$\boldsymbol{k}_0 \text{ fixed}, \quad E_A = E_B = E', \quad \theta_A = \theta_B = \theta, \quad \phi_A = 0, \quad \phi_B = \pi, \quad \theta \text{ varied};$$

noncoplanar symmetric geometry

$$\boldsymbol{k}_0 \text{ fixed}, \quad E_A = E_B = E', \quad \theta_A = \theta_B \text{ fixed}, \quad \phi_B = \pi, \quad \phi_A \text{ varied}.$$

From the measured momenta $\boldsymbol{k}_0$, $\boldsymbol{k}_A$ and $\boldsymbol{k}_B$ it is possible to calculate the momentum transfer $\boldsymbol{q}$ to the residual system. The most naive interpretation of the reaction is

the plane wave model in which the momentum transfer $\boldsymbol{q}$ is due merely to the removal of a particle whose momentum at the collision instant was $\boldsymbol{q}$. Of course in practice momentum is also transferred by elastic interactions of the particles 0, A and B with the remainder of the system.

If the plane wave interpretation were correct, then the reaction would be a tool of far-reaching significance in understanding the structure of quantum systems, because the momentum transfer distribution would then be related very directly to the momentum density of particles in the bound system. In fact, if eigenstates of the residual system could be resolved experimentally, we would have a measurement of the square of the single-particle wavefunction corresponding to that eigenstate, a quantity that is directly related to the structure problem or solution of the many-body Schrödinger equation.

The purpose of this talk is firstly to discuss the reaction mechanism with the object of finding out under what circumstances the structure information can be validly inferred from the differential cross section, and secondly to show what information has in fact been obtained from simple systems.

For over 20 years the (p, 2p) experiment has been known in nuclear physics. Much qualitative information has been obtained from it, but it has been a quantitative disappointment. With the advent of new accelerators and detection techniques there has been a revival of interest in this reaction, which is shared by several groups in Australia. In 1973 and 1974 the Flinders atomic scattering group perfected the (e, 2e) experiment on atoms and molecules. All the hopes of obtaining quantitative structure information about quantum systems have been fulfilled in these experiments. We will discuss them as an analogue of the (p, 2p) experiment that tells us how to obtain the structure information and therefore guides our design of (p, 2p) experiments.

The structure information is contained in the differential cross section. In order to extract it, we must have a good theory of the reaction emchanism that can be shown to give correct answers for targets whose structure is well known from independent information. We must know under what kinematic conditions the cross section is sensitive to structure information and less sensitive to other properties of the reaction.

Theory of the Reaction

The breakup reaction involves essentially a three-body system in which there are two light bodies, labelled 1 and 2, with degrees of freedom of translation and spin, and a heavy body with internal degrees of freedom denoted by ξ. We make the approximation that the disparity in energy between the unbound and bound particles means that unbound particles need not be antisymmetrized with bound particles. The two light particles are antisymmetrized with each other in the final state. The internal degrees of freedom ξ are regarded as independent of $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, the coordinates of the light particles. Spin–orbit coupling is not treated, since polarizations are not measured. The corresponding spins $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$ are involved only in determining the antisymmetric states of particles 1 and 2. For nucleons, isospin plays a similar role.

For simplicity of the three-body coordinate system we will assume that the third body is infinitely heavy. This is not an essential simplification. The equations to be derived are valid in the more general case with a slight redefinition of coordinates and momenta.

The Hamiltonian of the system is

$$\mathscr{H} = K_1 + K_2 + V_1(\boldsymbol{r}_1, \xi) + V_2(\boldsymbol{r}_2, \xi) + H(\xi) + v(\boldsymbol{r}), \tag{1}$$

where the centre-of-mass and relative coordinates are defined by

$$\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2, \qquad \boldsymbol{r}_1 = \boldsymbol{R} + \tfrac{1}{2}\boldsymbol{r}, \tag{2a}$$

$$\boldsymbol{R} = \tfrac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2), \qquad \boldsymbol{r}_2 = \boldsymbol{R} - \tfrac{1}{2}\boldsymbol{r}. \tag{2b}$$

Here we are treating the case in which particles 1 and 2 have equal masses as in (p, 2p) or (e, 2e). The relative and centre-of-mass kinetic energy operators obey the relation

$$K_r + K_R = K_1 + K_2. \tag{3}$$

We will now recall the general formulation of scattering theory. The total Hamiltonian $\mathscr{H}$ is partitioned in a convenient way,

$$\mathscr{H} = \mathscr{K} + \mathscr{V}, \tag{4}$$

where $\mathscr{K}$ contains all the kinetic energy operators. The scattering wavefunctions are defined for total energy E by

$$(E^{(\pm)} - \mathscr{H})\Psi^{(\pm)} = 0, \qquad (E^{(\pm)} - \mathscr{K})\Phi^{(\pm)} = 0, \tag{5,6}$$

where the $\pm$ superscipt indicates that the Schrödinger equation is solved for a complex energy $E \pm i\varepsilon$ and the limit $\varepsilon \to 0+$ is taken. The two cases correspond respectively to boundary conditions with outgoing and ingoing spherical waves in the open channels.

The scattering amplitude is

$$F = \langle \Phi^{(-)} | \mathscr{V} | \Psi^{(+)} \rangle = \langle \Psi^{(-)} | \mathscr{V} | \Phi^{(+)} \rangle. \tag{7}$$

We keep in mind that F must be appropriately antisymmetrized. Since we normally choose $\mathscr{K}$ so that we can solve equation (6), it is convenient to express the amplitude F in a representation in which $\mathscr{K}$ is diagonal:

$$F = \langle \Phi^{(-)} | T^{(\pm)} | \Phi^{(+)} \rangle, \tag{8}$$

where

$$T^{(\pm)}\Phi^{(\pm)} = \mathscr{V}\Psi^{(\pm)}, \qquad T^{(\pm)} = \mathscr{V} + \mathscr{V}\{E^{(\pm)} - \mathscr{H}\}^{-1}\mathscr{V}. \tag{9}$$

If $\mathscr{K}$ contains no terms representing interactions between separated bodies, F is called the T-matrix element for the whole system.

We now choose our partitions of the Hamiltonian for breakup reactions. For the entrance channel we use an auxiliary potential $\tilde{V}_0(r_1)$, which causes only elastic scattering of the incident particle 1 from the target system,

$$\mathscr{K}_i = [K_1 + \tilde{V}_0(r_1)] + [K_2 + V_2(\boldsymbol{r}_2, \xi) + H(\xi)], \tag{10a}$$

with

$$\mathscr{V}_i = v(\boldsymbol{r}) + [V_1(\boldsymbol{r}_1, \xi) - \tilde{V}_0(r_1)]. \tag{10b}$$

The Schrödinger equation for $\mathscr{K}$ separates as indicated by the square brackets in (10a), so that

$$\Phi^{(+)} = \chi^{(+)}(\boldsymbol{k}_0, \boldsymbol{r}_1)\, \Phi_0(\boldsymbol{r}_2, \xi)\,. \tag{11}$$

The first factor is the entrance channel distorted wave and the second factor is the ground state wavefunction of the target. In general a target eigenfunction is written as

$$\Phi_\alpha(\boldsymbol{r}_2, \xi) = \sum_{i\mu} f_{i\mu}^{(\alpha)} [\phi_i(\boldsymbol{r}_2) \times \psi_\mu(\xi)]_\alpha\,. \tag{12}$$

Equation (12) is a weak coupling expansion in terms of single-particle functions $\phi_i(\boldsymbol{r}_2)$, defined by some central single-particle potential $\mathscr{V}(r_2)$, and eigenstates $\psi_\mu(\xi)$ of the third body,

$$[\varepsilon_\mu - H(\xi)]\psi_\mu(\xi) = 0\,. \tag{13}$$

For simplicity we will assume that $\psi_\mu(\xi)$ is a bound state. If it is a decaying state, it can still be treated by appropriate choice of boundary conditions.

For the exit channel we may define auxiliary potentials $\tilde{V}_1(\boldsymbol{r}_1)$ and $\tilde{V}_2(\boldsymbol{r}_2)$, so that $\mathscr{K}_\mathrm{f}$ is defined and partitioned into separable parts as

$$\mathscr{K}_\mathrm{f} = [K_1 + \tilde{V}_1(\boldsymbol{r}_1)] + [K_2 + \tilde{V}_2(\boldsymbol{r}_2)] + H(\xi)\,, \tag{14a}$$

with

$$\begin{aligned} \mathscr{V}_\mathrm{f} &= v(\boldsymbol{r}) + [V_1(\boldsymbol{r}_1, \xi) - \tilde{V}_1(\boldsymbol{r}_1)] + [V_2(\boldsymbol{r}_2, \xi) - \tilde{V}_2(\boldsymbol{r}_2)] \\ &\equiv v(\boldsymbol{r}) + \tilde{v}_1(\boldsymbol{r}_1, \xi) + \tilde{v}_2(\boldsymbol{r}_2, \xi)\,. \end{aligned} \tag{14b}$$

The corresponding final state distorted wave is

$$\Phi^{(-)} = [\chi_A^{(-)}(\boldsymbol{k}_A, \boldsymbol{r}_1)\, \chi_B^{(-)}(\boldsymbol{k}_B, \boldsymbol{r}_2) - \chi_A^{(-)}(\boldsymbol{k}_A, \boldsymbol{r}_2)\, \chi_B^{(-)}(\boldsymbol{k}_B, \boldsymbol{r}_1)] \times \psi_\mu(\xi)\,, \tag{15}$$

where we have indicated the antisymmetrization explicitly.

In the actual experiment several final eigenstates $\psi_\mu(\xi)$ are detected and resolved. Unresolved states have trivial degeneracies due to different magnetic substates or spin–orbit coupling.

Since the final state momenta are measured completely, it will be simpler to treat the $T^{(-)}$ matrix element of equation (8),

$$F = \langle \Phi^{(-)} | \mathscr{V}_\mathrm{f} + \mathscr{V}_\mathrm{f} \{E^{(-)} - (K_1 + K_2 + H + V_1 + V_2 + v)\}^{-1} \mathscr{V}_\mathrm{i} | \Phi^{(+)} \rangle\,. \tag{16}$$

This is the exact amplitude for the problem in a distorted wave representation.

In order to obtain a computable approximation to equation (16) we will make two approximations:

(1) The quasi-three-body approximation. Here we replace the exact potential $V_1(\boldsymbol{r}_1, \xi)$ by an optical model potential $U_1(r_1)$. We thus ignore the possibility of inelastic excitations of the initial or final residual system by the small potentials $\tilde{v}_1$ and $\tilde{v}_2$. These potentials have been treated in first order for (e, 2e) by R. T. Janus and the author (unpublished results), and shown to have no measurable effect on the cross section.

(2) The optical potentials $U_1(r_1)$ and $U_2(r_2)$ are expanded in a Taylor series about $\boldsymbol{R}$ and the zeroth order is taken. In this series, for equal final state energies, the

first-order term in ∇_r is zero. The approximation depends on the neglect of terms of order ∇_r^2 over distances comparable with the range of $v(r)$. In both nuclear and atomic physics, optical potentials are quite smooth, so that this is an excellent approximation to the quasi-three-body problem. This is shown in the equation

$$U_1(r_1)+U_2(r_2) = \left[U_1(\boldsymbol{R})+U_2(\boldsymbol{R})\right] + \tfrac{1}{2}\boldsymbol{r}.\left[\nabla_r U_1 - \nabla_r U_2\right] + O\left[\nabla_r^2 U_1\right]. \tag{17}$$

For $E_A = E_B$ we have $U_1 = U_2$, so that the second term of equation (17) vanishes.

The second approximation enables us to redefine $\mathscr{K}_f$ as

$$\mathscr{K}_f = K_r + \left[K_R + U_1(\boldsymbol{R}) + U_2(\boldsymbol{R})\right] + H(\xi), \tag{18}$$

so that the distorted wave is

$$\Phi^{(-)} \approx \bar{\boldsymbol{X}}(\boldsymbol{k}_A, \boldsymbol{k}_B, \boldsymbol{R})\,\phi(\boldsymbol{r})\,\psi_\mu(\xi). \tag{19}$$

The point of the approximation is that we can now operate on $\Phi^{(-)}$ with the denominator of the Green's function in equation (16) in such a way as to eliminate the coordinate $\boldsymbol{R}$.

The separated Schrödinger equation in the approximation (19) is

$$\left[E_A+E_B-\varepsilon-(K_R+U_1+U_2+H)\right]\bar{\boldsymbol{X}}(\boldsymbol{R})\,\psi_\mu(\xi) = 0, \tag{20a}$$

$$\left[\varepsilon-K_r\right]\phi(\boldsymbol{r}) = 0. \tag{20b}$$

The separation constant ε is independent of U_1 and U_2. By setting $U_1 = U_2 = 0$, we may see that it is equal to the separation energy $\varepsilon \equiv \varepsilon_\mu$ or the energy eigenvalue of $\psi_\mu(\xi)$. Using this result and equations (20), the Green's function is treated as follows:

$$\bar{\boldsymbol{X}}^{(-)}(\boldsymbol{R})\,\phi(\boldsymbol{r})\,\psi_\mu(\xi)\; v(\boldsymbol{r})\{E-[K_r+K_R+H+U_1(\boldsymbol{R})+U_2(\boldsymbol{R})+v(\boldsymbol{r})]\}^{-1}$$
$$= \bar{\boldsymbol{X}}^{(-)}(\boldsymbol{R})\,\phi(\boldsymbol{r})\,\psi_\mu(\xi)\; v(\boldsymbol{r})\{\varepsilon_\mu-K_r-v(\boldsymbol{r})\}^{-1}. \tag{21}$$

Reverting to the approximately equivalent definition (15) for $\Phi^{(-)}$, we have

$$F = \mathscr{A}\langle\chi_A^{(-)}(\boldsymbol{k}_A)\,\chi_B^{(-)}(\boldsymbol{k}_B)\,\psi_\mu(\varepsilon_\mu)\,|\,T_v(\varepsilon_\mu)\,|\,\chi_0^{(+)}(\boldsymbol{k}_0)\,\Phi_0\rangle, \tag{22}$$

where the two-body T-matrix in three-body space is

$$T_v(\varepsilon_\mu) = \{\varepsilon_\mu-K_r-v(\boldsymbol{r})\}^{-1}\,\delta(\boldsymbol{R}'-\boldsymbol{R}). \tag{23}$$

Equations (22) and (23) constitute our basic approximation, which we have named the distorted wave off-shell impulse approximation.

Because of the nonlocal nature of the off-shell T-matrix T_v, this is a 9-dimensional integral with the usual problem of the coordinate transformation from the $\boldsymbol{r}_1, \boldsymbol{r}_2$ system to the $\boldsymbol{r}, \boldsymbol{R}$ system. It has never been evaluated for exact partial wave expansions of all quantities. Interesting results for 50 MeV (p, 2p) have been obtained by I. R. Afnan *et al.* (to be published) using distorted waves approximated as attenuated plane waves with a complex focus. The structure information in equation (22) is contained in the factor

$$\left(\psi_\mu(\varepsilon_\mu)\,|\,T_v(\varepsilon_\mu)\,|\,\Phi_0\right). \tag{24}$$

Since we have made the quasi-three-body approximation, T_v is independent of the core coordinates ξ. Therefore (24) can be written as

$$(\psi_\mu \mid \Phi_0)\, T_v(\varepsilon_\mu), \tag{25}$$

where the structure information is all contained in the overlap integral between the target system and the final system. This factor is a function only of the coordinate $\boldsymbol{r}_2$ of the struck particle (neglecting spin–orbit coupling in the absence of polarization measurements). We will discuss it in detail when we come to describe the structure information that can be obtained. At present we will concentrate on the reaction mechanism.

The necessity to make an approximation that enables the integral (22) to be evaluated confines this lecture to intermediate energies. For energies so high that the distorting potentials U_1 and U_2 are negligible, the *plane wave impulse approximation* is valid:

$$F_{\mathrm{PW}} = \mathscr{A}\langle \boldsymbol{k}_A \boldsymbol{k}_B \mid T_v(\varepsilon_\mu) \mid \boldsymbol{k}_0(\psi_\mu \mid \Phi_0)\rangle . \tag{26}$$

Since the coordinates $\boldsymbol{r}_1', \boldsymbol{r}_2', \boldsymbol{r}_1$ occur linearly in the exponents of the continuum wavefunctions (plane waves), the coordinate transformation to the $\boldsymbol{r}', \boldsymbol{R}', \boldsymbol{r}, \boldsymbol{R}$ system is trivial,

$$F_{\mathrm{PW}} = \mathscr{A}\langle \tfrac{1}{2}(\boldsymbol{k}_A - \boldsymbol{k}_B) \mid T_v(\tfrac{1}{4} \mid \boldsymbol{k}_A - \boldsymbol{k}_B \mid^2) \mid \tfrac{1}{2}(\boldsymbol{k}_0 + \boldsymbol{q})\rangle f_\mu(\boldsymbol{q}), \tag{27}$$

where

$$f_\mu(\boldsymbol{q}) = \int \mathrm{d}^3 r_2 \exp(\mathrm{i}\, \boldsymbol{q} \cdot \boldsymbol{r}_2)(\psi_\mu \mid \Phi_0), \qquad \boldsymbol{q} = \boldsymbol{k}_0 - \boldsymbol{k}_A - \boldsymbol{k}_B . \tag{28a, b}$$

The amplitude in the plane wave impulse approximation depends on the half-off-shell two-body T-matrix element and the structure factor in momentum space $f_\mu(\boldsymbol{q})$, which is the Fourier transform of $(\psi_\mu \mid \Phi_0)$.

Energies at which the approximation (27) is valid are called *high* energies. For lower energies the T-matrix element varies slowly with the momenta $\boldsymbol{k}_0$, $\boldsymbol{k}_A$, $\boldsymbol{k}_B$ and $\boldsymbol{q}$ so that it can be approximately factored out of the expression (22). This is the *factorization approximation*:

$$F_{\mathrm{fac}} = \mathscr{A}\langle \tfrac{1}{2}(\boldsymbol{k}_A - \boldsymbol{k}_B) \mid T_v(\tfrac{1}{4} \mid \boldsymbol{k}_A - \boldsymbol{k}_B \mid^2) \mid \tfrac{1}{2}(\boldsymbol{k}_0 + \boldsymbol{q})\rangle \langle \chi_A^{(-)}(\boldsymbol{k}_A)\, \chi_B^{(-)}(\boldsymbol{k}_B) \mid \chi_0^{(+)}(\boldsymbol{k}_0)(\psi_\mu \mid \Phi_0)\rangle . \tag{29}$$

The energy range where this is valid is the *intermediate* energy range. The (e, 2e) reaction will show that such a range exists.

Structure Factor

The structure factor is given by

$$(\psi_\mu \mid \Phi_0) = \sum_{i\mu} (\psi_\mu \mid f_{iv}^{(0)}[\phi_i(\boldsymbol{r}_2) \times \psi_v]_0) . \tag{30}$$

In general this is written as a linear combination of single-particle functions $\phi_i(\boldsymbol{r}_2)$ (called orbitals), where the quantum numbers i are restricted to values that obey total angular momentum and parity conservation:

$$(\psi_\mu \mid \Phi_0) = \sum_i f_{i\mu}^{(0)}\, \phi_i(\boldsymbol{r}_2) . \tag{31}$$

The factors $f_{i\mu}^{(0)}$ are spectroscopic amplitudes describing the probability amplitude that the overlap function contains the orbital ϕ_i.

It is a little easier to follow if we write the structure factor in terms of the target ground state as the core Φ_0 and the final state as a single hole $\phi_i^\dagger(\boldsymbol{r}_2)$ coupled to a target state Φ_α in such a way that all terms are members of the same representation of the rotation group:

$$\psi_\mu = \sum_{i\alpha} t_{i\alpha}^{(\mu)}[\phi_i^\dagger \times \Phi_\alpha]\,. \tag{32}$$

A structure calculation consists of diagonalizing the Hamiltonian in this representation and determining the eigenvectors $t_{i\alpha}^{(\mu)}$ and eigenvalues ε_μ. This is easily understood in the case where the target is a closed shell. The only terms in $(\psi_\mu \mid \Phi_0)$ that do not vanish by orthonormality of the core states are

$$(\psi_\mu \mid \Phi_0) = \sum_i t_{i0}^{(\mu)}\, \phi_i^\dagger(\boldsymbol{r}_2), \qquad i \supset \mu\,. \tag{33}$$

The angular momentum and parity quantum numbers in the set i are the same as those in the set μ. Only the radial quantum numbers are summed over. This is equivalent to the idea that there is a *best* ϕ_i and a best spectroscopic amplitude $t_{i0}^{(\mu)}$, defined so that there is only one term in the sum (33).

(i) An experimental definition of the *best* function ϕ_i is the one that best fits the coincidence cross section. We would like to know if this corresponds to any obvious theoretical definition.

The closure property of the target eigenstates leads to a sum rule over all states ψ_μ belonging to the same representation of the rotation group, provided we use the *best* function ϕ_i:

$$\sum_\mu S_{i0}^{(\mu)} = 1\,, \tag{34}$$

where the spectroscopic factors $S_{i0}^{(\mu)}$ are defined by

$$S_{i0}^{(\mu)} = |\, t_{i0}^{(\mu)}\,|^2\,. \tag{35}$$

If the approximation (22) for the coincidence amplitude is correct, the differential cross section is proportional to $S_{i0}^{(\mu)}$, provided there is only one term in the sum (33), i.e. provided we use the best function ϕ_i.

(ii) We have an independent check of the single-particle orbital ϕ_i. If we have the *best* function and the correct reaction theory, the spectroscopic factors for all final states belonging to the same representation will sum to 1.

We therefore have a very specific tool for measuring spectroscopic factors and thus checking structure calculations, if we can identify the representation to which a final state belongs. With the kinematic detail in the breakup experiment, this is simple.

(iii) At intermediate energies, where the plane wave approximation (27) is not a gross distortion of the truth, the differential cross section has the general shape of the square of the half-off-shell two-body T-matrix times the square of the Fourier transform of the *best* orbital ϕ_i. This shape is strongly characteristic of the quantum number l specifying the representation.

In some cases it may be possible to excite states whose overlap with the ground state is zero in simple structure models, but nonzero if both states are described by sums of configurations determined by sophisticated variational procedures. Such reactions would give very detailed information. An example is given in the next section.

Example: (e, 2e) Reaction on Atoms

Most of the reactions to be described are performed with noncoplanar symmetric geometry. This geometry has the fortunate advantage that the square of the half-off-shell Mott T-matrix (the antisymmetrized Coulomb T-matrix) is independent of the angle ϕ that is varied to give the distribution over the momentum $\boldsymbol{q}$. For this reason, one expects the factorization approximation to be an excellent one and the intermediate energy region to extend to quite low energies. In this approximation, the shape of the angular correlation is the square of the distorted wave transform in equation (29) of the structure factor or, for reasonably small distortions, roughly the square of the Fourier transform (28a). While the antisymmetrized off-shell T-matrix does not exactly have this property in nuclear physics, it is obviously slowly varying and noncoplanar symmetric geometry would be excellent for the extraction of structure information.

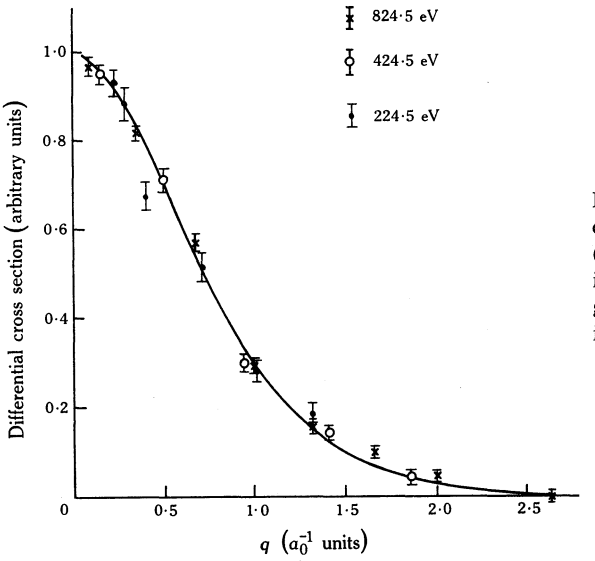

Fig. 1. Theoretical curve compared with experimental (e, 2e) angular correlations in in noncoplanar symmetric geometry for helium at the indicated incident energies.

For extraction of structure information, one could hope that the plane wave approximation would be reasonably valid. In fact it has been shown by Furness and McCarthy (1974) for atomic distorted waves and by Amos (1966) for nuclear distorted waves that the attenuated plane wave approximation is excellent in the surface region, to which the reaction is confined if valence shells are observed:

$$\chi^{(\pm)}(\boldsymbol{k}, \boldsymbol{r}) = \exp\{\mathrm{i}(1 \pm \mathrm{i}\gamma)\boldsymbol{k}.\boldsymbol{r}\}\exp(-\gamma kR). \tag{36}$$

In both cases the attenuation parameter is too small to affect the shape of the

angular correlation, and hence we expect the plane wave equation (27) to be roughly valid for the shape. Its validity is easily tested experimentally, since it requires the differential cross section shape to depend only on q, not on the total energy E,

$$E = E_A + E_B \tag{37}$$

or the separation energy ε_μ.

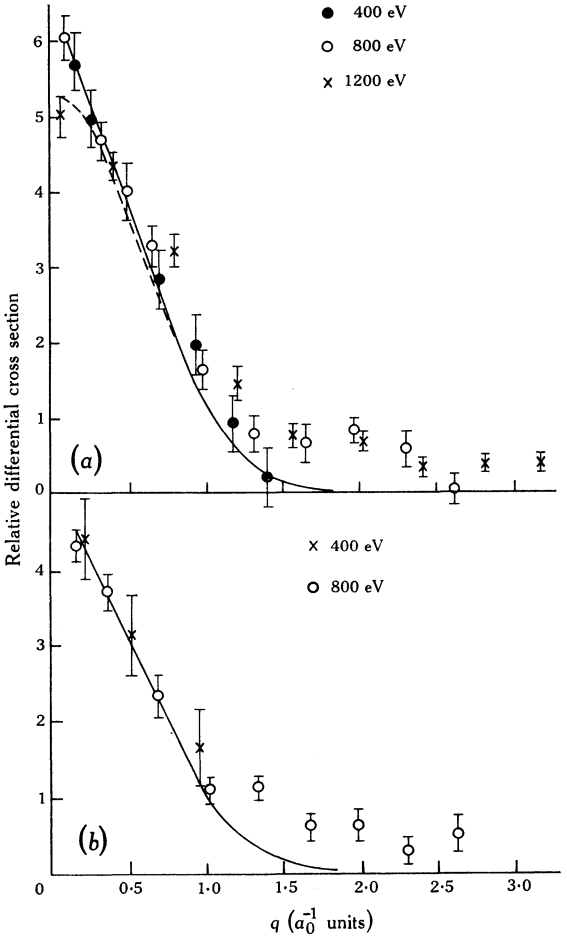

Fig. 2. Theoretical curves compared with experimental (e, 2e) angular correlations in noncoplanar symmetric geometry, with the indicated incident energies, for the 3s levels of argon at (*a*) 29·3 eV and (*b*) near 40 eV.

Figs 1 and 2 show that equation (27) is valid for (e, 2e) reactions on helium and argon over a wide range of energies. These reactions also check our early approximation (1), the quasi-three-body approximation. Core excitation terms are strongly energy-dependent. They are absent in any kinematic region where the breakup cross section depends only on q.

It is possible to fit the (e, 2e) angular correlation within experimental error. The structure factor used for the calculation is the *best* theoretical orbital multiplied by a spectroscopic factor for each state. The *best* theoretical orbital is the one obtained

by treating a determinant of single-particle orbitals as the trial function in a variational calculation. It is the Hartree–Fock orbital.

The Hartree–Fock calculation is numerically difficult and different numerical approximations have been used. As illustrated in Fig. 3, two such computations (A) by Herman and Skillman (1963) and (B) by Froese-Fischer (1972) fit the shape of the 3p excitation of argon well, while a third (C; Lu *et al.* 1974) fits it less well. This demonstrates the sensitivity of the method to details of the shape of the wavefunction.

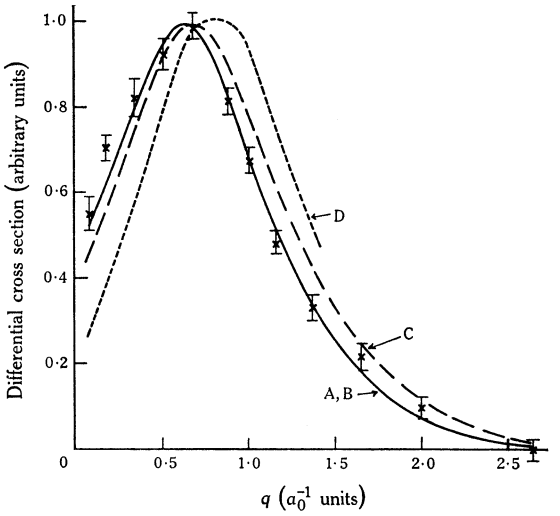

Fig. 3. Fits of bound-state wavefunctions to the 400 eV (e, 2e) angular correlations for the 3p state of argon at 815·76 eV:

A, B, Hartree–Fock computations by Herman and Skillman (1963) and Froese-Fischer (1972);

C, Hartree–Fock computation by Lu *et al.* (1974);

D, best variational Slater-type orbital.

There is only one 3p reaction observed for argon, at the separation energy 15·7 eV. It contains magnetic and spin–orbit degeneracies. The 3p spectroscopic factor for this level is therefore unity.

Three 3s levels are observed, at separation energies of 29·3, 38·6 and 41·2 eV. Their spectroscopic factors can be determined relative to the 3p spectroscopic factor. The sum is $0{\cdot}92 \pm 0{\cdot}07$, thus checking closely the structure factors A and B above.

There is a further check on the structure factor:

(iv) The independent-particle model eigenvalue for the 3s state in argon is defined as the expectation value of the Hamiltonian in the independent-particle state ϕ_i,

$$E_i = \langle \phi_i | H | \phi_i \rangle = \sum_{\mu\nu} \langle \phi_i | \psi_\mu \rangle \langle \psi_\mu | H | \psi_\nu \rangle \langle \psi_\nu | \phi_i \rangle = \sum_\mu S_{i0}^{(\mu)} \varepsilon_\mu . \qquad (38)$$

This is the centroid of the separation energies ε_μ, weighted by the spectroscopic factors.

The experimental value for argon is 34 ± 1 eV. The theoretical values for computations A and B are respectively 29 and 34·8 eV. The (e, 2e) reaction thus selects method B as the only acceptable structure theory.

What advantage does the breakup reaction have for analysing the structure of the residual system over other methods such as pickup or stripping, which also measure relative spectroscopic factors? The most important advantage is the sensitivity to the shape of the orbital, so that we can find the spectroscopic factor for

the *best* orbital. One can of course also verify structure calculations, based on various numerical Hartree–Fock methods, which attempt to correlate single-particle orbitals.

Brief mention should be made of the use of the breakup reaction in checking complicated configuration mixtures as models for many-body systems. The example is the helium atom. The ion can be left in an $N = 2$ state, even though there is only an $N = 1$ state in the Hartree–Fock wavefunction for the atom. A more sophisticated model gives nonzero overlap for $N = 2$ residual states and $N = 2$ configurations in the ground state. Using a very large basis, a helium wavefunction can be found which fits the (e, 2e) angular correlation exactly, while the Hartree–Fock prediction is clearly incorrect (McCarthy *et al.* 1974). This is shown in Table 1.

Table 1. Comparison of models for helium ion

The values shown are the differential cross section ratios for excitation of $N = 2$ and $N = 1$ states of He^+, expressed as percentages

θ (degrees)	Hartree–Fock prediction[A]	Correlated wavefunctions[B] 2s	2s+2p	Experimental ratio
45	2·75	0·65	0·67	0·72±0·04
49	2·07	0·77	0·88	0·97±0·10
53	1·94	1·42	1·74	1·54±0·30

[A] From Froese-Fischer (1972).
[B] From Joachain and Vanderpoorten (1970).

Is the breakup reaction so trivial that the plane wave theory is sufficient? This would be true at high enough energies, but experiments must be done at low enough energies to resolve states of the residual system. The coplanar symmetric geometry is one in which the factorized distorted wave off-shell impulse approximation does not work well for 400 eV (e, 2e) on argon or 100 MeV (p, 2p) on ^{12}C. The approximation does work for 1000 eV (e, 2e) on argon. In all these cases final states can be resolved. The calculations require distorted waves and an accurate model for the two-body T-matrix. In coplanar symmetric geometry, variation of θ is roughly equivalent to varying the energy in the elementary two-body collision. The T-matrix varies quite rapidly with energy in both atomic and nuclear physics in the regions where the factorization approximation is inaccurate. By contrast the T-matrix varies negligibly with ϕ in noncoplanar symmetric geometry, so that for this geometry the factorization method works at lower energies.

Conclusions

For this treatment of the breakup reaction, the intermediate energy range is defined at the lower end by the requirement that the factorized distorted wave T-matrix approximation must be an adequate description of the reaction and at the upper end by the experimental requirement that states of the residual system must be resolved.

We have seen that the energy range exists for (e, 2e) experiments on atoms. The reaction yields a very sensitive test of the shapes of the single-particle orbitals. The best numerical Hartree–Fock orbitals fit the data. Spectroscopic factors for the best orbitals are determined. In some cases it is possible to investigate ground state configuration interaction in the target.

For the (p, 2p) experiment on nuclei, noncoplanar symmetric geometry extends the energy range as low as possible and into the range where final states can be resolved.

References

Amos, K. A. (1966). *Nucl. Phys.* **77**, 225.
Froese-Fischer, C. (1972). *At. Data* **4**, 302.
Furness, J. B., and McCarthy, I. E. (1974). *J. Phys.* B **7**, 541.
Herman, F., and Skillman, S. (1963). 'Atomic Structure Calculations' (Prentice–Hall: New York).
Joachain, C. J., and Vanderpoorten, R. (1970). *Physica* **46**, 333.
Lu, C. C., Carlson, T. A., Malik, F. B., Tucker, T. C., and Nestor, C. W., Jr (1974). *At. Data* **3**, 1.
McCarthy, I. E., Ugbabe, A., Weigold, E., and Teubner, P. J. O. (1974). *Phys. Rev. Lett.* **33**, 459.

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