

ATOMIC PERTURBATIONS IN NUCLEAR REACTIONS

by

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Recent experimental advances in the resolution of cross section measurements of nuclear resonances have made it desirable to investigate the effects of the atomic environment on such measurements. Single-atom processes are studied in which the reacting projectile interacts with the atomic electrons, causing ionization. This ionization produces changes in the resonance line shape so that isolated nuclear resonances no longer have the simple, symmetric, Breit-Wigner form.

A simplified model of the atom is assumed in which there is only one excited state, and the electron-projectile potential is adjusted so that this single state can approximately represent the infinite number of real states. The criterion used requires that the total excitation probability for the model be equal to that for the particular atomic shell being considered.

The R -matrix theory of nuclear reactions forms the basis for the calculation. The two-state model of the atom allows the Schrödinger equation to be expressed as a pair of coupled differential equations with the elimination of the electronic coordinates. These equations permit the appropriate definition of internal and external states as required by the R -matrix theory. The theory is then developed for an isolated nuclear resonance.

In order to obtain a numerical estimate of the magnitude of the effect, the formal theory is specialized to the s -wave elastic scattering of 1.17 MeV protons on Ne^{20} with a width of 8 eV. The result is that ionization from the L_{II} or L_{III} subshells of Ne occurs in about 30% of the scattering processes. This value is shown to be consistent

with estimates obtained from Levinger's calculations of the effects of alpha and beta disintegrations on inner-shell electrons.

TABLE OF CONTENTS

	Page
ACKNOWLEDGMENTS	iii
INTRODUCTION	1
CHAPTER	
I THEORY OF NUCLEAR REACTIONS	5
II ATOMIC PERTURBATIONS: ELASTIC NUCLEAR SCATTERING	19
III ATOMIC PERTURBATIONS: NUCLEAR REACTIONS	35
IV THE MODEL PARAMETERS	48
V CONCLUSIONS	53
APPENDIX	
I CORRECTION FACTORS IN $(A_{res}^1)_{c'c}$	59
II DECOMPOSITION OF $(1 - RL^0)^{-1}R$	62
III THE QUANTITIES Γ AND ξ	63
IV EXCITATION CROSS SECTION FOR THE MODEL DURING PROTON IMPACT	66
FIGURES	69
REFERENCES	74

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INTRODUCTION

This thesis considers one of the small effects of physics, the influence of the atomic environment on nuclear reactions. Little work has been done in this field due to the coarseness of the experimental techniques, which have prevented observation of such phenomena. More recently, advances in the precision of nuclear experiments have made it desirable to re-examine the influence of atomic processes on nuclear reactions.

This is not to imply that the nuclear physicist has never seen atomic effects. The thick-target yield curve of a resonant nuclear reaction is an example to the contrary. At the resonant energy the yield curve rises sharply from zero to a level plateau. This happens because the incident particle with an energy greater than the resonant energy loses energy by atomic collisions until it has the resonant energy, whereupon it reacts with the nucleus (if at all). Hence, all particles with an energy greater than the resonant energy have an equal probability of reacting with the nucleus, leading to the flat plateau.

Actually, this view of the thick-target process must be modified slightly due to the Lewis effect, a more subtle example of the influence of atomic processes (1). In certain instances one sees a pronounced hump at the top of the rise in the yield curve, followed by a slight dip before the curve levels out. This phenomenon was explained by

Lewis as arising from the fact that the incident charged particle slows down by losing discrete amounts of energy to the atoms of the target. The hump is understood by noting that only incident particles with the resonant energy are assured of ever having the correct energy for reacting with the nucleus; particles with greater energy may completely jump the resonance during an atomic collision and never have the opportunity to react. The following dip, which is often not seen at all and is much smaller than the hump when it is seen, is understood by realizing that the incident particle of slightly more than resonant energy may jump entirely across the resonance and be unable to react. More energetic particles may do the same thing, of course, but there is also the possibility they will acquire the resonant energy, thereby reacting with greater probability. Thus, ideally the yield curve should dip, then rise again. This effect is often lost in the imperfections of the experiment.

These two examples are really instances of the bulk properties of matter in that they involve the interaction of the incident particle with many atoms of the target. On the other hand the process to be investigated here concerns the interaction of the particle with a single atom. In contrast to the above, the projectile reacts with the nucleus and electrons of the same atom.

A lone voice in the literature, Christy has made rough estimates of the atomic effects in such single-atom events (2). He is concerned with the atomic corrections to nuclear Q values, the Q value being the difference in the ground-state energies of the initial and final atoms. The corrections arise for various reasons. First, the recoiling nucleus carries off a certain amount of energy as well as causing atomic excitation.

Second, the change in nuclear charge during a (p,n) reaction, for example, induces atomic excitation and changes the ground state energy of the atom. Third, the passage of a charged particle through the atom produces atomic excitation through the Coulomb perturbation. Christy finds that these effects are unimportant until the experimental resolution becomes less than about 100 eV. Unattainable at that time, such resolutions are now fact, pointing up the need for newer and more detailed calculations on such processes.

This work addresses itself to the third aspect of Christy's paper, the atomic excitation produced by a charged particle undergoing a nuclear reaction. More specifically, we consider the effects of such excitations on the shape of nuclear resonances. This calculation was suggested a number of years ago by H. W. Newson. The physical process is easy to imagine. The incoming charged particles interact via the Coulomb field with the atomic electrons, and an occasional projectile will lose energy by ionizing the atom. The particle then strikes the nucleus with diminished energy and, consequently, altered probability for undergoing the nuclear reaction. The end result is a different resonance shape; specifically, the symmetric isolated resonance is expected to become asymmetric. This is the classical picture. When the calculation is done quantum-mechanically, one includes the fact that the outgoing particle (if charged) can also excite the atom. Since the two processes are generally indistinguishable, both contribute to the cross section of the event and interfere with each other.

Actually, neither incident nor outgoing particle need be charged for ionization to occur. It is well known from studies of ionization probabilities during nuclear decays and reactions that even the recoil

accompanying the capture and emission of neutral particles induces significant ionization (3,4). However, nuclear recoil will be neglected here so that such processes will not contribute.

CHAPTER I
THEORY OF NUCLEAR REACTIONS

Nuclear reaction theory has its beginning in the 1936 suggestion by Bohr (5) of the compound nucleus mechanism, which was elaborated by Bethe (6) the following year. But the first real quantitative success came in the application of the Weisskopf-Wigner theory (7) of atomic resonance fluorescence to nuclear resonances. This time-dependent perturbation treatment of nuclear reactions by Breit and Wigner (8) yielded the correct energy dependence but was unable to make quantitative statements concerning the cross section. This was of course due to the application of the perturbation method to strong nuclear forces.

In 1938, Kapur and Peierls (9) published the first rigorous nuclear reaction theory, which, although completely general, is especially well suited to the description of reactions proceeding by the compound nucleus mechanism. However, the energy dependence of the cross section is not exhibited explicitly, but rather certain quantities are themselves energy dependent in an unknown way. This led Wigner and Eisenbud (10) in 1947 to develop the "*R*-matrix theory of nuclear reactions," in which the energy dependence of the cross section was made as explicit as possible.

R-matrix theory has been attacked on grounds which are mainly aesthetic. This dissatisfaction produced other reaction theories,

notably those of Rosenfeld (11) and Feshbach (12). They claim, among other advantages, a more natural application to the various types of nuclear reactions. However, the R -matrix theory is particularly well suited to the description of resonances, so it will be used here. In the remainder of this chapter we present a brief outline of the theory of the R matrix in order to establish certain rules of notation and to provide a useful reference for the following calculations.

General Description of R -Matrix Theory

The basic idea behind the theory is quite simple; it is only in the details of the calculation that matters become complicated. The first step in any quantum-mechanical scattering problem is to relate the cross section for a given process to the amplitude of the corresponding outgoing wave in the wavefunction. This is done in terms of the U matrix, each element of which is defined as the amplitude of the outgoing wave of the pair of product particles c' produced by an incoming pair of reacting particles c . The U matrix contains all the physics of the process but is rather far removed from the actual dynamics producing the scattering. In addition, for nuclear scattering all the interactions are not even known.

This latter problem is dealt with in a manner which is peculiar to R -matrix theory (and the Kapur-Peierls theory). The configuration space of the N nucleons (those in the nucleus plus those in the projectile) is divided into two regions, the external region in which any pair of nuclei formed from the N nucleons interact via non-nuclear forces only, and the internal region. It is assumed that for each pair of nuclei c , there is a separation distance a_c beyond which there is no nuclear interaction. There is of course a lower bound on a_c ,

but any greater value is formally valid. Next, for each pair of nuclei we define incoming and outgoing wavefunctions in the external region where the interactions are known. In the internal region the interactions are incompletely known, but formal eigenstates can nevertheless be defined in terms of boundary conditions on the surface separating the two regions. The total scattering wavefunction is expanded in each region in terms of an appropriate set of functions, and the logarithmic derivatives of the two expansions are matched at the surface. The external quantities are expressed in terms of the L and Ω matrices, yet to be defined, and the internal quantities are expressed in terms of the R matrix. By joining the two solutions, the U matrix is written in terms of the L , Ω , and R matrices, which are more closely related to the interactions involved in the reaction. Now the rationale behind the division of configuration space into exterior and interior regions becomes apparent. In the exterior all interactions are known and, at least in principle, can be treated exactly. For the internal region where the forces are not known, we can nevertheless determine the various internal quantities appearing in the cross section by fitting from experiment.

The theory of the R matrix is useful in the description of nuclear resonances as one may be able to identify one of the internal states with the compound nucleus state by which the reaction proceeds. If this is possible, one can often neglect all but that single internal state, yielding the famous "one-level resonance formula."

In summary, we list the four assumptions of the R -matrix theory:

- 1) Correctness of non-relativistic quantum mechanics.
- 2) No creation or annihilation processes.

- 3) No processes producing more than two final nuclei.
 4) The assumption, for any pair of nuclei c , of a finite distance a_c beyond which the nuclear interaction is absent.

Assumptions 2) and 3) can be relaxed somewhat, but this additional freedom is not required in this paper.

Definitions and Notation

So far, a pair of nuclei has been given the vague label c . This notation is now made more precise by introducing the concept of "channel," which is defined as a pair of nuclei each in a definite quantum state. The description of the quantum state includes the quantum numbers of relative motion as well as those of the internal and spin states of the nuclei. Thus, for a pair of nuclei in quantum states α_1 and α_2 with spins I_1 and I_2 , spin projections i_1 and i_2 , and relative angular momentum ℓ and projection m , the channel c is written

$$c = (\alpha i_1 i_2 \ell m)$$

where α is written for the pairs $\alpha_1 \alpha_2$ and $I_1 I_2$. Alternatively, the two spins can be coupled to form a channel spin s and projection v so that

$$c = (\alpha s v \ell m)$$

Again, it is often useful to combine the spin and orbital angular momenta into a total angular momentum J and projection M , giving

$$c = (\alpha \ell J M)$$

External Wavefunctions

In the center-of-mass system the Hamiltonian H_N can be written as the sum of three terms,

$$H_N = H_c + H_{\alpha_1} + H_{\alpha_2}$$

Here, H_c involves the relative motion of the two fragments under consideration (i. e., H_c = relative kinetic energy plus long-range interactions), and H_{α_1} and H_{α_2} contain the internal coordinates of the fragments α_1 and α_2 .

The total external wavefunction can be written as the product of three parts, the wavefunction of relative motion and the two wavefunctions of the internal states. The internal channel spin wavefunctions $\psi_{\alpha_1 I_1 i_1}$ and $\psi_{\alpha_2 I_2 i_2}$, which are eigenfunctions of H_{α_1} and H_{α_2} , are not the most convenient internal functions to use. Since H_c does not depend on the orientations of the spins I_1 and I_2 , the spin wavefunctions can be vector-coupled to form wavefunctions of channel spin s and projection v , $\psi_{\alpha s v}$, which are assumed to be orthogonal.

The wavefunction of relative motion is

$$\chi_c = \frac{1}{R_\alpha} u_{\alpha s l}(R_\alpha) i^\ell Y_{\ell m}(\Omega_\alpha)$$

where the radial function satisfies

$$\frac{d^2 u_{\alpha l}}{d\rho_\alpha^2} - \left(\frac{\ell(\ell+1)}{\rho_\alpha^2} + \frac{2\eta_\alpha}{\rho_\alpha} - 1 \right) u_{\alpha l}(\rho_\alpha) = 0$$

where $\eta_\alpha = Z_1 Z_2 / \hbar v_\alpha$, $\rho_\alpha = k_\alpha R_\alpha$, and R_α is the relative coordinate of separation of the pair α . The energy is taken to be positive. The most natural choice for the two independent solutions is made in terms of their asymptotic behavior as

$$\begin{aligned} I_c &\equiv I_{\alpha l} \sim \exp[-i(\rho_\alpha - \eta_\alpha \log 2\rho_\alpha - \frac{\ell\pi}{2} + \sigma_{\alpha 0})] \\ O_c &\equiv O_{\alpha l} \sim \exp[+i(\rho_\alpha - \eta_\alpha \log 2\rho_\alpha - \frac{\ell\pi}{2} + \sigma_{\alpha 0})] \end{aligned}$$

where $\sigma_{\alpha l} = \arg \Gamma(\ell + 1 + i\eta_\alpha)$. In the absence of the Coulomb field ($\eta_\alpha = 0$), these two solutions are simply related to the Hankel functions

of half-odd order.

The complete external channel wavefunctions in the $(\alpha s l \nu m)$ scheme are

$$I_{\alpha s l \nu m} = \frac{1}{R_\alpha} I_{\alpha l} i^l Y_{l m} \psi_{\alpha s \nu}$$

$$O_{\alpha s l \nu m} = \frac{1}{R_\alpha} O_{\alpha l} i^l Y_{l m} \psi_{\alpha s \nu}$$

and in the $(\alpha s l J M)$ scheme they are

$$I_{\alpha s l J M} = \sum_{\nu+m=M} (\alpha s l \nu m | J M) I_{\alpha s l \nu m}$$

$$O_{\alpha s l J M} = \sum_{\nu+m=M} (\alpha s l \nu m | J M) O_{\alpha s l \nu m}$$

Finally, it is useful to introduce the surface wavefunctions,

$$\phi_{\alpha s l \nu m} = \frac{1}{R_\alpha} i^l Y_{l m} \psi_{\alpha s \nu}$$

They are similarly defined in the $(\alpha s l J M)$ scheme. In both cases they are mutually orthonormal on S , the hypersphere in configuration space separating the internal and external regions.

The U Matrix and Cross Section

The most general form for the scattering wavefunction is

$$\begin{aligned} \psi &= \sum_c (y_c I_c + x_c O_c) \\ &= \sum_{c c'} (\delta_{c c'} I_c - U_{c' c} O_{c'}) y_c \end{aligned}$$

where the U matrix is defined by

$$x_{c'} = -\sum_c U_{c' c} y_c$$

The y_c are determined by the requirement that the only incoming waves be those in the incident plane wave:

$$y_c = y_{\alpha s l \nu 0} = \frac{i\pi^{\frac{1}{2}}}{k_\alpha} (2l + 1)^{\frac{1}{2}}$$

All other y_c are zero. Then,

$$\psi = \psi^{\text{inc}} + \sum_{cc'} (\delta_{cc'} - U_{c'c}) O_{c'} y_c$$

The amplitude $f_{\alpha' s' \nu', \alpha s \nu}$ for the inelastic outgoing spherical wave of the type $\alpha' s' \nu'$ associated with the incident plane wave of type $\alpha s \nu$ is

$$f_{\alpha' s' \nu', \alpha s \nu} = -\frac{i\pi^{\frac{1}{2}}}{k_\alpha} \sum_{\ell \ell'} (2\ell + 1)^{\frac{1}{2}} U_{\alpha' s' \ell' \nu' m', \alpha s \ell \nu m} Y_{\ell' m'}(\Omega_{\alpha'})$$

The differential cross section for the process is given by the outgoing flux divided by the incoming flux:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\alpha' s' \nu', \alpha s \nu} = \frac{\pi}{k_\alpha^2} \frac{v_{\alpha'}}{v_\alpha} \left| \sum_{\ell \ell'} (2\ell + 1)^{\frac{1}{2}} U_{\alpha' s' \ell' \nu' m', \alpha s \ell \nu 0} Y_{\ell' m'}(\Omega_{\alpha'}) \right|^2$$

In order to sum over ν and s for unpolarized beams and targets, it is useful to change to the $(\alpha s \ell J M)$ system. The U matrices in the two schemes are related by

$$U_{\alpha' s' \ell' \nu' m', \alpha s \ell \nu m} = \sum_{JM} (s \ell \nu m | JM) (s' \ell' \nu' m' | JM) U_{\alpha' s' \ell', \alpha s \ell}^J$$

Integrating the differential cross section over angle, substituting the relation between the two U matrices, summing over ν' , and averaging over ν , we obtain the total cross section for reactions of unpolarized beams with given channel spin:

$$\sigma_{\alpha' s', \alpha s} = \frac{\pi}{k_\alpha^2} \frac{v_{\alpha'}}{v_\alpha} \frac{1}{2s + 1} \sum_{J \ell \ell'} (2J + 1) |U_{\alpha' s' \ell', \alpha s \ell}^J|^2$$

Since one does not measure the spins s or s' , the experimental cross section is given by summing over s' and averaging over s . The total number of initial spin states is $(2I_1 + 1)(2I_2 + 1)$, so that

$$\sigma_{\alpha', \alpha}^J = \frac{v_{\alpha'} \pi}{v_{\alpha} k_{\alpha}^2} \sum_{J, \ell, \ell', s, s'} g_{\alpha}^J |U_{\alpha', s', \ell', \alpha s \ell}^J|^2 \quad (1)$$

where

$$g_{\alpha}^J = \frac{2J + 1}{(2I_1 + 1)(2I_2 + 1)}$$

Equation (1) is valid for inelastic scattering, $\alpha \neq \alpha'$. For elastic scattering U must be replaced by $1 - U$, and the Coulomb amplitude must be included if charged particles are incident. For simplicity, in this chapter we treat only inelastic scattering.

The R-Matrix Relation

The Schrödinger equations for two arbitrary solutions at energies E_1 and E_2 are

$$H\psi_1 = E_1\psi_1$$

$$H\psi_2 = E_2\psi_2$$

Forming $\psi_2^\dagger \times (\text{first}) - \psi_1 \times (\text{second})^\dagger$, and integrating over the internal region τ , we obtain

$$(E_2 - E_1) \int_{\tau} \psi_2^\dagger \psi_1 \, d\tau = \int_{\tau} [(H\psi_2)^\dagger \psi_1 - \psi_2^\dagger H\psi_1] \, d\tau$$

If the interaction term is self-adjoint, it drops out, and the remaining kinetic energy terms may be integrated by the 3A-dimensional form of Green's theorem, giving

$$(E_2 - E_1) \int_{\tau} \psi_2^\dagger \psi_1 \, d\tau = \int_S \frac{\hbar^2}{2M_c} (\psi_2^\dagger \text{grad}_n \psi_1 - \psi_1 \text{grad}_n \psi_2^\dagger) \, dS \quad (2)$$

It is convenient to introduce certain quantities on the boundary surface S , namely, the value quantity,

$$V_c = \left(\frac{a_c^2}{2M_c a_c} \right)^{1/2} u_c(a_c)$$

and the derivative quantity,

$$D_c = \left(\frac{a_c^2}{2M_c} \right)^{1/2} \left(\frac{du_c}{dR_c} \right)_{R_c=a_c}$$

where u_c is the radial solution on S (in general, one cannot separate variables inside S). These quantities may be expressed as surface integrals,

$$V_c = \left(\frac{a_c^2}{2M_c a_c} \right)^{1/2} \int_S \phi_c^\dagger \psi \, dS$$

$$D_c = V_c + \left(\frac{a_c^2}{2M_c} \right)^{1/2} \int_S \phi_c^\dagger \text{grad}_n \psi \, dS$$

Finally, ψ and its normal gradient on S are expanded in terms of the ϕ_c ,

$$\psi = \sum_c \left(\frac{2M_c a_c}{a_c^2} \right)^{1/2} V_c \phi_c$$

$$\text{grad}_n \psi = \sum_c \left(\frac{2M_c}{a_c^2} \right)^{1/2} (D_c - V_c) \phi_c$$

Substitution of these expansions into Equation (2) gives

$$(E_2 - E_1) \int_\tau \psi_2^\dagger \psi_1 \, d\tau = \sum_c (V_{2c}^* D_{1c} - V_{1c} D_{2c}^*) \quad (3)$$

We introduce the complete set of internal states $X_{\lambda J}$ which satisfy

$$H X_{\lambda J M} = E_{\lambda J} X_{\lambda J M}$$

with boundary conditions on the surface S ,

$$\frac{D_{\lambda c}}{V_{\lambda c}} \equiv \frac{\delta_{\lambda c}}{\gamma_{\lambda c}} = B_c$$

where the constants B_c are independent of the λ . The states $X_{\lambda JM}$ are chosen to be eigenstates of the total angular momentum J and its projection M . The label λ completes the specification of the states. Equation (3) shows that these internal solutions form an orthogonal set. The solutions are also assumed to be normalized so that, dropping the JM designation,

$$\int_{\tau} X_{\lambda}^{\dagger} X_{\lambda} d\tau = \delta_{\lambda\lambda'}$$

Any wavefunction ψ can be expanded in terms of the X_{λ} inside S :

$$\begin{aligned}\psi &= \sum_{\lambda} A_{\lambda} X_{\lambda} \\ A_{\lambda} &= \int_{\tau} X_{\lambda}^{\dagger} \psi d\tau\end{aligned}$$

The A_{λ} are determined by another application of Equation (3) using the expansions for ψ and $\text{grad}_n \psi$,

$$A_{\lambda} = \frac{1}{E_{\lambda} - E} \sum_c D_c^{\circ} Y_{\lambda c}$$

where

$$D_c^{\circ} = D_c - B_c V_c$$

Therefore,

$$\psi = \sum_c \left[\sum_{\lambda} \frac{1}{E_{\lambda} - E} X_{\lambda} Y_{\lambda c} \right] D_c^{\circ}$$

and operating on this with $\int_S \phi_c^{\dagger} dS$, one obtains the fundamental R-matrix relation,

$$\begin{aligned}V_{c'c} &= \sum_c R_{c'c} D_c^{\circ} \\ R_{c'c} &\equiv \sum_{\lambda} \frac{1}{E_{\lambda} - E} Y_{\lambda c'} Y_{\lambda c}\end{aligned}$$

In matrix notation,

$$V = RD^0$$

$$R = \sum_{\lambda} \frac{1}{E_{\lambda} - i} \gamma_{\lambda} \times \gamma_{\lambda}$$

The matrices V and D^0 are column vectors with components V_c and D_c^0 .

The matrix $\gamma_{\lambda} \times \gamma_{\lambda}$ is the direct product of the vector γ_{λ} with components $\gamma_{\lambda c}$. Note that the R matrix is symmetrical and real (because the $\gamma_{\lambda c}$ are real).

Relation between the R and U Matrices

Since the R matrix specifies the form of the wavefunction inside S , and the U matrix specifies it in the external region, by joining the two segments of the wavefunction on S , we obtain a relation between U and R . Recalling that in the exterior the wavefunction has the form,

$$\Psi = \sum_c (x_c O_c + y_c I_c)$$

we write the value and derivative quantities as

$$V_c = \left(\frac{\hbar^2}{2M_c a_c} \right)^{1/2} (O_c x_c + I_c y_c)_{R_c = a_c}$$

$$D_c^0 = \left(\frac{\rho_c^2 \hbar^2}{2M_c a_c} \right)^{1/2} \left(\frac{dO_c}{d\rho_c} x_c + \frac{dI_c}{d\rho_c} y_c \right)_{R_c = a_c}$$

The R -matrix relation becomes, in matrix notation,

$$[O - R(\rho \frac{dO}{d\rho} - BO)](Ma)^{-1/2} x = -[I - R(\rho \frac{dI}{d\rho} - BI)](Ma)^{-1/2} y \quad (4)$$

By definition,

$$x = -Uy$$

so that by comparison with Equation (4), we have

$$U = IO^{-1} + 2i(\text{Ma})^{\frac{1}{2}}O^{-1}(1 - RL^O)^{-1}RPI(\text{Ma})^{-\frac{1}{2}}$$

where the following quantities have been introduced:

$$L \equiv \rho \frac{dO}{d\rho} O^{-1}$$

$$L^O \equiv L - B$$

The One-Level Approximation

The only remaining problem is the inversion of the channel matrix $(1 - RL^O)$. If only one or two channels participate, the inversion is simple. But in general there are an infinite number of channels so we are faced with the prospect of inverting an infinite-dimensional matrix. This inversion can be circumvented by transforming it into the inversion of a level matrix. If, as is often the case, only one or two levels are important in the reaction, we need invert only a one- or two-dimensional matrix, no matter how many channels are involved.

First, R is written as the sum of two terms,

$$R = R^O + R'$$

corresponding to the division of the levels into two groups. Eventually, the approximation will come about in the assumption that R' is large compared to R^O , but for the present the division is arbitrary. Then,

$$(1 - RL^O)^{-1}R = (1 - R^OL^O)^{-1}R^O + (1 - R^OL^O)^{-1}(1 - R'L')^{-1}R'(1 - L^OR^O)^{-1}$$

If R is split up so that $(1 - R^OL^O)$ can be inverted easily (at least in some approximation), the problem reduces to the inversion of $(1 - R'L')$, where L' is

$$L' \equiv L^0(1 - R^0L^0)^{-1}$$

This inversion can be done with the result that

$$U = U_0 + 2i(\text{Ma})^{\frac{1}{2}}O^{-1}(1 - R^0L^0)^{-1} \sum_{\lambda\mu} A_{\lambda\mu}(\gamma_\lambda \times \gamma_\mu)(1 - L^0R^0)^{-1}PI(\text{Ma})^{-\frac{1}{2}} \quad (5a)$$

where

$$U_0 = O^{-1}I + 2i(\text{Ma})^{\frac{1}{2}}O^{-1}(1 - R^0L^0)^{-1}R^0PI(\text{Ma})^{-\frac{1}{2}} \quad (5b)$$

The level matrix A is

$$A = (e - E - \xi)^{-1}$$

where e is the diagonal matrix with components E_λ , E is the energy times the unit matrix, and ξ has components $\xi_{\mu\lambda} = \sum_c (L'\gamma_\mu)_c \gamma_{\lambda c}$.

The level sum in U is restricted to those levels contained in R' so that A is determined by inverting a matrix whose size is given by the number of levels included in R' . In the "one-level approximation" it is assumed that in the neighborhood of a resonance one term in the expansion of R will be dominant. This term comprises R' :

$$R' = \frac{\gamma_\lambda \times \gamma_\mu}{E_\lambda - E}$$

The approximation comes in the assumption concerning R^0 . The strongest assumption, and the one usually used in practice, is that $R^0L^0 = 0$, giving

$$U = IO^{-1} + 2i(\text{Ma})^{\frac{1}{2}}O^{-1} \frac{\gamma_\lambda \times \gamma_\lambda}{E_\lambda + \Delta_\lambda - E - \frac{1}{2}i\Gamma_\lambda} PI(\text{Ma})^{-\frac{1}{2}}$$

where

$$\Delta_\lambda \equiv - \sum_c \gamma_{\lambda c} (S - B)_c \gamma_{\lambda c}$$

$$\Gamma_\lambda \equiv 2 \sum_c \gamma_{\lambda c} P_c \gamma_{\lambda c} = \sum_c \Gamma_{\lambda c}$$

The general element of the U matrix is

$$U_{cc'} = \begin{pmatrix} I_c \\ 0_c \end{pmatrix}^{1/2} \begin{pmatrix} I_{c'} \\ 0_{c'} \end{pmatrix}^{1/2} \left[\delta_{cc'} + i \begin{pmatrix} v_{c'} \\ v_c \end{pmatrix}^{1/2} \frac{\Gamma_{\lambda c}^{1/2} \Gamma_{\lambda c'}^{1/2}}{E_\lambda + \Delta_\lambda - E - \frac{1}{2}i\Gamma_\lambda} \right]$$

Insertion of this expression into Equation (1) for the cross section gives the famous Breit-Wigner one-level resonance formula for the reaction cross section ($\alpha \neq \alpha'$) for an isolated resonance of definite parity and J ,

$$\sigma_{\alpha\alpha'} = g_\alpha^J \frac{\pi}{k_\alpha^2} \frac{(\sum_{\ell s} \Gamma_{\lambda c}) (\sum_{\ell' s'} \Gamma_{\lambda c'})}{(E_\lambda + \Delta_\lambda)^2 + \frac{1}{4}\Gamma_\lambda^2}$$

where the primed sums are such that $\vec{\ell} + \vec{s} = \vec{\ell}' + \vec{s}' = J$.

As a general reaction theory, the S -matrix method is applicable to more than isolated resonances. Such applications, as well as a more detailed treatment of the material presented here, are contained in the article by Lane and Thomas (13).

CHAPTER II

ATOMIC PERTURBATIONS: ELASTIC NUCLEAR SCATTERING

In order to introduce the basic ideas involved in the calculation as simply as possible, we consider the following special case: the elastic nuclear scattering of a spinless charged particle for which the Coulomb interaction with the nucleus is neglected. Thus, we eliminate the complicating effects of Rutherford scattering which otherwise would interfere with the nuclear scattering. On the other hand, the really important features are retained intact.

The Two-State Approximation

It is assumed throughout the remainder of the paper that the atom consists of a single electron for which there exist but two states separated by an energy δ . Thus, the fundamental process by which the scattered particle gives up energy to the atom is included while the mathematics is kept to manageable proportions. It will be shown that the assumption of a single possible energy loss is a reasonable approximation. The assumption of a single atomic electron must, and will, be corrected for.

The basis for the calculation is the R -matrix theory of nuclear reactions. Although the formalism of the theory could be applied *in toto* to the problem, this would involve enclosing the entire atom inside the sphere separating internal and external regions. The resulting density of internal states would then be much too great to allow

the one-level approximation. Instead, the electronic coordinates can be eliminated at the outset by introducing the expansion,

$$\Psi(\vec{r}, \vec{R}) = \phi_0(\vec{r}) \psi_0(\vec{R}) + \phi_1(\vec{r}) \psi_1(\vec{R})$$

Here, Ψ is the total scattering wavefunction, ϕ_0 and ϕ_1 are the ground and excited states of the atom (with electronic coordinate \vec{r}), and ψ_0 and ψ_1 are the expansion coefficients which depend on the incident particle coordinate \vec{R} . We shall always use hydrogenic s-states for ϕ_0 and ϕ_1 , and neglect the electron spin as far as the dynamics is concerned.

The calculation is performed in the center-of-mass coordinate system of the nuclear masses. Since elastic scattering only is treated, in this system there is just the one nuclear coordinate \vec{R} for the external region. The nucleus is treated as infinitely massive with respect to the electron; this amounts to the neglect of nuclear recoil from the viewpoint of the electron.

It is useful to cast the various equations in matrix form.

Thus,

$$\Psi(\vec{r}, \vec{R}) = \phi^T(\vec{r}) \psi(\vec{R})$$

where

$$\phi = \begin{pmatrix} \phi_0 \\ \phi_1 \end{pmatrix} \quad \text{and} \quad \psi = \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}$$

To simplify matters further, we assume that the nuclear potential is central and expand $\psi(\vec{R})$ accordingly:

$$\psi(\vec{R}) = \frac{1}{k_0 R} \sum_{\ell} (2\ell + 1) G_{\ell}(R) P_{\ell}(\cos \theta)$$

where

$$G_{\ell} = \begin{pmatrix} G_{0\ell} \\ G_{1\ell} \end{pmatrix}$$

and the angle θ is measured from the incident beam direction. Substitution of this expansion into the previous equation for ψ , putting the result into the Schrödinger equation for Ψ , then operating alternately with $\int d\vec{r} \phi_0^*(r)$ and $\int d\vec{r} \phi_1^*(r)$ one obtains a pair of coupled differential equations which replace the Schrödinger equation in the usual theory:

$$\begin{aligned} \left[\frac{d^2}{dR^2} + k_0^2 - \frac{\ell(\ell+1)}{R^2} - U_{00} \right] G_{0\ell} &= U_{01} G_{1\ell} \\ \left[\frac{d^2}{dR^2} + k_1^2 - \frac{\ell(\ell+1)}{R^2} - U_{11} \right] G_{1\ell} &= U_{10} G_{0\ell} \end{aligned} \quad (1)$$

where

$$U_{mn} \equiv \frac{2M}{\hbar^2} \left[V_p(R) \delta_{mn} + \int \phi_m^*(r) V_{ep}(|\vec{r} - \vec{R}|) \phi_n(r) d\vec{r} \right]$$

V_p = nuclear potential seen by the projectile

V_{ep} = electron-projectile potential

In the above k_0 and k_1 are the wave numbers of the projectile when the atom is in its ground and excited states, respectively. They are related by

$$\frac{\hbar^2 k_0^2}{2M} = \frac{\hbar^2 k_1^2}{2M} + \delta$$

Definition of External States

As an alternate form of the radial Schrödinger equation, Equation (1) is the central equation of the calculation. In particular, it is used to define the necessary external wavefunctions. Since Equation (1) is a set of two coupled second-order differential equations, there will be four independent solutions instead of the customary two solutions

(incoming and outgoing, for example). The two equations decouple at infinity so the four solutions can be defined in terms of their asymptotic forms:

$$O_{\ell}^{\pm} \equiv \begin{pmatrix} O_{0\ell}^{\pm} \\ O_{1\ell}^{\pm} \end{pmatrix} \sim \begin{pmatrix} \exp[+i(k_0 R - \frac{1}{2}\pi\ell)] \\ \pm \exp[+i(k_1 R - \frac{1}{2}\pi\ell)] \end{pmatrix}$$

$$I_{\ell}^{\pm} \equiv \begin{pmatrix} I_{0\ell}^{\pm} \\ I_{1\ell}^{\pm} \end{pmatrix} \sim \begin{pmatrix} \exp[-i(k_0 R - \frac{1}{2}\pi\ell)] \\ \pm \exp[-i(k_1 R - \frac{1}{2}\pi\ell)] \end{pmatrix}$$

Finally,

$$O_{\ell} \equiv \begin{pmatrix} O_{0\ell}^{+} & O_{0\ell}^{-} \\ O_{1\ell}^{+} & O_{1\ell}^{-} \end{pmatrix} \quad I_{\ell} \equiv \begin{pmatrix} I_{0\ell}^{+} & I_{0\ell}^{-} \\ I_{1\ell}^{+} & I_{1\ell}^{-} \end{pmatrix}$$

and

$$O_{\ell m} \equiv i^{\ell} \frac{1}{R} O_{\ell} Y_{\ell m}(\theta, \phi) \quad I_{\ell m} \equiv i^{\ell} \frac{1}{R} I_{\ell} Y_{\ell m}(\theta, \phi)$$

The U Matrix and Cross Section

The most general external wavefunction is

$$\begin{aligned} \Psi(r, R) &= \phi^T(r) \sum_{\ell m} (O_{\ell m} x_{\ell m} + I_{\ell m} y_{\ell m}) \\ &= \phi^T(r) \sum_{\ell m} (I_{\ell m} - O_{\ell m} U_{\ell m}) y_{\ell m} \end{aligned}$$

where $x_{\ell m} = -U_{\ell m} y_{\ell m}$, $x_{\ell m}$ and $y_{\ell m}$ are two-component column matrices, and $U_{\ell m}$ is a 2×2 matrix. The $y_{\ell m}$ are determined by the condition that all the incoming part of Ψ be included in the incident plane wave:

$$\Psi^{\text{inc}}(r, R) = \frac{i\pi^{\frac{1}{2}}}{2k_0} \phi^T(r) \sum_{\ell} (2\ell + 1) (O_{\ell 0} - I_{\ell 0}) \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Comparing the last two equations, we obtain

$$y_{\ell m} = \frac{i\pi^{3/2}}{2k_0} (2\ell + 1)^{3/2} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$= 0, \text{ for } m \neq 0,$$

and

$$\begin{aligned} \psi(\mathbf{r}, R) &= \psi^{\text{inc}}(\mathbf{r}, R) + \phi^{\text{T}}(\mathbf{r}) \sum_{\ell} O_{\ell 0} (1 - U_{\ell 0}) y_{\ell 0} \\ &\sim \phi_0(\mathbf{r}) e^{ik_0 Z} + \phi^{\text{T}}(\mathbf{r}) \sum_{\ell} \frac{i}{4k_0} (2\ell + 1) \frac{1}{R} \begin{pmatrix} e^{ik_0 R} & e^{ik_0 R} \\ e^{ik_1 R} & -e^{ik_1 R} \end{pmatrix} \\ &\quad \times (1 - U_{\ell 0}) P_{\ell}(\cos \theta) \begin{pmatrix} 1 \\ 1 \end{pmatrix} \end{aligned}$$

using $Y_{\ell 0} = \left[\frac{2\ell + 1}{4\pi} \right]^{1/2} P_{\ell}(\cos \theta)$. More explicitly,

$$\psi(\mathbf{r}, R) \sim [e^{ik_0 Z} + f_0(\theta) \frac{e^{ik_0 R}}{R}] \phi_0(\mathbf{r}) + f_1(\theta) \frac{e^{ik_1 R}}{R} \phi_1(\mathbf{r})$$

where

$$f_0 = \frac{i}{4k_0} \sum_{\ell} (2\ell + 1) V_0^{\text{T}} (1 - U_{\ell 0}) V_0 P_{\ell}(\cos \theta), \quad V_0 = \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$

The differential cross sections for scattering without atomic excitation, $\left(\frac{d\sigma}{d\Omega} \right)_0$, and with excitation, $\left(\frac{d\sigma}{d\Omega} \right)_1$, are

$$\left(\frac{d\sigma}{d\Omega} \right)_0 = \frac{v_0}{v_0} \frac{1}{16 k_0} \left| \sum_{\ell} (2\ell + 1) V_0^{\text{T}} (1 - U_{\ell 0}) V_0 P_{\ell}(\cos \theta) \right|^2$$

The total cross sections are

$$\sigma_0 = \frac{v_0}{v_0} \frac{\pi}{4k_0} \sum_{\ell} (2\ell + 1) |V_0^{\text{T}} (1 - U_{\ell 0}) V_0|^2$$

and the total cross section for the nuclear process irrespective of the final state of the atom is

$$\sigma = \frac{\pi}{4k_0} \sum_{\ell} (2\ell + 1) \left[|V_0^{\text{T}} (1 - U_{\ell 0}) V_0|^2 + \frac{v_1}{v_0} |V_1^{\text{T}} (1 - U_{\ell 0}) V_0|^2 \right] \quad (2)$$

The Fundamental R-Matrix Relation

If the two-component column matrices G_ℓ and G'_ℓ are two solutions to Equation (1), then, dropping the ℓ subscript,

$$\begin{aligned} G_0 \frac{d^2 G'_0}{dR^2} - G'_0 \frac{d^2 G_0}{dR^2} + \frac{2M}{\hbar^2} (E'_0 - E_0) G_0 G'_0 &= 0 \\ G_1 \frac{d^2 G'_1}{dR^2} - G'_1 \frac{d^2 G_1}{dR^2} + \frac{2M}{\hbar^2} (E'_1 - E_1) G_1 G'_1 &= 0 \end{aligned}$$

Adding the two equations and using the fact that $E'_1 - E_1 = E'_0 - E_0$, we obtain

$$G^T \frac{dG'}{dR} - G'^T \frac{dG}{dR} + \frac{2M}{\hbar^2} (E' - E) G'^T G = 0$$

where the subscript is dropped on E_0 , the projectile energy. Finally, applying $\int_0^a dR$ gives

$$\left(G^T \frac{dG'}{dR} - G'^T \frac{dG}{dR} \right)_{R=a} + \frac{2M}{\hbar^2} (E' - E) \int_0^a G'^T G dR = 0 \quad (3)$$

Here, we have used the boundary condition, $G(0) = G'(0) = 0$, for any regular solution, and a is the radius of the boundary sphere S .

The eigenfunctions G_λ are defined by the homogeneous boundary condition (in addition to the above-mentioned boundary condition at the origin),

$$\left(\frac{dG_\lambda}{dR} \right)_{R=a} = 0$$

We could have used the more general boundary conditions of the type described in Chapter I, but for simplicity we set $B = 0$ here. Then Equation (3) shows that the eigenfunctions are orthogonal in the sense that

$$\int_0^a G_\lambda^T G_\lambda dR = \delta_{\lambda\lambda'}$$

assuming all eigenfunctions are normalized. The labels λ and λ' denote eigenstates with the same ℓ .

In Equation (3), G is now identified with the reduced radial part of the actual scattering wavefunction, and the replacement $G' \rightarrow G_\lambda$ is made, giving

$$\int_0^a G_\lambda^T G dR = \frac{\hbar^2}{2M} \frac{1}{E_\lambda - E} \left(G_\lambda \frac{dG}{dR} \right)_{R=a} \quad (4)$$

On the other hand G can be expanded in terms of the G_λ inside S :

$$G = \sum_\lambda b_\lambda G_\lambda$$

and the b_λ are determined by applying Equation (4):

$$\begin{aligned} b_\lambda &= \int_0^a G_\lambda^T G dR \\ &= \frac{\hbar^2}{2M} \frac{1}{E_\lambda - E} \left(G_\lambda^T \frac{dG}{dR} \right)_{R=a} \end{aligned}$$

So, inside S ,

$$G(R) = \frac{\hbar^2}{2M} \sum_\lambda \frac{1}{E_\lambda - E} G_\lambda(R) G_\lambda^T(R) \left(\frac{dG}{dR} \right)_{R=a}$$

The fundamental R -matrix relation is obtained by setting $R = a$,

$$G_\ell(a) = R_\ell a \left(\frac{dG_\ell}{dR} \right)_{R=a} \quad (5)$$

with the matrix R_ℓ defined by

$$R_\ell = \frac{\hbar^2}{2Ma} \sum_\lambda \frac{1}{E_\lambda - E} G_{\ell\lambda}(a) G_{\ell\lambda}^T(a)$$

and the ℓ 's have been restored. Note that the forms of the equations are identical with those in Chapter I, but some of the quantities have become matrices. For example, the quantity R_ℓ is a 2×2 matrix but would have been a scalar if the atomic interactions had been neglected.

Connection between U and R Matrices

Since the radial part of the external wavefunction has the form

$$G_{\ell m} = O_{\ell m} x_{\ell m} + I_{\ell m} y_{\ell m}$$

Equation (5) becomes

$$\begin{aligned} (O_{\ell m} x_{\ell m} + I_{\ell m} y_{\ell m})_{R=a} &= R_{\ell} a \left(\frac{dO_{\ell m}}{dR} x_{\ell m} + \frac{dI_{\ell m}}{dR} y_{\ell m} \right)_{R=a} \\ x_{\ell m} &= - \left(O_{\ell m} - a R_{\ell} \frac{dO_{\ell m}}{dR} \right)^{-1} \left(I_{\ell m} - a R_{\ell} \frac{dI_{\ell m}}{dR} \right) y_{\ell m}, \quad R = a. \end{aligned}$$

According to the definition of the U matrix, $x_{\ell m} = -U_{\ell m} y_{\ell m}$,

$$U_{\ell m} = \left(O_{\ell m} - a R_{\ell} \frac{dO_{\ell m}}{dR} \right)^{-1} \left(I_{\ell m} - a R_{\ell} \frac{dI_{\ell m}}{dR} \right), \quad R = a.$$

Under our assumptions, there is no m -dependence, so we can drop the m label:

$$U_{\ell} = O_{\ell}^{-1}(a) (1 - R_{\ell} L)^{-1} (1 - R_{\ell} L^*) I_{\ell}(a)$$

where

$$\begin{aligned} L_{\ell} &= a \left(\frac{dO_{\ell}}{dR} \right)_{R=a} O_{\ell}^{-1}(a) \\ &= S_{\ell} + iP_{\ell} \end{aligned}$$

The Cross Section: the "One-Level" Approximation

As a rule it is not correct to make a true one-level approximation now that the possibility of atomic transitions is included. Even if the perturbation V_{ep} is turned off, there are twice as many eigenstates and eigenenergies as in the conventional R -matrix theory. For each eigenenergy \bar{E}_{λ} in the usual theory, here there are two energies, \bar{E}_{λ} and $\bar{E}_{\lambda} + \delta$, which correspond to the atom being in the ground and excited states, respectively. As V_{ep} is turned on, both eigenvalues shift due to the perturbation, but the two different eigenstates remain.

Thus, unless the two states are separated by many resonance widths (i. e., $\delta \gg \Gamma$), there will be two overlapping levels which must be treated as a single object. Yet, from the viewpoint of the nucleus there is still only one level involved; the atom induces the second level.

In light of the above, the R matrix is approximated by (again, the λ label is dropped)

$$\begin{aligned} R &= R_{\lambda_0} + R_{\lambda_1} \\ &= \frac{\gamma_{\lambda_0} \gamma_{\lambda_0}^T}{E_{\lambda_0} - E} + \frac{\gamma_{\lambda_1} \gamma_{\lambda_1}^T}{E_{\lambda_1} - E} \end{aligned}$$

where $\gamma_{\lambda} = \left(\frac{\hbar^2}{2Ma} \right)^{1/2} G_{\lambda}$. The quantities γ_{λ_0} and γ_{λ_1} are the internal eigenfunctions corresponding to the single nuclear level mentioned above and referring to the ground and excited states of the atom, respectively. The energies, E_{λ_0} and E_{λ_1} , are eigenenergies of these states, and E is the incident projectile energy.

The important quantity is [see the expression for the cross section, Equation (2)]

$$\begin{aligned} |V_0^T (1 - U) V_0|^2 &= |V_0^T [1 - O^{-1} (1 - RL)^{-1} (1 - RL^*) I] V_0|^2 \\ &= |V_0^T [1 - O^{-1} \left(1 - \frac{\gamma_{\lambda_0} \gamma_{\lambda_0}^T L}{E_{\lambda_0} - E} - \frac{\gamma_{\lambda_1} \gamma_{\lambda_1}^T L}{E_{\lambda_1} - E} \right) \\ &\quad \times \left(1 - \frac{\gamma_{\lambda_0} \gamma_{\lambda_0}^T L}{E_{\lambda_0} - E} - \frac{\gamma_{\lambda_1} \gamma_{\lambda_1}^T L}{E_{\lambda_1} - E} \right) I] V_0|^2 \\ &= |V_0^T [(1 - O^{-1} I) i + O^{-1} (\Delta E_0 \Delta E_1 - \Delta E_1 \Lambda^0 - \Delta E_0 \Lambda^1)^{-1} \\ &\quad \times (\Delta E_1 \Gamma^0 + \Delta E_0 \Gamma^1) I] V_0|^2 \\ &\equiv |A^0|^2 \end{aligned}$$

where the following quantities have been introduced:

$$\begin{aligned}\Delta E_0^0 &\equiv E_{\lambda_0} - E \\ \Lambda^0 &\equiv \gamma_{\lambda_0} \gamma_{\lambda_0}^T L \\ \Gamma^0 &\equiv 2 \operatorname{Im} \Lambda^0\end{aligned}$$

The first term in A^0 produces a slow variation of the cross section (the so-called "hard-sphere" scattering) which is negligible in the neighborhood of the resonance. Keeping only the resonance term (i. e., the second term in A^0), we have the important equation,

$$A_{\text{res}}^0 = V_0^T O^{-1} (\Delta E_0 \Delta E_1 - \Delta E_1 \Lambda^0 - \Delta E_0 \Lambda^1)^{-1} (\Delta E_1 \Gamma^0 + \Delta E_0 \Gamma^1) I V_0 \quad (6)$$

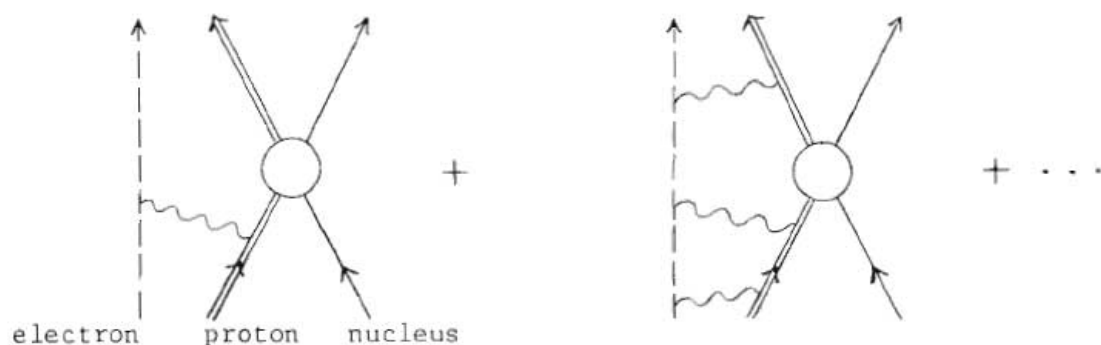
The hard-sphere term separates naturally from the resonance term because of the division of space into the internal and external regions. In the remainder of this chapter the hard-sphere term is neglected as small in the neighborhood of the resonance.

At this point it is necessary to expand A_{res}^0 more explicitly, that is, to perform the matrix inversion and multiplication. This can be done without difficulty, but the result is not particularly useful in that the atomic and nuclear contributions are mixed together. The goal is to write the cross section solely in terms of nuclear quantities which can be determined from experiment (the resonance energy and the partial widths) and atomic quantities which can be calculated. To this end the coefficients of the various resonance terms are expanded in a power series in the perturbation V_{ep} . This allows the desired separation of nuclear and atomic quantities, as will be seen.

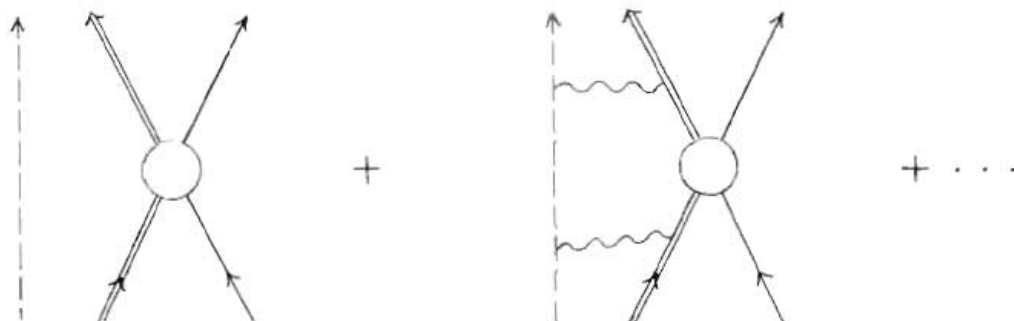
Before performing the expansion itself, it is useful to discuss what one might expect in qualitative terms, the purpose being two-fold:

to show that, to lowest order, only the zero-order term of A_{res}^0 and the first-order term of A_{res}^1 need be retained, and to show that certain terms in the first-order term in A_{res}^1 can be neglected.

The amplitude A_{res}^0 corresponds to nuclear scattering which leaves the atom in its ground state. As such, it contains a zero-order term, as well as higher ones. On the other hand, A_{res}^i represents scattering which raises the atom to its excited state. Clearly, it must go to zero as V_{ep} is turned off, so its leading term is of first, or higher, order. The amplitude A_{res} represents processes such as



so that its leading term is actually first-order. Since A_{res}^i corresponds to excitation of the atom, it is expected to contribute the primary correction to the cross section and must surely be included in such a correction. Thus, the cross section should be expanded to second order but no higher, as we are concerned with only lowest-order corrections. It would seem that, to be consistent, A_{res}^0 should be expanded to second order since the cross term in its square is second-order. This can be understood if one realizes that A_{res}^0 contains only terms of even order -- it requires two interactions to leave the atom in its ground state, one to excite it and one to de-excite it. Schematically, A_{res}^0 is of the form,



Note that in this, and the preceding, schematic diagram only a representative term of each order is included.

Yet, for a real atom with its infinity of excited states, it is extremely unlikely that the atom would be excited, then de-excited, to precisely the initial state. Rather, the second interaction would cause a second transition but, with over-whelming probability, to some state other than the ground state, especially since there would be many states much nearer the energy of the excited atom. The second-order (and higher) terms in A_{res}^0 thus represent processes which are extremely improbable. They arise from approximating the atom with only two states and, as such, should be discarded. The more probable second-order processes would actually appear in A_{res}^1 in an exact treatment of the atom. Such terms would not contribute to the cross section to lowest order so their omission is not crucial. Thus, only the leading terms of A_{res}^0 and A_{res}^1 (zero- and first-order, respectively) are retained.

The perturbation corrections arise from two sources, the internal and external wavefunctions. In the first-order term of A_{res}^1 there is one term which comes from the correction to the internal wavefunction corresponding to the level being considered. This term is negligible compared to the other terms, which arise from external corrections.

The correction to this internal wavefunction is obtained by Rayleigh-Schrödinger perturbation theory and involves off-diagonal matrix elements of V_{ep} between internal states. But V_{ep} (actually U_{01}) is almost constant inside the nucleus so that such matrix elements are approximately zero owing to orthogonality. A calculation using internal wavefunctions appropriate to a square-well nuclear potential indicates that internal corrections are three to four orders of magnitude smaller than external ones. This is the same result one obtains from a rough estimate using the ratio of nuclear to atomic radius. So, barring a fortuitous cancellation of terms, the internal correction may be neglected compared to the external ones. This is just as well since the internal matrix elements cannot be calculated due to our ignorance of the internal wavefunctions.

Therefore, A_{res}^0 is expanded keeping only the zero-order term, which gives the usual Breit-Wigner resonance. Likewise, only the first-order terms coming from external corrections are retained in A_{res}^1 . The results are

$$A_{res}^0 = 2 \frac{I_0}{O_0} \frac{(\Gamma_{11}^0)^{(0)}}{\Delta E_0 - \Lambda_{11}^0 - \Lambda_{22}^0}$$

$$A_{res}^1 = - \frac{I_0}{O_0} \frac{(O_{21} + O_{22})^{(1)}}{O_1} \frac{(\Gamma_{11}^0)^{(0)}}{\Delta E_0 - \Lambda_{11}^0 - \Lambda_{22}^0} + 2 \frac{I_0}{O_1} \frac{(\Gamma_{11}^0)^{(0)} (\Lambda_{21}^1)^{(1)}}{(\Delta E_0 - \Lambda_{11}^0 - \Lambda_{22}^0) (\Delta E_1 - \Lambda_{11}^1 - \Lambda_{22}^1)}$$

$$+ \left(2 \frac{I_0}{O_1} (\Gamma_{21}^1)^{(1)} + \frac{(I_{21} + I_{22})^{(1)}}{O_1} (\Gamma_{22}^1)^{(0)} \right) \frac{1}{\Delta E_1 - \Lambda_{11}^1 - \Lambda_{22}^1}$$

where the superscripts in parentheses indicate the orders of the leading terms of those quantities. The functions I_0 and O_0 are the usual in and out spherical solutions introduced in Chapter I, and

they appear as diagonal components of the zero-order expression for the I and O matrices. The subscripts refer to the projectile energy, E_0 or E_r , corresponding to the atom being in the ground or excited state.

Instead of the boundary condition, $\left(\frac{d\gamma_\lambda}{dR}\right)_{R=a} = 0$, we could have used the more general one of Chapter I for which $\left(\frac{d\gamma_\lambda}{dR}\right)_{R=a} = B$. In general this is indeed necessary, for to insure the validity of the one-level approximation, B must be chosen so that the level energy lies within the width of the observed resonance; i. e., we require that $(\Delta_{11}^0)^{(1)} = (\Gamma_{11}^0)^{(0)}$, where $(\Delta_{11}^0)^{(0)} = - (S_{11}^{(0)} - B) \gamma_{0\lambda_0}^2$ and $(\Gamma_{11}^0)^{(0)}$ are the unperturbed level shift and level width. This condition is certainly satisfied if we choose $B = S_{11}^{(0)}(E_r)$, although any other choice which satisfies the condition is equally valid. The quantity E_r is the resonance energy.

One can show that

$$(\Lambda_{21}^1)^{(1)} \approx \frac{1}{2} \frac{L_{21}^{(1)}}{P_{11}^{(0)}} (\Gamma_{11}^0)^{(0)}$$

if only external corrections are retained. Therefore, for each partial wave,

$$A_{\text{res}}^0 \approx - \frac{2\Gamma}{E - E_r + \frac{1}{2}i\Gamma}$$

$$A_{\text{res}}^1 \approx \frac{I_0}{O_0} \frac{(O_{21} + O_{22})^{(1)}}{O_1} \frac{\Gamma}{E - E_r + \frac{1}{2}i\Gamma} + \frac{I_0}{O_1} \frac{L_{21}^{(1)}}{P_{11}^{(0)}} \frac{\Gamma^2}{(E - E_r + \frac{1}{2}i\Gamma)(E - E_r - \delta + \frac{1}{2}\frac{k_1}{k_0}i\Gamma)}$$

$$- \left[2 \frac{I_0}{O_1} \frac{P_{21}^{(1)}}{P_{11}^{(0)}} + \frac{(I_{21} + I_{22})^{(1)}}{O_1} \frac{P_{22}^{(0)}}{P_{11}^{(0)}} \right] \frac{\Gamma}{E - E_r - \delta + \frac{1}{2}\frac{k_1}{k_0}i\Gamma}$$

where $\Gamma \equiv (\Gamma_{11}^0)^{(0)}$; $E_r = E_{\lambda_0}$; δ is the energy difference between the

two atomic states; Λ_{11}^1 and Λ_{22}^0 , the (second-order) corrections to the level shift and width, are neglected; the angular momentum label l is omitted.

To proceed further, the atomic wavefunctions must be specified. They are taken to be K- and L-shell hydrogenic s-state wavefunctions. This choice is made for convenience only. The guiding principle is that the important quantities are the value for δ and the ionization probability for the reaction. In Chapter IV, the duplication of these values by the model is described. On the other hand, the results should be independent of the precise form of the atomic wavefunctions to a good approximation so these wavefunctions are chosen for ease of computation.

Squaring A_{res}^0 and A_{res}^1 and substituting the results into Equation (2) give the corrected cross section for free s-waves (the projectile-nucleus Coulomb potential is neglected):

$$\begin{aligned} \sigma \approx & \frac{\pi}{k^2} \left\{ \frac{\Gamma^2}{(E-E_r)^2 + \frac{1}{4}\Gamma^2} + \frac{512}{729} \frac{1}{k^2 a_0^2 \rho} \frac{1}{(1+\rho)^4} \left[(1+\rho)^2 + 2\frac{E}{\delta} \left(1 + \frac{8}{3}\rho\right) \right]^2 + 16 \left(\frac{E}{\delta}\right)^2 \rho^3 \right\} \\ & \times \frac{\Gamma^2}{(E-E_r-\delta)^2 + \frac{1}{4}\Gamma^2} - \frac{512}{81} \frac{1}{k^2 a_0^2 \rho} \frac{\Gamma^2}{(E-E_r)^2 + \frac{1}{4}\Gamma^2} \frac{\Gamma^2}{(E-E_r-\delta)^2 + \frac{1}{4}\Gamma^2} \left\{ \frac{E-E_r}{\frac{1}{2}\Gamma} \frac{E-E_r-\delta}{\frac{1}{2}\Gamma} \right. \\ & \times \frac{E}{\delta} \frac{1}{(1+\rho)^4} \left[\left(1 + \frac{8}{3}\rho\right) (1+\rho)^2 + 4\frac{E}{\delta} \left(\frac{1}{2}\left(1 + \frac{8}{3}\rho\right)^2 - 2\rho^3\right) \right] + 8\rho^{\frac{3}{2}} \left(\frac{E}{\delta}\right)^2 \frac{1}{(1+\rho)^2} \\ & \times \left[\frac{1}{2} \frac{E-E_r}{\frac{1}{2}\Gamma} \frac{\delta}{E} + 2\frac{\delta}{\Gamma} \frac{1 + \frac{8}{3}\rho}{(1+\rho)^2} \right] + \frac{1}{4} - 2 \left(\frac{E}{\delta}\right)^2 \frac{1}{(1+\rho)^4} \left[4\rho^3 - \left(1 + \frac{8}{3}\rho\right)^2 \right] \\ & \left. + \frac{1}{\delta} \frac{1}{(1+\rho)^2} \left(1 + \frac{8}{3}\rho\right) \right\} \end{aligned} \quad (7)$$

Here, a_0 is the first Bohr radius of hydrogen, $\rho = 12 \frac{m}{M} \frac{E}{\delta}$, and k_1

is set equal to k_0 . The correction factors in A_{res}^1 are derived in Appendix I. Note that Equation (7) is valid only for E and δ such that $\frac{\delta}{E} \ll 1$.

CHAPTER III

ATOMIC PERTURBATIONS: NUCLEAR REACTIONS

The general approach to solving the many-channel scattering problem is very close to that of the previous chapter. Again, the spectrum of the atom is approximated by only two states, and Schrödinger's equation takes the form of a two-dimensional matrix equation once the electronic coordinates are eliminated. The differences amount to additional complication arising from the possibility of several channels.

The Two-State Approximation

As above, we work in the center-of-mass coordinate system (CM of the nucleons). In Chapter I the Hamiltonian was separated into a sum of several parts in a channel-dependent manner. The same separation is performed here except that an additional term, the Hamiltonian of the electron, is added:

$$H_{e,\alpha} = -\frac{\hbar^2}{2M} \nabla_{\mathbf{r}}^2 + V_{e,\alpha_1} + V_{e,\alpha_2}$$

The V_{e,α_i} terms are simply the Coulomb interactions with the two nuclear fragments. It is an extremely good approximation to assume that for any reaction proceeding through an isolated resonance, one of the reaction products will be much more massive and highly charged than the other. This fragment will be labeled α_1 , and we assume the electron is bound to it in the final state.

The total scattering wavefunction is expanded in terms of the two atomic states,

$$\text{Total Wavefunction} = \phi^T \Psi$$

where the two-component column matrix Ψ depends on the nuclear coordinates.

Definition of External States

The nuclear part of the wavefunction in state $(\alpha s v)$ is decomposed into partial waves,

$$\psi_{\alpha s v} = \frac{1}{R_\alpha} \sum_{\ell m} (2\ell + 1) Y_{\ell m}(\Omega_\alpha) G_{\ell m}^\alpha(R_\alpha) \psi_{\alpha s v}$$

is substituted into the wave equation, and the result is operated on successively by $\int \phi_0^* d\vec{r}$ and $\int \phi_1^* d\vec{r}$ to obtain the pair of equations,

$$\left(\frac{d^2}{dR_\alpha^2} + k_0^2 - \frac{\ell(\ell+1)}{R_\alpha^2} - U_{00}^\alpha \right) G_{0\ell m}^\alpha = U_{01}^\alpha G_{1\ell m}^\alpha$$

$$\left(\frac{d^2}{dR_\alpha^2} + k_1^2 - \frac{\ell(\ell+1)}{R_\alpha^2} - U_{11}^\alpha \right) G_{1\ell m}^\alpha = U_{10}^\alpha G_{0\ell m}^\alpha$$

The quantities k_0 and k_1 are defined as in Chapter II, and

$$U_{ij}^\alpha = \frac{2M_\alpha}{\hbar^2} [V_c(R_\alpha) \delta_{ij} + \int \phi_i^*(\mathbf{r}) V_{e,\alpha_2}(|\mathbf{r}-\vec{R}_\alpha|) \phi_j(\mathbf{r}) d\vec{r}]$$

For each channel there are four independent solutions defined by their asymptotic forms:

$$O_c^\pm = O_{\alpha\ell}^\pm = \begin{pmatrix} O_{0\alpha\ell}^\pm \\ O_{1\alpha\ell}^\pm \end{pmatrix}$$

$$\sim \begin{pmatrix} \exp[i(k_0 R_\alpha - \eta_{0\alpha} \log 2k_0 R_\alpha - \frac{1}{2}\ell\pi + \sigma_{0\alpha 0})] \\ \pm \exp[i(k_1 R_\alpha - \eta_{1\alpha} \log 2k_1 R_\alpha - \frac{1}{2}\ell\pi + \sigma_{1\alpha 0})] \end{pmatrix}$$

where $\eta_{i\alpha} = \frac{Z_1 Z_2 e^2}{\hbar v_i}$, and $\sigma_{i\alpha\ell} = \arg \Gamma(\ell + 1 + i\eta_{i\alpha}) = \sigma_0 + \sum_{s=1}^{\ell} \tan^{-1} \frac{\eta_{i\alpha}}{s}$.

The other two solutions, I_c^+ , are similarly defined and equal the complex conjugate of the O_c^+ , asymptotically.

Finally, we define

$$O_c = O_{\alpha l} = \begin{pmatrix} O_{0\alpha l}^+ & O_{0\alpha l}^- \\ O_{l\alpha l}^+ & O_{l\alpha l}^- \end{pmatrix}$$

and $O_c \equiv i \frac{k}{R_\alpha} O_c Y_{lm} \psi_{\alpha s v}$. The I_c and I_c^+ are defined similarly.

The U Matrix and Cross Section

Externally, the most general form for ψ is

$$\begin{aligned} \psi &= \sum_c (O_c x_c + I_c y_c) \\ &= \sum_c (I_c - \sum_{c'} O_{c'} U_{c'c}) y_c \end{aligned}$$

where $x_{c'} = -\sum_c U_{c'c} y_c$, and $U_{c'c}$ is an infinite-dimensional matrix with components which are two-dimensional matrices. The incident wave is

$$\psi_{\alpha s v}^{\text{inc}} = \sum_c (I_c - e^{2i\omega_0 c} O_c) y_c$$

with

$$\begin{aligned} y_c &= \frac{i^{n-\frac{1}{2}}}{2k_{0\alpha}} (2l+1)^{\frac{1}{2}} \delta_{m0} \begin{pmatrix} 1 \\ 1 \end{pmatrix} && \text{for state } \alpha s v \\ &= 0 && \text{otherwise} \end{aligned}$$

and $\omega_{0c} = \omega_{0\alpha l} = \sigma_{0\alpha l} - \sigma_{0\alpha 0} = \sum_{s=1} \tan^{-1} \frac{n_{0\mu}}{s}$. The positive z -axis has been chosen to lie along the incident beam direction. Separating out the incident part, the total wavefunction becomes

$$\phi_{\alpha s v}^{\text{inc}} + \phi_{\alpha s v}^{\text{sc}} = \sum_c (e^{2i\omega_0 c} O_c - \sum_{c'} O_{c'} U_{c'c}) y_c$$

and the amplitude for scattering into the different state ($\alpha's'v'$) is

$$f_{\alpha's'v',\alpha s} = -\frac{i\pi^{3/2}}{2k_{0\alpha}} \phi^T \sum_{\ell\ell'} (2\ell+1)^{3/2} O_{\alpha'\ell'm's'v'} U_{\alpha'\ell'm's'v',\alpha\ell s v} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

There is no m' sum since $m' = v - v'$. This amplitude is the sum of two parts, one representing elastic and one inelastic atomic scattering. The corresponding differential cross sections are

$$\left(\frac{d\sigma}{d\Omega}\right)_{\alpha's'v',\alpha s v}^{\text{elastic}} = \frac{\pi}{4k_0^2} \frac{v_{0\alpha'}}{v_{0\alpha}} \left| \sum_{\ell\ell'} (2\ell+1)^{3/2} V_0^T U_{\alpha'\ell'm's'v',\alpha\ell s v} V_0 Y_{\ell'm'} \right|^2$$

and we have used the fact that, asymptotically, $i^\ell O_\ell$ has components of unit modulus independent of ℓ . As in Chapter I, in order to do the sums and averaging we convert to the $(\alpha s \ell J M)$ scheme. Then, integrating the differential cross sections over angle, summing over v' and s' , and averaging over v and s , we obtain

$$\sigma_{\alpha'\alpha}^{\text{elastic}} = \frac{\pi}{4k_0^2} \frac{v_{0\alpha'}}{v_{0\alpha}} \sum_{J\ell\ell'} g_\alpha^J |V_0^T U_{\alpha's'\ell',\alpha s \ell} V_0|^2$$

for $\alpha \neq \alpha'$; i. e., inelastic nuclear collisions. For elastic scattering U is replaced by $T = 1 - U$, and the Coulomb amplitude must be included if charged particles are incident.

The Fundamental R-Matrix Relation

The procedure here is a straightforward combination of the methods of Chapters I and II. It is no accident that the results have a familiar look about them; the notation was developed with just this in mind.

Writing H_N for the nuclear part of the Hamiltonian, the complete Hamiltonian is

$$H = H_N + T_e + V_{e,\alpha_1} + V_{e,\alpha_2}$$

so that Schrödinger's equation becomes

$$[H_N \phi^T + (\epsilon_\alpha \phi)^T + V_{e,\alpha_2} \phi^T] \psi = E \phi^T \psi$$

where

$$\epsilon_{\alpha} = \begin{pmatrix} \epsilon_{\alpha 0} & 0 \\ 0 & \epsilon_{\alpha 1} \end{pmatrix}$$

$$(T_e + V_{e,\alpha_1}) \phi_{\alpha i} = \epsilon_{\alpha i} \phi_{\alpha i}$$

Applying $\int \phi^* dr$ from the left, we eliminate the atomic coordinates and obtain

$$(H_N + V_{e,\alpha_2}) \Psi = E \Psi$$

with $E = E - \epsilon_{\alpha}$, and $V_{e,\alpha_2} = \int \phi^* V_{e,\alpha_2} \phi^T$ is a 2×2 matrix.

Given two solutions to this equation, Ψ_1 and Ψ_2 , we form

$$\Psi_2^\dagger E_2 \Psi_1 - \Psi_1^\dagger E_1 \Psi_2 = (H_N \Psi_2)^\dagger \Psi_1 - \Psi_2^\dagger H_N \Psi_1 + (V_{e,\alpha_2} \Psi_2)^\dagger \Psi_1 - \Psi_2^\dagger V_{e,\alpha_2} \Psi_1$$

where \dagger indicates Hermitian conjugation as well as transposition of the two-dimensional matrices. Since $V_{e,\alpha_2} = V_{e,\alpha_2}^\dagger$ (assuming real atomic wavefunctions) and $E_2 - E_1$ is a multiple of the unit matrix, we have

$$(E_2 - E_1) \Psi_2^\dagger \Psi_1 = (H_N \Psi_2)^\dagger \Psi_1 - \Psi_2^\dagger H_N \Psi_1$$

If the nuclear interaction term is self-adjoint, then integration over a volume τ in 3A-dimensional configuration space gives

$$\begin{aligned} (E_2 - E_1) \int_{\tau} \Psi_2^\dagger \Psi_1 d\tau &= \int_{\tau} [(T_N \Psi_2)^\dagger \Psi_1 - \Psi_2^\dagger T_N \Psi_1] d\tau \\ &= \int_S \frac{\hbar^2}{2M_c} [\Psi_2^\dagger \text{grad}_n \Psi_1 - (\text{grad}_n \Psi_2)^\dagger \Psi_1] dS \end{aligned} \quad (1)$$

As before, the value and derivative quantities are defined using the surface functions ϕ_c :

$$V_c = \left(\frac{\hbar^2}{2M_c a_c} \right)^{1/2} \int_S \phi_c^\dagger \Psi dS$$

$$\begin{aligned}
 D_c &= \left(\frac{\hbar^2}{2M_c a_c} \right)^{1/2} \int_S \phi_c^\dagger \text{grad}_n (R_c \psi) dS \\
 &= V_c + \left(\frac{a_c \hbar^2}{2M_c} \right)^{1/2} \int_S \phi_c^\dagger \text{grad}_n \psi dS
 \end{aligned}$$

The expressions for ψ and its normal derivative in terms of these quantities are

$$\begin{aligned}
 \psi &= \sum_c \left(\frac{2M_c a_c}{\hbar^2} \right)^{1/2} V_c \phi_c \\
 \text{grad}_n \psi &= \sum_c \left(\frac{2M_c}{a_c \hbar^2} \right)^{1/2} (D_c - V_c) \phi_c
 \end{aligned}$$

Putting these expansions into Equation (1) yields

$$(E_2 - E_1) \int_\tau \psi_2^\dagger \psi_1 d\tau = \sum_c (V_{2c}^\dagger D_{1c} - D_{2c}^\dagger V_{1c}) \quad (')$$

which is identical in form to Equation (3) of Chapter I, though the meanings of some of the quantities are different.

Following the usual procedure, we define a set of internal eigenfunctions,

$$(H_N + V_{e, \alpha_2}) X_{\lambda JM} = E_{\lambda J} X_{\lambda JM}$$

by the boundary conditions,

$$\delta_{\lambda c} = B_c \gamma_{\lambda c}$$

where B_c is a constant independent of λ , and $\gamma_{\lambda c}$ and $\delta_{\lambda c}$ are the value and derivative quantities, respectively, of the internal eigenfunctions $X_{\lambda JM}$. According to Equation (2), the X_λ (dropping the JM subscripts) are orthogonal, and they are assumed to be normalized.

The actual ψ can be expanded inside S in terms of the X_λ :

$$\begin{aligned}
 \psi^{\text{internal}} &= \sum_\lambda A_\lambda X_\lambda \\
 A_\lambda &= \int_\tau X_\lambda^\dagger \psi^{\text{internal}} d\tau
 \end{aligned}$$

According to Equation (2), with $\psi_2 = X_\lambda$ and $\psi_1 = \psi^{\text{internal}}$, the A_λ

can be written

$$A_\lambda = \frac{1}{E_\lambda - E} \sum_c \gamma_{\lambda c}^T D_c^O$$

assuming time-reversal invariance (so that the $\gamma_{\lambda c}$ are real), and $D_c^O \equiv D_c - B_c V_c$ has been introduced. Finally,

$$\psi^{\text{internal}} = \sum_c \left(\sum_\lambda \frac{X_\lambda \gamma_{\lambda c}^T}{E_\lambda - E} \right) D_c^O$$

so that operating with $\left(\frac{\hbar^2}{2M_c a_c} \right)^{1/2} \int_S \phi_{c'}^* dS$, we obtain the desired result,

$$V_{c'} = \sum_c R_{c'c} D_c^O$$

where

$$R = \sum_\lambda \frac{\gamma_\lambda^* \gamma_\lambda}{E_\lambda - E}$$

and γ_λ is a column matrix with components labeled by the different channels, and each component is a two-component column matrix.

In taking the transpose of γ_λ , the transpose of the column matrix as a whole as well as that of each component is taken.

Connection between U and R Matrices

In the external region Ψ has the form

$$\Psi = \sum_c (O_c x_c + I_c y_c)$$

so the value and derivative quantities are

$$V_c = \left(\frac{\hbar^2}{2M_c a_c} \right)^{1/2} (O_c x_c + I_c y_c)$$

$$D_c = \left(\frac{\hbar^2}{2M_c a_c} \right)^{1/2} a_c \left(\frac{dO_c}{dR_c} x_c + \frac{dI_c}{dR_c} y_c \right)$$

In matrix notation

$$V = \left(\frac{\hbar^2}{2}\right)^{1/2} (Ma)^{-1/2} (Ox + Iy)$$

$$D = \left(\frac{\hbar^2}{2}\right)^{1/2} M^{-1/2} a^{1/2} (O'x + I'y)$$

where

$$(M)_{cc'} = M_c \delta_{cc'} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$(O)_{cc'} = O_c \delta_{cc'} \quad (O')_{cc'} = \frac{dO_c}{dR_c} \delta_{cc'} \quad \text{etc.}$$

Insertion of these expressions for V and D into the R -matrix relation,

$V = RD^O$, gives

$$[(Ma)^{-1/2}O - RM^{-1/2}a^{1/2}O' + RB(Ma)^{-1/2}O] x = -[(Ma)^{-1/2}I - RM^{-1/2}a^{1/2}I' + RB(Ma)^{-1/2}I] y$$

By definition, $x = -Uy$, so that

$$U^J = O^{-1}I + 2i(Ma)^{1/2}O^{-1}(1 - RL^O)^{-1}RPI(Ma)^{-1/2}$$

where

$$L \equiv M^{-1/2}a^{1/2}O'O^{-1} \equiv S + iP$$

$$L^O \equiv L - B$$

Use is made of the fact that, except for R , the various matrices involved are diagonal (with their components being 2×2 matrices) and that the components of the matrices M and a are scalar multiples of the unit matrix.

The "One-Level" Approximation

As in Chapter I, the inversion of $(1 - RL^O)$ is begun by dividing R into the sum of two parts, $R = R^O + R'$. Then (see Appendix II),

$$(1 - RL^0)^{-1} = (1 - R^0L^0)^{-1}R^0 + (1 - R^0L^0)^{-1}(1 - R'L')^{-1}R'(1 - L^0R^0)^{-1}$$

where $L' = L^0(1 - R^0L^0)^{-1}$. So if $(1 - R^0L^0)$ and $(1 - L^0R^0)$ can be inverted (approximately), the problem reduces to the inversion of $(1 - R'L')$. This inversion is complicated somewhat due to the fact that quantities which were scalar in Chapter I are now 2×2 matrices. However, the end result is not affected; in its form, it is exactly the same as the corresponding result of the conventional theory.

It is assumed that in the neighborhood of the resonance only one nuclear level will be important. As in Chapter II, it is necessary to include two states as defined here. The matrix R' is composed of these two levels, and R^0 is set equal to zero. We label these two states with $\mu, \nu = 0, 1$, and treat reaction channels only, $\alpha \neq \alpha'$. In this approximation the collision matrix U becomes

$$U = 2i(Ma)^{\frac{1}{2}}O^{-1} \sum'_{\mu\nu} A_{\mu\nu} (\gamma_{\mu} \times \gamma_{\nu}) PI(Ma)^{-\frac{1}{2}}$$

where the prime restricts the sum to $\mu, \nu = 0, 1$, and

$$A_{\mu\nu} = (\Delta E_1 \delta_{\mu 0} \delta_{\nu 0} + \Delta E_0 \delta_{\mu 1} \delta_{\nu 1} + \xi_{\mu\nu}) \frac{1}{F}$$

$$F = (\Delta E_0 - \xi_{00})(\Delta E_1 - \xi_{11}) - \xi_{10} \xi_{01}$$

$$\Delta E_0 = E_{\lambda_0} - E$$

Actually, this expression for U contains the resonant part of elastic, as well as inelastic, scattering. This elastic part is eliminated by taking the cc' component of U for $c \neq c'$:

$$U_{c'c} = i \left(\frac{M_{c'a'}}{M_{ca}} \right)^{\frac{1}{2}} O_{c'}^{-1} \sum'_{\mu\nu} A_{\mu\nu} \Gamma_{c'c}^{\mu\nu} I_c$$

where

$$\Gamma^{\mu\lambda} \equiv 2(\gamma_\mu \times \gamma_\lambda)P$$

The interesting quantity is

$$A_{\text{res}}^0 = V_Q^T / V_0$$

and V_Q acts on the two-dimensional space labeled by the two atomic states. Taking the $c'c$ component ($c \neq c'$), we have

$$\begin{aligned} (A_{\text{res}}^0)_{c'c} &= i \left[\frac{M_{c'c}}{M_c a_c} \right]^{1/2} \frac{1}{F} \frac{1}{\det O_c} \left\{ (O_{c',22} \mp O_{c',21}) \left[(I_{c,11} + I_{c,12}) \right. \right. \\ &\quad \times [(\Delta E_1 - \xi_{11})(\Gamma_{c'c}^{00})_{11} + \xi_{01}(\Gamma_{c'c}^{01})_{11} + \xi_{10}(\Gamma_{c'c}^{10})_{11} \\ &\quad \left. \left. + (\Delta E_0 - \xi_{00})(\Gamma_{c'c}^{11})_{11} \right] + (I_{c,21} + I_{c,22}) [(\Delta E_1 - \xi_{11})(\Gamma_{c'c}^{00})_{12} \right. \\ &\quad \left. + \xi_{01}(\Gamma_{c'c}^{01})_{12} + \xi_{10}(\Gamma_{c'c}^{10})_{12} + (\Delta E_0 - \xi_{00})(\Gamma_{c'c}^{11})_{12} \right] \\ &\quad - (O_{c',12} \pm O_{c',11}) \left[(I_{c,11} + I_{c,12}) [(\Delta E_1 - \xi_{11})(\Gamma_{c'c}^{00})_{21} \right. \\ &\quad \left. + \xi_{01}(\Gamma_{c'c}^{01})_{21} + \xi_{10}(\Gamma_{c'c}^{10})_{21} + (\Delta E_0 - \xi_{00})(\Gamma_{c'c}^{11})_{21} \right] \\ &\quad \left. + (I_{c,21} + I_{c,22}) [(\Delta E_1 - \xi_{11})(\Gamma_{c'c}^{00})_{22} + \xi_{01}(\Gamma_{c'c}^{01})_{22} \right. \\ &\quad \left. + \xi_{10}(\Gamma_{c'c}^{10})_{22} + (\Delta E_0 - \xi_{00})(\Gamma_{c'c}^{11})_{22} \right] \} \end{aligned}$$

As in Chapter II only the zero-order term of A_{res}^0 and the first-order terms of A_{res}^1 are retained. Also, terms which arise from internal corrections are dropped for the same reasons as before. Referring to Appendix III and dropping the appropriate terms, we have

$$(A_{\text{res}}^0)_{c',c} = 2i \left(\frac{M_{c',a_{c'}}}{M_{c,c}} \right)^{\frac{1}{2}} \frac{I_{0c} (\Gamma_{c',c}^{00})_{11}}{O_{0c', \Delta E_{\lambda_0} - \epsilon_{00}}} \quad (3a)$$

$$(A_{\text{res}}^1)_{c',c} = i \left(\frac{M_{c',a_{c'}}}{M_{c,c}} \right)^{\frac{1}{2}} \left(- \frac{I_{0c} O_{c',21} + O_{c',22}}{O_{0c'} O_{1c'}} \frac{(\Gamma_{c',c}^{00})_{11}}{\Delta E_{\lambda_0} - \epsilon_{00}} \right. \\ \left. + 2 \frac{I_{0c}}{O_{0c'}} \frac{\epsilon_{10} (\Gamma_{c',c}^{10})_{21}}{(\Delta E_{\lambda_0} - \epsilon_{00}) (\Delta E_{\lambda_1} - \epsilon_{11})} + \left[2 \frac{I_{0c}}{O_{0c'}} (\Gamma_{c',c}^{11})_{21} \right. \right. \\ \left. \left. + \frac{I_{c,21} + I_{c,22}}{O_{1c'}} (\Gamma_{c',c}^{11})_{22} \right] \frac{1}{\Delta E_{\lambda_1} - \epsilon_{11}} \right) \quad (3b)$$

The I_{0c} , etc., are the many-channel extensions of the unperturbed incoming and outgoing spherical solutions introduced in Chapter II.

If the reaction takes place via an isolated resonance of definite J and parity, the cross section is given by

$$\sigma_{\alpha'\alpha} = \frac{\pi}{4k_{0\alpha}^2} g_{\alpha}^J \sum'_{\ell s \ell' s'} \left(\frac{v_{0\alpha'}}{v_{0\alpha}} \right) | (A_{\text{res}}^0)_{c',c} |^2 + \frac{v_{1\alpha'}}{v_{0\alpha}} | (A_{\text{res}}^1)_{c',c} |^2$$

where the prime on the sum indicates the restriction to values such that $\vec{\ell} + \vec{s} = \vec{\ell}' + \vec{s}' = \vec{j}$, and that parity is conserved. In order that the problem be carried to its most complete conclusion, it is necessary that every unperturbed partial width for each reaction, proceeding via the intermediate state being considered, be known from experiment. In principle it is possible to determine these widths from the differential cross sections, but in practice such a procedure would be extremely difficult. In general, the most one might hope for is knowledge of the total width and the partial widths for the various possible reaction products summed over ℓ and s . This is the situation to which the remainder of the chapter is addressed.

Under such restrictions on the knowledge of the partial widths, we can make further progress if only one ℓ and s value contributes

to the various reaction widths, in an approximate sense at least. Then, instead of each reaction partial width being a sum over ℓ and s , it consists of a single term corresponding to a single ℓ and s value. For purposes of illustration, here we assume $\ell = 0$ in all cases; other orbital angular momenta are treated similarly. By considering this special case, one is able to carry the calculation through to the final result which will indicate the importance of the atomic excitations. In the final analysis each orbital angular momentum has to be worked out individually; the method is illustrated here by treating the case $\ell = 0$.

Before proceeding, it is useful to convert to a more standard notation. For example, we introduce Γ_c , which was defined in Chapter I and involves the level λ_0 ; i. e., $\Gamma_c = 2\gamma_{\lambda_0}^2 P_c$. Also, $\Gamma = \sum_c \Gamma_c$ appears. In the approximation that only s-waves contribute, the cross section does not contain the sums over orbital and spin angular momenta, so that

$$\begin{aligned} \sigma_{\alpha'\alpha} = g_{\alpha}^J \frac{\pi}{k_{\alpha}^2} & \left(\frac{\Gamma_{c'} \Gamma_c}{(E - E_{\lambda_0})^2 + \frac{1}{4} \Gamma^2} + \frac{1}{4} \frac{v_{1\alpha'}}{v_{0\alpha'}} \Gamma_{0c'} \Gamma_{0c} \left| \frac{O_{c',21} + O_{c',22}}{O_{1c'}} \frac{1}{E - E_{\lambda_0} + \frac{1}{2} i \Gamma} \right. \right. \\ & + \frac{O_{0c'}}{O_{1c'}} \left\{ \sum_{c''} \frac{L_{c'',21}}{P_{0c''}} \Gamma_{c''} \right\} \frac{1}{(E - E_{\lambda_0} + \frac{1}{2} i \Gamma) (E - E_{\lambda_1} + \frac{1}{2} i \sum_{c''} \frac{P_{1c''}}{P_{0c''}} \Gamma_{c''})} \\ & \left. \left. - \left\{ 2 \frac{O_{0c'}}{O_{1c'}} \frac{P_{c,21}}{P_{0c}} + \frac{O_{0c'}}{O_{1c'}} \frac{P_{1c}}{P_{0c}} \frac{I_{c,21} + I_{c,22}}{I_{0c}} \right\} \frac{1}{E - E_{\lambda_1} + \frac{1}{2} i \sum_{c''} \frac{P_{1c''}}{P_{0c''}} \Gamma_{c''}} \right| \right)^2 \end{aligned}$$

where the results of Appendix III have been used, and the quantities $O_{c',21}$, etc., are the many-channel generalizations of the quantities introduced in Chapter II. The c'' sum is over only the different partitions α'' since the orbital angular momentum is zero before and after the collision so that s , J , and M are constants of the motion. Using Appendix I, we obtain the generalization of Equation (7), Chapter II:

$$\begin{aligned}
\sigma_{\alpha',\alpha} = & g_{\alpha}^J \frac{\pi}{k_{\alpha}^2} \left(\frac{\Gamma_{c'}\Gamma_c}{(E-E_r)^2 + \frac{1}{4}\Gamma^2} + \frac{512}{729} \frac{1}{k_{\alpha}^2 a_{\alpha}^2 \rho_{\alpha}} \frac{1}{(1+\rho_{\alpha})^4} \left\{ [(1+\rho_{\alpha})^2 + 2 \frac{E}{\delta} (1 + \frac{8}{3}\rho_{\alpha})]^2 \right. \right. \\
& + 16 \left(\frac{E}{\delta} \right)^2 \left. \left. \frac{\Gamma_{c'}\Gamma_c}{(E-E_r-\delta)^2 + \frac{1}{4}\Gamma^2} + \frac{32}{729} \frac{1}{k_{\alpha}^2 a_{\alpha}^2 \rho_{\alpha}} \frac{\Gamma_{c'}}{(E-E_r)^2 + \frac{1}{4}\Gamma^2} \frac{\Gamma_c}{(E-E_r-\delta)^2 + \frac{1}{4}\Gamma^2} \right. \right. \\
& \times \left\{ 4 \left| \sum_{\alpha''} \frac{k_{\alpha} \rho_{\alpha}^{\frac{1}{2}}}{k_{\alpha''} \rho_{\alpha''}^{\frac{1}{2}}} \frac{\Gamma_{c''}}{\Gamma} \right|^2 + 2 \sum_{\alpha''} \frac{k_{\alpha} \rho_{\alpha}^{\frac{1}{2}}}{k_{\alpha''} \rho_{\alpha''}^{\frac{1}{2}}} \frac{\Gamma_{c''}}{\Gamma} \left[8 \frac{E}{\delta} \left(\frac{k_{\alpha} \rho_{\alpha}^{\frac{1}{2}}}{k_{\alpha''} \rho_{\alpha''}^{\frac{1}{2}}} \frac{1 + \frac{8}{3}\rho_{\alpha'}}{(1+\rho_{\alpha'})^2} \right. \right. \right. \\
& - \left. \left. \frac{1 + \frac{8}{3}\rho_{\alpha'}}{(1+\rho_{\alpha'})^2} \right) + 32 \frac{\delta}{\Gamma} \frac{E}{\delta} \frac{k_{\alpha} \rho_{\alpha}^{\frac{1}{2}}}{k_{\alpha''} \rho_{\alpha''}^{\frac{1}{2}}} \frac{\rho_{\alpha'}^{\frac{3}{2}}}{(1+\rho_{\alpha'})^2} - 16 \frac{E-E_r}{\frac{1}{2}\Gamma} \frac{E}{\delta} \left(\frac{\rho_{\alpha'}^{\frac{3}{2}}}{(1+\rho_{\alpha'})^2} \right. \right. \\
& + \left. \left. \frac{k_{\alpha} \rho_{\alpha}^{\frac{1}{2}}}{k_{\alpha''} \rho_{\alpha''}^{\frac{1}{2}}} \frac{\rho_{\alpha'}^{\frac{3}{2}}}{(1+\rho_{\alpha'})^2} \right) - 4 \right] + \frac{32}{(1+\rho_{\alpha'})^2} \left(\frac{E}{\delta} \right)^2 \frac{k_{\alpha} \rho_{\alpha}^{\frac{1}{2}}}{k_{\alpha''} \rho_{\alpha''}^{\frac{1}{2}}} \left[\frac{E-E_r}{\frac{1}{2}\Gamma} \frac{E-E_r-\delta}{\frac{1}{2}\Gamma} + 1 \right] \\
& \times \frac{1}{(1+\rho_{\alpha'})^2} \left[4(\rho_{\alpha'} \rho_{\alpha'})^{\frac{3}{2}} - (1 + \frac{8}{3}\rho_{\alpha'}) (1 + \frac{8}{3}\rho_{\alpha'}) \right] - \frac{128}{(1+\rho_{\alpha'})^2} \frac{k_{\alpha} \rho_{\alpha}^{\frac{1}{2}}}{k_{\alpha''} \rho_{\alpha''}^{\frac{1}{2}}} \left(\frac{E}{\delta} \right)^2 \\
& \times \left. \left. \frac{1}{(1+\rho_{\alpha'})^2} \left[\rho_{\alpha'}^{\frac{3}{2}} (1 + \frac{8}{3}\rho_{\alpha'}) + \rho_{\alpha'}^{\frac{3}{2}} (1 + \frac{8}{3}\rho_{\alpha'}) \right] \right\} \right)
\end{aligned}$$

where $\rho_{\alpha} = 12 \frac{m}{M_{\alpha}} \frac{E}{\delta}$. Again, δ and E are limited to values such that $\frac{\delta}{E} \ll 1$, and the result is derived for free s-waves and K- and L-shell ($l = 0$) hydrogenic atomic wavefunctions.

CHAPTER IV
THE MODEL PARAMETERS

The use of a model for the atom with only two atomic states is the only fundamental assumption that has been made. There are two parameters which must be chosen to fit the model to the actual physical atom: the strength of the excitation-producing perturbation and the energy difference δ between the two atomic states.

The appropriate choice for the energy δ is simply determined as the ionization energy of the particular electron of the atom being treated since the preponderance of excitation in the real atom is to the lower edge of the continuum. This is a well-known fact in collisions between heavy charged particles and atoms, and recent calculations indicate the same for nuclear reactions and decay (3,4). Thus, although the physical atom can absorb infinitely many energies, it is a good approximation to replace this continuous range of energies by a set of discrete energies corresponding to the ionization energies of the various electrons.

The perturbation strength corrects for the fact that the two-state model contains a single excited state whereas in fact the actual atom contains an infinite number of such states. For each electron in the atom there is a separate perturbation strength which is introduced so that the model electron has the same total ionization probability during the nuclear reaction as the appropriate electron in the atom.

If the reaction is treated as accurately as possible in the context of the model, the nuclear cross section consists of the zero-order resonance and a series of perturbed resonant terms. There is one term for each of the electrons in the atom, and each term has its own energy shift δ and perturbation strength, corresponding to the electron's ionization energy and ionization probability, respectively.

The most obvious method of estimating this strength factor is to compare the ionization probabilities for the reaction for the model and physical atoms. This can be done with the methods of Ciocchetti and Molinari (4), although it would be simpler, and sufficient, to treat the case of nuclear decay rather than nuclear reaction. This is more than is necessary for our purposes so that we simply compare the ionization cross sections for the model and physical atoms during a collision with a heavy charged particle, specifically, a proton. The strength factor is obtained as the ratio of the two cross sections and should be accurate enough for the present purposes.

The ionization cross section for the real electron is approximated using the tables of Khandelwal and Choi (14), the atom being represented by hydrogenic electron states. They have calculated the ionization cross section during charged-particle impact for a wide range of projectile energy and charge and atomic screening constants in the Bethe-Born approximation. The corresponding model calculation is done with time-dependent perturbation theory with plane waves for the initial and final projectile states. See Appendix IV for a detailed derivation of the cross section.

As mentioned above, ideally the entire calculation should be performed for each electron of the atom, thereby accounting for the

different ionization cross sections and energies of the various electrons. This would lead to a fine structure in the nuclear cross section curve which, however, will be beyond experimental detection for some time to come. In addition, the contributions to the nuclear cross section by the inner shell electrons will generally be so small that such shells can be neglected altogether. Often only the outermost shell need be treated at all. For example, for the 5.3 MeV alpha decay of Po^{210} , the K-, L-, and M-shell ionization probabilities are 2×10^{-6} , 7×10^{-4} , and 2×10^{-2} , respectively (15). This indicates that the inner shells of an atom can probably be neglected compared with the outer shell since we are concerned with the largest effect only. This example also suggests that for the loosely-bound outer shell electrons the ionization probability may become appreciable (note the rapid increase in the probability as one goes from the inner to outer shells).

To complete the calculation and obtain specific results it is necessary to fix attention upon a particular atom. From the outset it is possible to restrict the atoms to be considered to a relatively small group. For example, in order to eliminate the complicating effects of multi-atom processes, it is necessary to use gaseous targets. Of the gases, Ne is particularly suitable for two reasons. First, it has an extremely low boiling point which allows the experiment to be performed at temperatures low enough to obtain maximum relief from the resolution-destroying effects of Doppler broadening. Second, since Ne (like the other rare gases) remains in the atomic state even at low temperatures, the wave-mechanical treatment of its electronic states is much simpler than those of the diatomic molecules.

Ne^{20} is chosen for detailed study. This isotope is particularly

suitable as it has an elastic proton resonance at 1.17 MeV which is the subject of a very precise cross section measurement (16). The experiment was performed at 20°K (to reduce Doppler broadening) and attained a resolution of 110 eV with substantial improvements foreseen in the near future. The natural width was determined to be about 8 eV. We will perform the calculation for this resonance.

In addition to the energy and width of the resonance given above, the value for δ and the perturbation strength for Ne are needed. In the spirit of the above discussion, we neglect the K shell in comparison with the L shell. The L-shell ionization energies are 48.3 eV (L_I), 21.6 eV (L_{II}), and 21.4 eV (L_{III}). Since the nuclear resonance is only 8 eV wide, the L_I terms will not overlap the other two terms to any appreciable extent. Its intensity will be down by a factor of three due to the smaller number of electrons when compared with the L_{II} and L_{III} terms which are essentially coincident and therefore add. In addition, the L_I intensity will be lowered in comparison due to its greater ionization energy. So for purposes of concentrating on the largest effect, we can neglect the L_I term and treat the L_{II} and L_{III} terms as coincident with an intermediate ionization energy, 21.5 eV.

The "ionization" cross section for the model, using plane waves for the proton, is (See Appendix IV)

$$\sigma_{\text{model}} \approx 0.444 \frac{\pi}{k^Z} \left(\frac{M}{m}\right)^2 \left(\frac{\delta}{\text{Ryd}}\right)^4 \left\{ \frac{\delta}{\text{Ryd}} + \frac{1}{9} k^2 a_o^2 \left(\frac{\delta}{E}\right)^2 \right\}^{-5}$$

For this example, $k^2 a_o^2 \left(\frac{\delta}{E}\right)^2 \ll 9 \frac{\delta}{\text{Ryd}}$, so the cross section simplifies to

$$\sigma_{\text{model}} \approx 0.444 \frac{\pi}{k^Z} \left(\frac{M}{m}\right)^2 \frac{\text{Ryd}}{\delta}$$

According to the tables of Khandelwal and Choi, the cross section for L-shell ionization of the Ne atom by 1.17 MeV incident protons is

$$\sigma_{\text{atom}} = 1.59 \pi a_0^2$$

The ratio of these two terms gives the desired correction factor:

$$\frac{\sigma_{\text{atom}}}{\sigma_{\text{model}}} = 266$$

Since the nuclear process is elastic with no other open channels, the result of Chapter II can be used [Equation (7)]. Including the correction factor and simplifying, we obtain the final result,

$$\begin{aligned} \sigma = \frac{\pi}{k^2} & \left(\frac{\Gamma^2}{(E-E_r)^2 + \frac{1}{4}\Gamma^2} + 0.22 \left[2 \frac{\Gamma^2}{(E-E_r-\delta)^2 + \frac{1}{4}\Gamma^2} \right. \right. \\ & \left. \left. + \left[\frac{E-E_r}{\frac{1}{2}\Gamma} \frac{E-E_r-\delta}{\frac{1}{2}\Gamma} + 0.240 \right] \frac{\Gamma^2}{(E-E_r)^2 + \frac{1}{4}\Gamma^2} \frac{\Gamma^2}{(E-E_r-\delta)^2 + \frac{1}{4}\Gamma^2} \right] \right) \quad (1) \end{aligned}$$

The quantity δ equals the ionization energy of the shell considered: 21.5 eV in this example. The unperturbed resonance width Γ and energy E_r must be determined from experiment. This is particularly simple in this case since the unperturbed and displaced terms are well separated so that either peak in the cross section may be examined to determine δ and E_r . In cases for which there is significant overlap, they are determined by a two-parameter fit to the data.

CHAPTER V

CONCLUSIONS

The ionization energy of Ne (L_{II} and L_{III} subshells) is equal to approximately five nuclear resonance half-widths. Therefore, it is not surprising that the interference term of Equation (1), Chapter IV, is only a small fraction of the total perturbation—less than two percent. This means the process is essentially classical in the sense that the compound nucleus exists long enough to determine whether the ionization occurred before or after the nuclear interaction took place. Thus, it is valid to think of the reaction as nothing more than two nuclear decays, one of which is time-reversed. The total ionization that occurs before the nuclear reaction, i. e., during the "time-reversed decay," will contribute to the line shape.

The surprising aspect of the result of Chapter IV is the magnitude of the effects. The indication is that ionization occurs (before the nuclear reaction) in about 30% of the events. This is in sharp contrast to the ionization probabilities associated with the 5.3 MeV alpha decay of Po^{210} described in the previous chapter. However, even the M shell of Po is much more tightly bound than the L shell of Ne so that another order-of-magnitude increase in the probability in going from the M shell of Po to the L shell of Ne is not unexpected.

Levinger's beta decay calculations (3) provide further support for the 30% figure for the ionization probability derived here.

The beta decay results are used instead of the alpha decay ones because the 1.17 MeV proton of the example travels much faster than the L-shell electrons of Ne. Thus, it is appropriate to use the "sudden approximation" that Levinger employed in his treatment of beta decay instead of the "adiabatic approximation" appropriate to alpha decay. In the former the perturbation is taken as the sudden change in nuclear charge due to the emission of the beta ray; the passage of the beta particle through the electronic cloud is neglected. In the adiabatic approximation just the opposite assumption is made. The perturbation is taken as the Coulomb interaction between the charged particle and the atomic electrons as the particle passes (adiabatically) through the atom. Using Levinger's beta decay results with an effective $Z_L = 5.85$ for Ne, we find the ionization probability for the $L_{II,III}$ shells is 0.037. This result does not include outer screening. It will be shown that such corrections can account for the factor of 8 required for agreement with this work.

If the parameters, E and Γ , of our example are fixed while δ is allowed to vary, Equation (7) of Chapter II shows that the size of the perturbation term decreases quite slowly as δ increases from approximately a Rydberg to a keV. Compare this with the very rapid variation of ionization probability with ionization energy described above for Po^{210} . This seeming inconsistency is illusory, however. For example, in passing from the K to L shell there is a factor of 4 increase in the ionization probability simply due to the four-fold increase in the number of electrons available for ionization. This amounts to an effective δ -dependence in addition to that expressed in Equation (7), Chapter II. If this dependence were made explicit,

it would appear in the perturbation strength factor applied to that equation.

The effect of screening induces a second implicit δ -dependence which, again, would appear in the strength factor if made explicit. There is no screening in the model (there is only one electron). If this were true for the physical atom, one would expect that, except for the factor of four discussed in the previous paragraph, the strength factor would be approximately the same for the K and L shells. However, screening (more importantly, outer screening) does occur, and it is more important for the outer electron states. This makes it relatively easier to ionize the L shell than the K shell compared with the no-screening case. Hence, here is another source of an implicit δ -dependence. For example, in Ne the strength factor is 18.5 times larger for the entire L shell than for the K shell. A factor of four is accounted for by the differential in the number of electrons. This leaves a 4.6-fold increase due to screening (and other sources, but mainly screening). So in some cases at least, the effect of screening can be considerable.

In the example, the interference term is much smaller than the "classical" correction term [See Equation (1) of the previous chapter] and can be neglected for most purposes. In less extreme cases (i. e., broader resonances) the interference term will be comparable to the "classical" one. In fact the more important result of this calculation is the size of the interference term rather than that of the "classical" term. The latter result can be obtained to a fair approximation by the methods of Ciocchetti and Molinari (4), but these authors have difficulties when they try to treat the interference between

incoming and outgoing particles. The effect of such interference comes out automatically in the present work. As much as anything the elucidation of these interference effects was the objective of this calculation. The existence of interference explains why the nuclear and atomic processes were treated together as a single event.

Now that we know the shape of the resonance cross section, we can bridge the gap to the experiment by asking the question: What line shape does the experimentalist, with his imperfect energy resolution, see? He will certainly not see the two separate resonances of Ne^{20} unless his resolution is about 20 eV or better. With poorer resolution the experiment will detect only a single resonance which will be asymmetric (unless the sizes of the two theoretical resonances are equal).

It is assumed that the total experimental energy resolution is represented by a normal distribution. At 8 eV, the Ne^{20} resonance is quite narrow, especially compared with current resolutions. So, for purposes of performing the necessary integrations, we replace the Lorentzian resonances with delta functions (which the Lorentzians approach for small Γ). Then, the experimental curve is proportional to

$$\begin{aligned} I(E) &= \int_0^\infty \frac{1}{\sigma_0 \sqrt{2\pi}} \exp\left[-\frac{(E-E')^2}{2\sigma_0^2}\right] [a \delta(E'-E_r) + b \delta(E'-E_r-\delta)] dE' \\ &= \frac{1}{\sigma_0 \sqrt{2\pi}} \left[a \exp\left[-\frac{(E-E_r)^2}{2\sigma_0^2}\right] + b \exp\left[-\frac{(E-E_r-\delta)^2}{2\sigma_0^2}\right] \right] \end{aligned}$$

where a and b give the sizes of the primary and correction terms, respectively, and $a + b = 1$. For Ne^{20} , $a = 0.7$, and $b = 0.3$. The corresponding graphs for resolution curves with variances of 5 eV,

10 eV, 20 eV, and 30 eV are displayed in Figures 1-4. Of course, the delta function approximation breaks down for the higher resolutions, particularly the 5 eV curve, but the qualitative trend indicated by the figures is still valid. The variance of the resolution curve is approximately one-half what one might normally call the resolution. It is clear from the figures that the asymmetry is going to be past detection for even the best statistics unless the resolution is better than about 60 eV.

A measure of the asymmetry of the cross section is given by the skewness. This is the third central moment of the cross section divided by its variance to the $\frac{3}{2}$ power:

$$\text{Skewness} = \frac{\langle (E - \langle E \rangle)^3 \rangle}{[\langle (E - \langle E \rangle)^2 \rangle]^{3/2}}$$

In the delta-function approximation, the skewness can be expressed in closed form as

$$\text{Skewness} = \frac{b(1-b)(1-2b) \left(\frac{\delta}{\sigma_0} \right)^3}{\left[1 + b(1-b) \left(\frac{\delta}{\sigma_0} \right)^2 \right]^{3/2}}$$

where σ_0 is the variance of the resolution curve. The graph of this function is exhibited in Figure 5 for Ne^{20} ($\delta = 21.5$ eV). It is clear that for resolutions greater than 100 eV no visible asymmetry can be expected. Somewhere between 50 eV and 100 eV, one might hope to see the asymmetry, depending on the statistics and extent of isolation of the resonance.

The greatest single improvement that could be made in this work would be to divest the theory of the two-state model. Then one would have no need for calculating the perturbation strength, and most other possible criticisms of the theory would be met. However,

to eliminate the model would almost certainly require the abandonment of the R -matrix formalism for some other reaction theory. The difficulty lies in the fact that, just as the two-state model leads to two coupled differential equations and elements of the R matrix which are two-dimensional matrices, the real atom with its infinite number of states would lead to an infinite number of coupled differential equations and infinite-dimensional elements of the R matrix. In addition, the definition of the external states would become much more complicated.

In summary, the methods developed here give results which are consistent with experimental data and other calculations where comparison is possible. In addition, the interference between incoming and outgoing particles is described rigorously as compared with the previous attempts which are heuristic, at best. It is found that the effects of screening can be important and should be reckoned with in future calculations of ionization probabilities in nuclear reactions and decay. The resonance for the elastic scattering of 1.17 MeV protons on Ne^{20} is studied. It is found that the term for ionization is large (almost half the size of the primary term) and should be detectable with modest improvements in present experimental resolution. It appears that a resolution of at least 60 eV is needed for the observation of the asymmetry for Ne^{20} .

APPENDIX I

CORRECTION FACTORS IN $(A_{\text{res}}^1)_{c'c}$

For simplicity of notation the channel labels are omitted. The quantities to be determined are L_{21} , $O_{21} + O_{22}$, and $I_{21} + I_{22}$, all to first order in the atomic perturbation.

Section A: Calculation of L_{21}

Since L_{21} is given by

$$L_{21} = \frac{O_{22}' O_{21} - O_{21}' O_{22}}{2O_0 O_1}$$

the relevant quantity is $(O_{22}' O_{21} - O_{21}' O_{22})$. The equations for O_{21} and O_{22} are

$$\left(\frac{d^2}{dR^2} + k_1^2 - \frac{\ell(\ell+1)}{R^2} - U_{11} \right) O_{21} = U_{01} O_{11}$$

$$\left(\frac{d^2}{dR^2} + k_1^2 - \frac{\ell(\ell+1)}{R^2} - U_{11} \right) O_{22} = U_{01} O_{12}$$

Therefore,

$$O_{22} \frac{d^2 O_{21}}{dR^2} - O_{21} \frac{d^2 O_{22}}{dR^2} = -2U_{01} O_0 O_1$$

to first order. Integrating from R to ∞ , we have

$$\begin{aligned} O_{22}'(R) O_{21}(R) - O_{21}'(R) O_{22}(R) &= O_{22}'(\infty) O_{21}(\infty) - O_{21}'(\infty) O_{22}(\infty) \\ &- 2 \int_R^\infty U_{01}(R') O_0(R') O_1(R') dR' \end{aligned}$$

$$\begin{aligned}
&= -2 \int_R^{\infty} U_{01}(R') O_0(R') O_1(R') dR' \\
&\approx \frac{1}{2} D \left\{ \alpha \left(\frac{1}{3} \frac{m}{M} \frac{\delta}{E} \right)^{\frac{3}{2}} + \frac{4}{3} \alpha \right\} O_0(R) O_1(R)
\end{aligned}$$

for free s-waves, and $D \equiv \frac{32}{9 a_0 \rho^{\frac{1}{2}}}$. The quantity δ is the energy between the two atomic states, a_0 is the first Bohr radius for hydrogen, and $\rho = 12 \frac{m}{M} \frac{E}{\delta}$.

Section B: Calculation of $I_{21} + I_{22}$ and $O_{21} + O_{22}$

We compute $O_{21} + O_{22}$ and determine $I_{21} + I_{22}$ using

$$I_{21} + I_{22} = (O_{21} + O_{22})^*$$

Referring to Section A, we write the equations for the first-order corrections to O_{21} and O_{22} as

$$\left(\frac{d^2}{dR^2} + k_1^2 - \frac{\ell(\ell+1)}{R^2} + \frac{Ze^2}{R} \right) O_{21}^{(1)} = \bar{U}_{11} O_{21}^{(0)} + \bar{U}_{01} O_{11}^{(0)}$$

$$\left(\frac{d^2}{dR^2} + k_1^2 - \frac{\ell(\ell+1)}{R^2} + \frac{Ze^2}{R} \right) O_{22}^{(1)} = \bar{U}_{11} O_{22}^{(0)} + \bar{U}_{01} O_{12}^{(0)}$$

where $\bar{U}_{ij} \equiv U_{ij} + \frac{Ze^2}{R}$. Since $O_{21}^{(0)} = -O_{22}^{(0)}$, and $O_{11}^{(0)} = O_{21}^{(0)} = O_0$, then

$$\left(\frac{d^2}{dR^2} + k_1^2 - \frac{\ell(\ell+1)}{R^2} + \frac{Ze^2}{R} \right) [O_{21}^{(1)} + O_{22}^{(1)}] = 2 U_{01} O_0$$

The Green's function, $G(R, R')$, is defined by

$$\left(\frac{d^2}{dR^2} + k_1^2 - \frac{\ell(\ell+1)}{R^2} + \frac{Ze^2}{R} \right) G(R, R') = \delta(R - R') \quad (1)$$

so that

$$O_{21}^{(1)} + O_{22}^{(1)} = 2 \int_0^{\infty} G(R, R') U_{01}(R') O_0(R') dR'$$

Since $O_{21}^{(1)}$ and $O_{22}^{(1)}$ go to zero as $R \rightarrow \infty$, the boundary condition

on $G(R, R')$ is: $G(R, R') \rightarrow 0$ as $R \rightarrow \infty$. Writing

$$G(R, R') = \begin{cases} E O_1(R) + F I_1(R) & R > R' \\ S O_1(R) + T I_1(R) & R < R' \end{cases}$$

we see that the boundary condition is satisfied if $E = F = 0$.

Continuity at R' sets the condition,

$$S O_1(R') + T I_1(R') = 0$$

Integration of Equation (1) from $R' - \epsilon$ to $R' + \epsilon$ gives

$$\left. \frac{dG}{dR} \right|_{R=R'-\epsilon}^{R=R'+\epsilon} = 1 = -S O_1'(R') - T I_1'(R')$$

The solutions for S and T are obtained by combining the previous two equations:

$$S = T^* = -\frac{1}{2ik_1} I_1(R')$$

The value for the Wronskian, $O_1' I_1 - I_1' O_1 = 2ik_1$, was used. Finally,

$$\begin{aligned} O_{21}^{(1)} + O_{22}^{(1)} &= \frac{1}{ik_1} \int_R^\infty [O_1(R') I_1(R) - I_1(R') O_1(R)] U_{01}(R') O_0(R') dR' \\ &= \frac{8D}{k_0} \frac{E}{\delta} \frac{1}{(1+\rho)^2} \left\{ \frac{1}{6} (1 + \frac{8}{3}\rho) + \frac{1}{3} \rho^{\frac{3}{2}} i \right\} \end{aligned}$$

The last expression is for free s-waves.

APPENDIX II

DECOMPOSITION OF $(1 - RL^O)^{-1}R$

$$\begin{aligned}
 (1 - RL^O)^{-1}R &= (1 - RL^O)^{-1}(R^O + R') \\
 &= (1 - RL^O)^{-1}[R^O - (R'L^OR^O - R')(1 - L^OR^O)] \\
 &= (1 - RL^O)^{-1}[R^O - R'L^O(1 - R^OL^O)^{-1}(R^O - R^OL^OR^O)(1 - L^OR^O)^{-1} \\
 &\quad + R'(1 - L^OR^O)] \\
 &= (1 - RL^O)^{-1}[R^O - R'L^O(1 - R^OL^O)^{-1}R^O + R'(1 - L^OR^O)^{-1}] \\
 &= (1 - RL^O)^{-1}[1 - R'L^O(1 - R^OL^O)^{-1}]R^O \\
 &\quad + (1 - R^OL^O)^{-1}(1 - R^OL^O)(1 - RL^O)^{-1}R'(1 - L^OR^O)^{-1} \\
 &= (1 - R^OL^O)^{-1}R^O + (1 - R^OL^O)^{-1}[(1 - RL^O)(1 - R^OL^O)^{-1}]^{-1} \\
 &\quad \times R'(1 - L^OR^O)^{-1} \\
 &= (1 - R^OL^O)^{-1}R^O + (1 - R^OL^O)^{-1}[1 - R'L^O(1 - R^OL^O)^{-1}]^{-1} \\
 &\quad \times R'(1 - L^OR^O)^{-1} \\
 &= (1 - R^OL^O)^{-1}R^O + (1 - R^OL^O)^{-1}(1 - R'L')^{-1}R'(1 - L^OR^O)^{-1}
 \end{aligned}$$

where $L' = L^O(1 - R^OL^O)^{-1}$.

APPENDIX III

THE QUANTITIES Γ AND ξ

In Section A we derive the order of each quantity. Section B gives the explicit form of those quantities which, according to Section A, contribute to the second-order expansion of the cross section.

Section A

First, we recall that

$$\Gamma_{c'c}^{\mu\nu} \equiv 2(\gamma_{\mu c'}^* \gamma_{\nu c}) P_c$$

Also, P_c is given by

$$P = \text{Im} \frac{1}{O_{11}O_{22} - O_{12}O_{21}} \begin{pmatrix} O'_{11}O_{22} - O'_{12}O_{21} & O'_{12}O_{11} - O'_{11}O_{12} \\ O'_{21}O_{22} - O'_{22}O_{21} & O'_{22}O_{11} - O'_{21}O_{12} \end{pmatrix}$$

dropping the channel label. Thus, symbolically,

$$P = \begin{pmatrix} 1 & g \\ g & 1 \end{pmatrix}$$

where g is the strength of the perturbation.

The lower (upper) component of γ_{0c} (γ_{1c}) is proportional to an internal correction. According to the discussion in Chapter II, internal corrections do not contribute to the cross section to second order, so these components are set equal to zero; symbolically, we write

$$\gamma_{0c} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \gamma_{1c} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and

$$\Gamma_{c'c}^{\mu\nu} = (\gamma_{\mu c'}^T \times \gamma_{\nu c}) \begin{pmatrix} 1 & g \\ g & 1 \end{pmatrix}$$

There are four possible combinations for μ and ν , giving

$$\Gamma_{c'c}^{00} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 \quad 0) \begin{pmatrix} 1 & g \\ g & 1 \end{pmatrix} = \begin{pmatrix} 1 & g \\ 0 & 0 \end{pmatrix}$$

$$\Gamma_{c'c}^{01} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} (0 \quad 1) \begin{pmatrix} 1 & g \\ g & 1 \end{pmatrix} = \begin{pmatrix} g & 1 \\ 0 & 0 \end{pmatrix}$$

$$\Gamma_{c'c}^{10} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1 \quad 0) \begin{pmatrix} 1 & g \\ g & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & g \end{pmatrix}$$

$$\Gamma_{c'c}^{11} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} (0 \quad 1) \begin{pmatrix} 1 & g \\ g & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ g & 1 \end{pmatrix}$$

Since

$$\epsilon_{ij} = \sum_c \gamma_{ic}^T (L_c - B_c) \gamma_{jc}$$

we have

$$\epsilon_{01} = \sum_c (1 \quad 0) \begin{pmatrix} 1 & g \\ g & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \sum_c g$$

$$\epsilon_{10} = \sum_c (0 \quad 1) \begin{pmatrix} 1 & g \\ g & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \sum_c g$$

So ϵ_{01} and ϵ_{10} are first-order terms.

Section B

The object of this section is to express the relevant Γ and ϵ quantities in terms of atomic corrections and nuclear factors which

can be determined from experiment.

$$\begin{aligned}
 (\Gamma_{c',c}^{00})_{11} &= [2(\gamma_{0c'} \times \gamma_{0c}) P_c]_{11} \approx 2 (\gamma_{0c'}^{(0)})_1 (\gamma_{0c}^{(0)})_1 P_{0c} \\
 &= \Gamma_{c'}^{\frac{1}{2}} \Gamma_c^{\frac{1}{2}} \left(\frac{P_{0c}}{P_{0c'}} \right)^{\frac{1}{2}} \\
 &= \left(\frac{M_c}{M_{c'}} \frac{v_{0c}}{v_{0c'}} \frac{a_c}{a_{c'}} \frac{I_{0c'}}{I_{0c}} \frac{O_{0c'}}{O_{0c}} \Gamma_{c'} \Gamma_c \right)^{\frac{1}{2}}
 \end{aligned}$$

where $(\gamma_{0c'})_i$ is the i^{th} component of γ_{0c} ($i = 1, 2$), and the identity

$$P_c = \left(\frac{M_c a_c v_{0c}}{\hbar} \right)^{\frac{1}{2}} \left(\frac{1}{I_{0c} O_{0c}} \right)^{\frac{1}{2}}$$

was used. The remaining quantities are

$$(\Gamma_{c',c}^{10})_{21} = [2(\gamma_{1c'} \times \gamma_{0c}) P_c]_{21} \approx 2 (\gamma_{0c'}^{(0)})_1 (\gamma_{0c}^{(0)})_1 P_{0c} = (\Gamma_{c',c}^{00})_{11}$$

$$\begin{aligned}
 (\Gamma_{c',c}^{11})_{22} &= [2(\gamma_{1c'} \times \gamma_{1c}) P_c]_{22} \approx 2 (\gamma_{0c'}^{(0)})_1 (\gamma_{0c}^{(0)})_1 P_{1c} \\
 &= \frac{P_{1c}}{P_{0c}} (\Gamma_{c',c}^{00})_{11}
 \end{aligned}$$

$$(\Gamma_{c',c}^{11})_{21} = [2(\gamma_{1c'} \times \gamma_{1c}) P_c]_{21} \approx \frac{P_{c,21}}{P_{0c}} (\Gamma_{c',c}^{00})_{11}$$

$$\xi_{00} = \sum_c \gamma_{0c}^T L_c^O \gamma_{0c} \approx \sum_c (\gamma_{0c}^{(0)})_1 (\gamma_{0c}^{(0)})_1 L_{c,11}^O = \frac{1}{2} \sum_c \Gamma_c, \text{ if } B = S.$$

$$\xi_{11} \approx \frac{1}{2} \sum_c \frac{P_{1c}}{P_{0c}} \Gamma_c, \text{ similarly.}$$

$$\xi_{10} \approx \frac{1}{2} \sum_c \frac{L_{c,21}}{P_{0c}} \Gamma_c$$

APPENDIX IV

EXCITATION CROSS SECTION FOR THE MODEL DURING PROTON IMPACT

The calculation is performed according to Section 30 of Schiff's Quantum Mechanics (2nd edition)(17).

As usual, the atomic wavefunctions are hydrogenic K and L ($l = 0$) states:

$$\phi_0 = \left(\frac{\alpha^3}{\pi}\right)^{1/2} e^{-\alpha r}$$

$$\phi_1 = \frac{1}{4} \left(\frac{\alpha^3}{2\pi}\right)^{1/2} (2 - \alpha r) e^{-1/2 \alpha r}$$

with α being given by the energy gap between the two atomic states:

$$\alpha^2 = \frac{1}{a_0^2} \frac{\delta}{\text{Ryd}}$$

The initial and final proton wavefunctions are taken to be plane waves:

$$\psi_0 = L^{-3/2} e^{i\vec{k}_0 \cdot \vec{R}} \quad \text{Initial}$$

$$= L^{-3/2} e^{i\vec{k}_1 \cdot \vec{R}} \quad \text{Final}$$

where \vec{k}_0 and \vec{k}_1 are initial and final proton wave vectors.

The total Hamiltonian is

$$H = H_0 + H^1$$

where

$$H_0 = -\frac{\hbar^2}{2m} \nabla_{\vec{r}}^2 - \frac{\hbar^2}{2M} \nabla_{\vec{R}}^2 - \frac{e^2}{r}$$

$$H' = -\frac{e^2}{|\vec{r} - \vec{R}|} + \frac{e^2}{R}$$

The transition rate is given by the Golden Rule,

$$\omega = \frac{2\pi}{\hbar} \rho(k_1) |H'_{01}|^2$$

and the cross section by

$$\frac{d\sigma}{d\Omega} = L^6 \frac{M}{2\pi\hbar^2} |H'_{01}|^2$$

for $\frac{k_1}{k_0} \approx 1$.

The transition matrix element H'_{01} is

$$\begin{aligned} H'_{01} &= \iint d\vec{r} d\vec{R} \phi_1^* \psi_1^* \left(-\frac{e^2}{|\vec{r} - \vec{R}|} + \frac{e^2}{R} \right) \phi_0 \psi_0 \\ &= \iint d\vec{r} d\vec{R} \phi_1^* \psi_1^* \left(-\frac{e^2}{|\vec{r} - \vec{R}|} \right) \phi_0 \psi_0 \end{aligned}$$

since the atomic states are orthogonal. Therefore,

$$H'_{01} = -\frac{e^2 \alpha^3}{4\pi L^3 \sqrt{2}} \int d\vec{r} (2 - \alpha r) e^{-\frac{3}{2}\alpha r} \int d\vec{R} e^{i\vec{K} \cdot \vec{R}} \frac{1}{|\vec{r} - \vec{R}|}$$

where $\vec{K} = \vec{k}_0 - \vec{k}_1$.

The \vec{R} integration is done by first transforming to $\vec{\rho} = \vec{R} - \vec{r}$. Then, the angular integration of $\vec{\rho}$ is easy, and the ρ integration is done by introducing an ϵ -cutoff. The result is

$$H'_{01} = -\frac{e^2 \alpha^3}{K^2 L^3 \sqrt{2}} \int d\vec{r} (2 - \alpha r) e^{-3(\frac{3}{2}\alpha r - \frac{1}{3}i\vec{K} \cdot \vec{r})}$$

The \vec{r} integration is straightforward, giving

$$H'_{01} = -\frac{32\pi e^2 \alpha^4}{L^3 \sqrt{2}} \left[\frac{9}{4}\alpha^2 + K^2 \right]^{-3}$$

The differential cross section is

$$\frac{d\sigma}{d\Omega} = \frac{128M^2 e^4 \alpha^8}{\hbar^4} \left(\frac{9}{4}\alpha^2 + K^2 \right)^{-6}$$

and the total cross section is

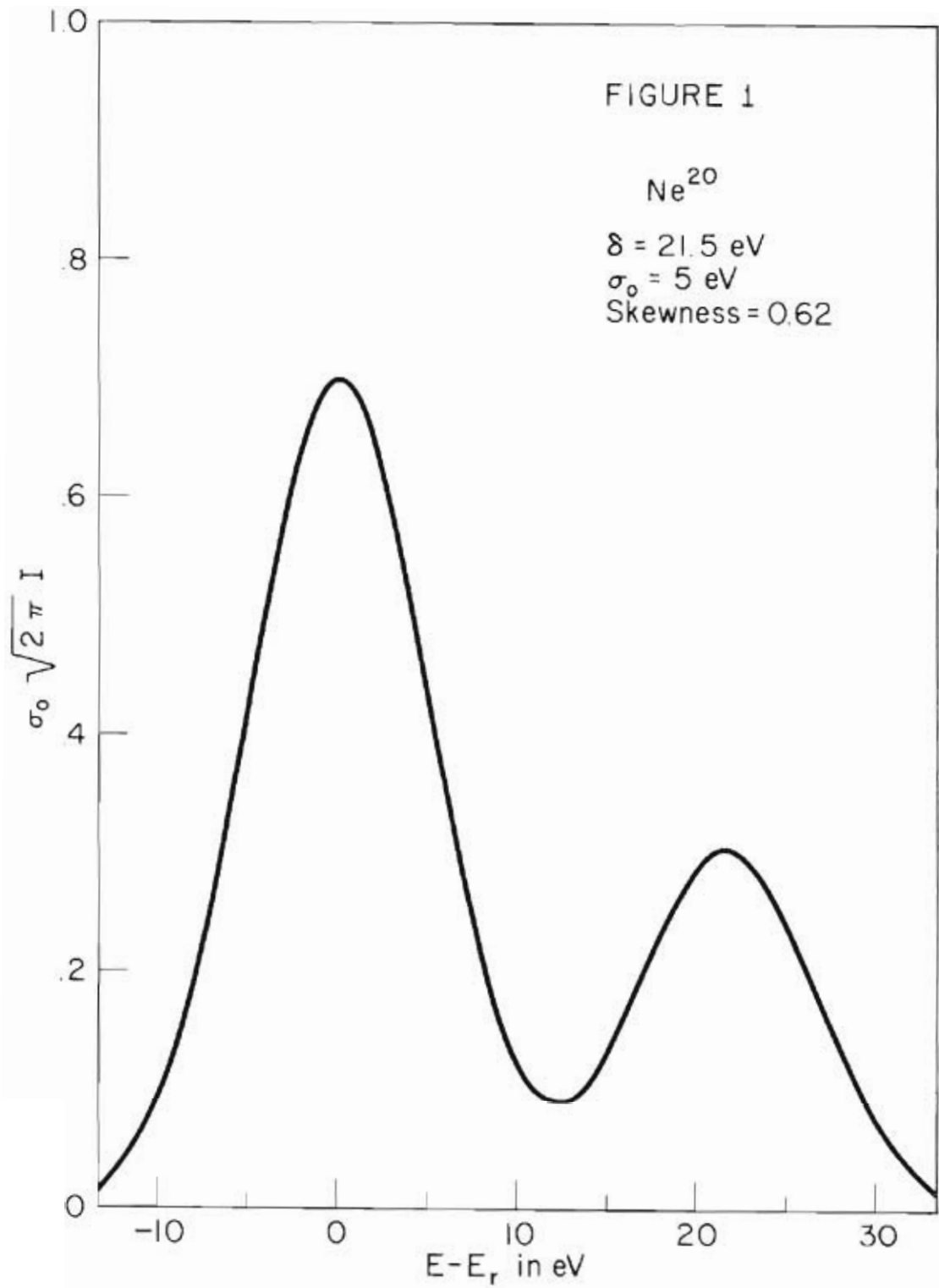
$$\sigma = \int_{\vec{k}_1} d\Omega \frac{d\sigma}{d\Omega}$$

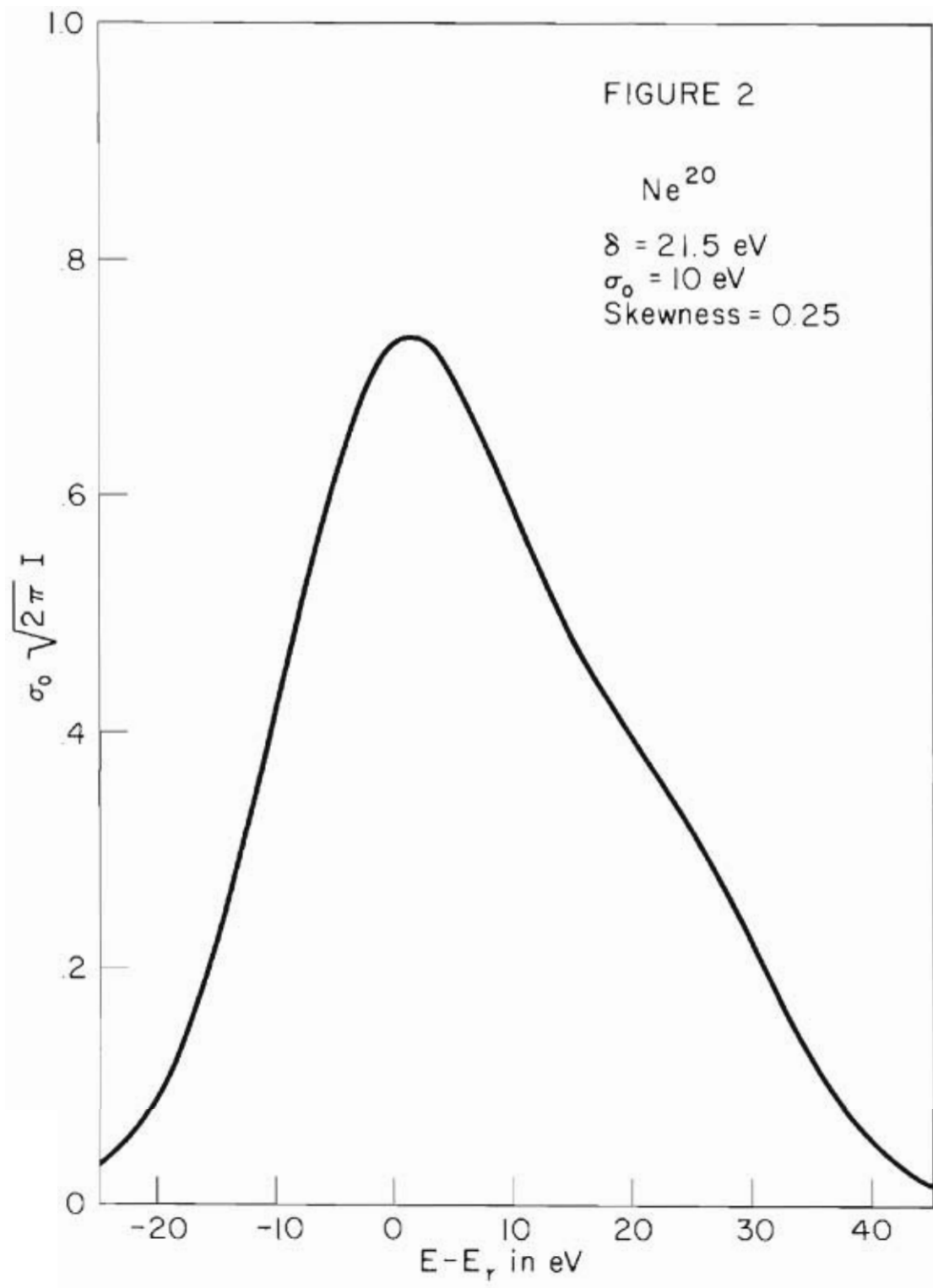
Transforming from an integration over directions of \vec{k}_1 to directions of \vec{K} , we get

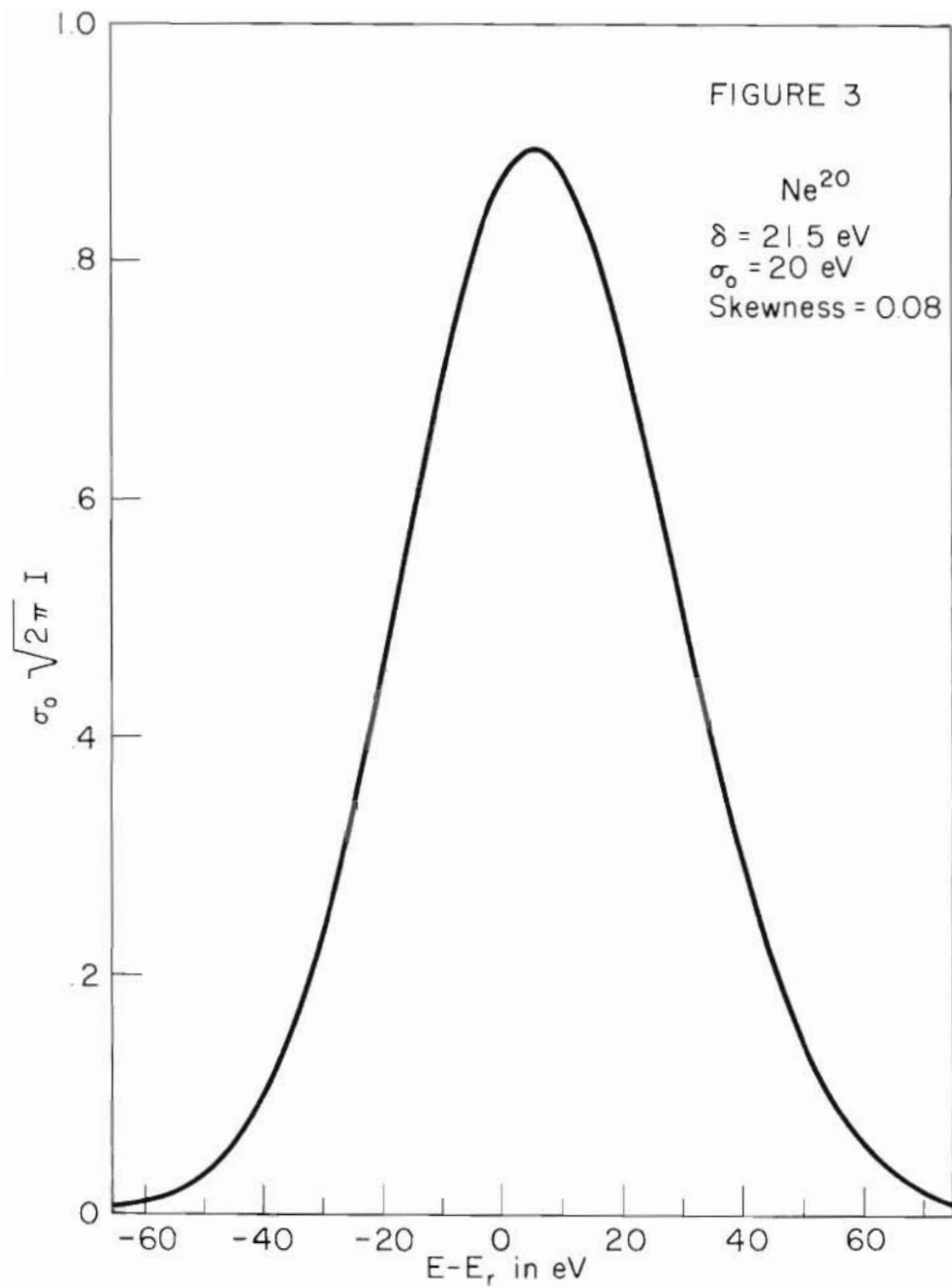
$$\begin{aligned} \sigma &= \frac{256\pi M^2 e^4 \alpha^8}{\hbar^2} \int_{\vec{k}_0 - \vec{k}_1}^{\vec{k}_0 + \vec{k}_1} d\vec{K} \frac{K}{k_0 k_1} \left(\frac{9}{4}\alpha^2 + K^2 \right)^{-6} \\ &\approx \frac{128\pi M^2 e^4 \alpha^8}{5k_0^2 \hbar^4} \left(\frac{9}{4}\alpha^2 + (k_0 - k_1)^2 \right)^{-5} \end{aligned}$$

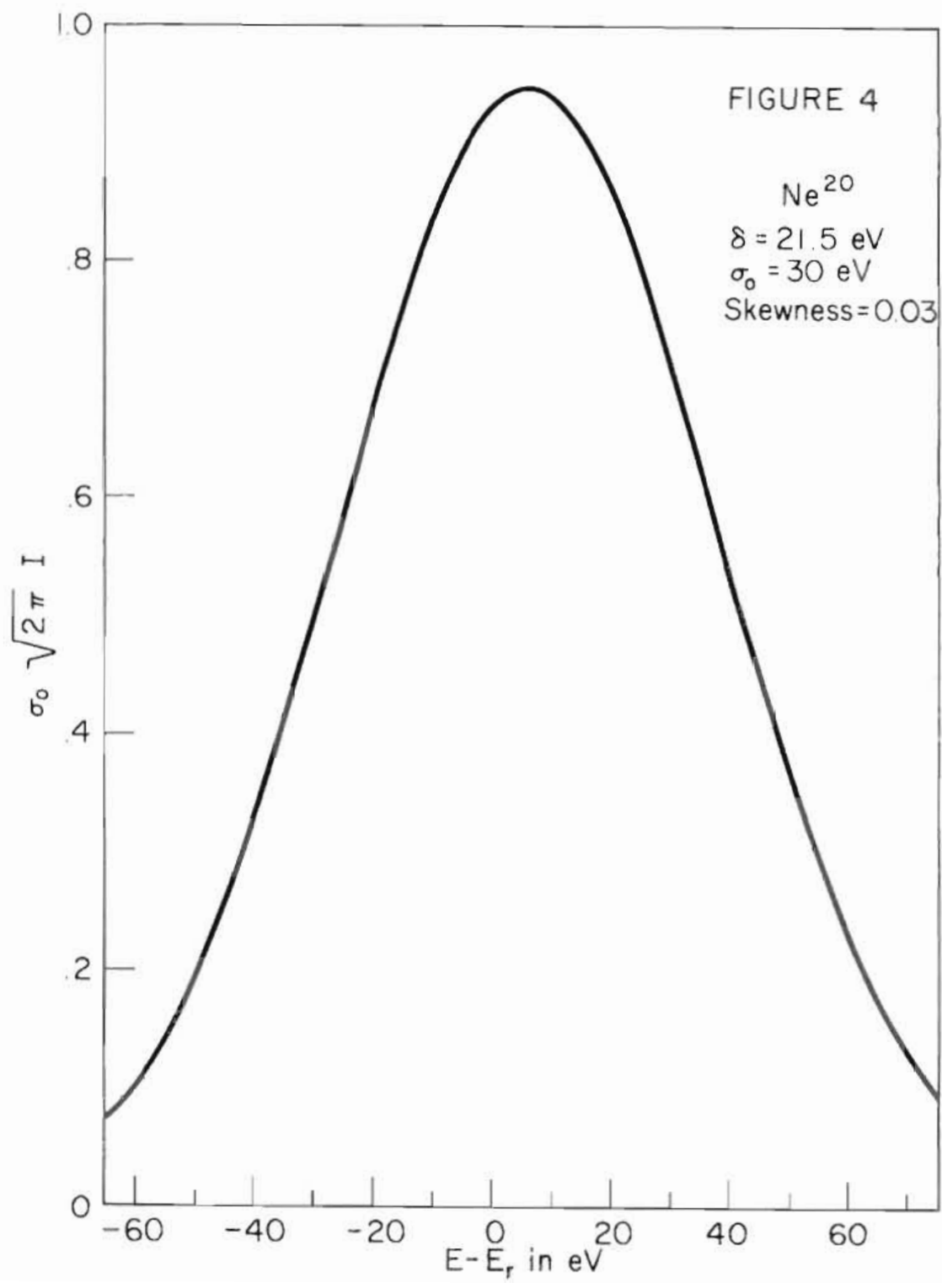
for $k_0 \approx k_1$, and $(k_0 + k_1)^2 \gg (k_0 - k_1)^2, \alpha^2$.

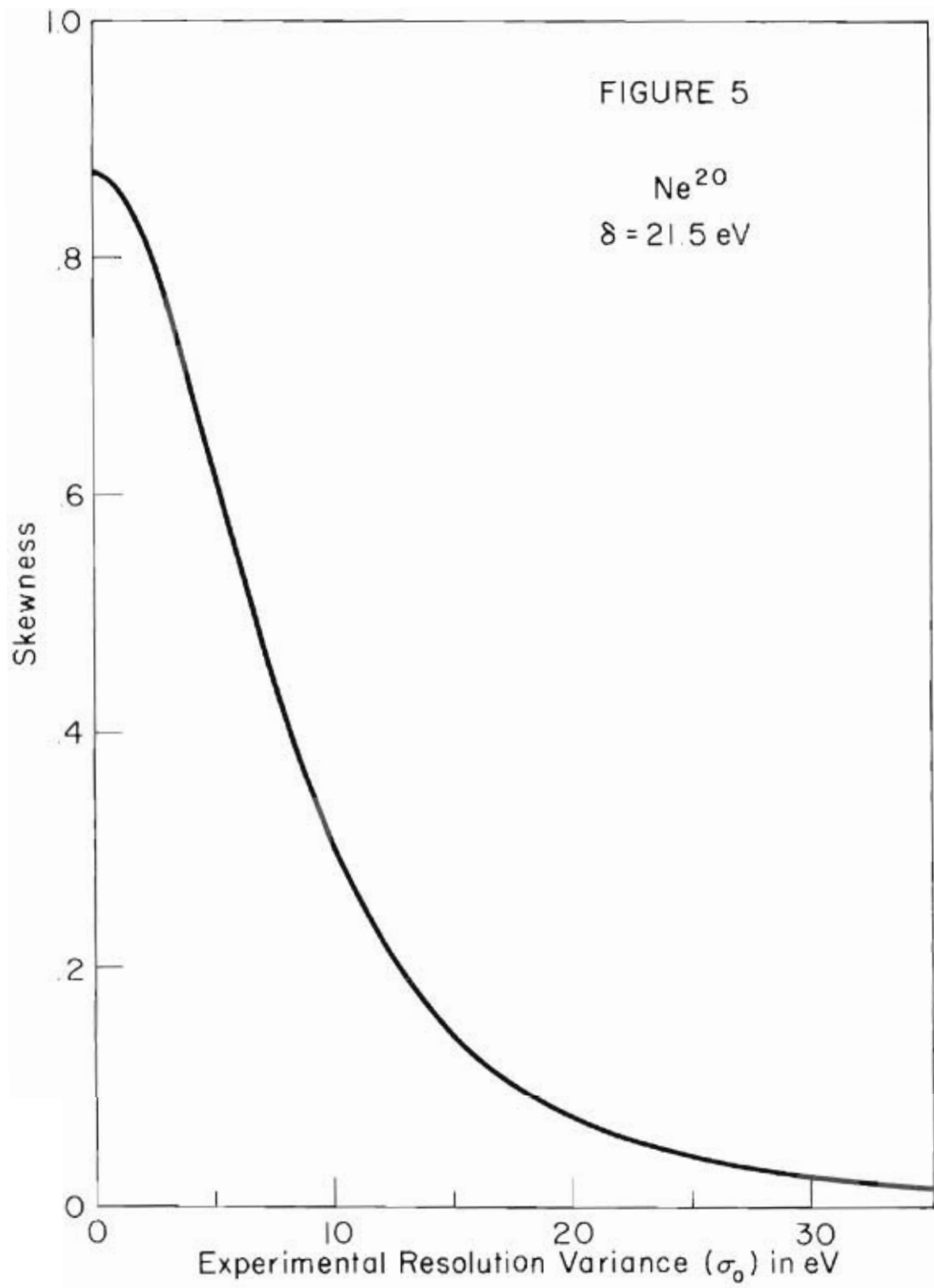
$$\sigma = \frac{(128)(1024)\pi}{5k_0^2} \left(\frac{M}{m} \right)^2 \left(\frac{\delta}{\text{Ryd}} \right)^4 \left\{ 9 \frac{\delta}{\text{Ryd}} + a_0^2 k_0^2 \left(\frac{\delta}{E} \right)^2 \right\}^{-5}$$











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