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OPTIMIZED AVERAGE EXCITED STATE OF ATOMS, INTERMEDIATE - ENERGY SCATTERING

by

ARTHUR BENJAMIN WEGLEIN

A dissertation submitted to the Graduate Faculty in Physics in partial fulfillment of the requirements for the degree of Doctor of Philosophy, The City University of New York.

1975

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Abstract

OPTIMIZED AVERAGE EXCITED STATE OF ATOMS,

INTERMEDIATE - ENERGY SCATTERING

by

Arthur Benjamin Weglein

Adviser: Professor Marvin H. Mittleman

The optimization of the average excited state of an atom (via a Kohn variational principle) is investigated. The resulting non-linear coupled integro-differential equations for the optimized excited state and the elastic and inelastic scattering coefficients are studied with two purposes in mind: (1) to extract electron-atom scattering information from this optimized two state model and (2) to attempt to assign some physical reality to the optimized excited state of an atom.

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Fig.3. v versus R.

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Fig.5. Q_0^{00} versus incident energy.

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Chapter One: Introduction

A technique used to calculate scattering amplitudes of projectiles off targets with structure is to choose a finite basis set in which to expand the total wave function and then to optimize the choice using a variational principle. If target eigenstates are chosen as a basis and the coefficients (which are functions of the projectiles coordinates) are optimized by the Kohn principle this leads to the usual close coupling equations[1].

This program has been widely applied[2,3] in scattering problems often yielding reliable amplitudes whenever a small number of channels dominate the particular process. The expansion basis, however, need not consist of target eigenstates. In fact they may not correspond to any physical state, and, among others, the pseudostate expansions[4,5,6] and effective channel methods[7] have been considered.

We are thereby naturally lead to the idea of choosing average inelastic channels. The concept of prechoosing an average inelastic channel has also been applied, in the context of an optical potential expansion[8] (at high energies), yielding rather good results for e-He scattering.

At intermediate energies (50-500 e.V.), where neither high nor low energy expansion techniques are expected to work, it seems unlikely that scattering will be easily describable by a systematic expansion technique where we prechoose a finite basis set.

The next step in the growth (and exploitation) of the average inelastic channel(s) concept was to optimize the choice of basis set[9]. That is, rather than prechoosing the basis set, we ask how we should make the best choice under certain criteria. The choice of criteria for optimizing the basis is in itself deserving of serious attention.

The program of optimizing a single excited state has been considered[9]. The criteria chosen was a Kohn-type of variational principle to optimize the average inelastic channel; although an alternate method of optimizing the optical potential operator was also outlined[9].

The former variational principle method, carried out on a trial wave function of the form:

$$\psi_t^{\pm}(\vec{r}, \vec{x}) = \varphi_0(\vec{x}) F^{\pm}(\vec{r}) + \omega(\vec{x}) G^{\pm}(\vec{r}) \quad (1.1)$$

where φ_0 = the target ground state, assumed known,

F = the elastic scattering coefficient,

ω = the average excited state

G = the coefficient describing inelastic scattering into the average inelastic channel,

leads to a set of three <u>non-linear</u> coupled integro-differential equations for the functions F, G and ω[9].

To avoid the non-linear problems involved in the trial function (1.1) an alternate trial function[(10)] was considered which incorporated features of

both low and high energy collisions:

$$\Psi(\vec{r},\vec{X}) = \gamma_0(\vec{X})\,F(\vec{r}) + \varphi_t(\vec{r},\vec{X})\,\omega(\vec{r}) + \chi(\vec{X})\,\gamma_t(\vec{r},\vec{X}) \tag{1.2}$$

where γ_0, φ_t and γ_t are assumed known (prechosen) while F, ω and χ are to be obtained optimally from a set of coupled equations.

In (1.2):

γ_0 = the target ground state

φ_t = the adiabatic component of Ψ

γ_t = the impulse component of Ψ.

The basis functions are chosen and the relative importance of the various terms was decided optimally by a set of linear coupled differential equations.

Although the above scheme avoids the non-linearity and could be a valuable calculational tool at intermediate energies it does avoid the optimized average inelastic channel concept.

It seems, however, that if we want to deal with at least a single non-prechosen average excited state within the Kohn principle, a general feature of the technique will be the non-linearity.

The purpose of this paper is to further explore and use the concept of a single optimized (non-prechosen) average excited state determined via a Kohn principle. There are two basic and related reasons to justify this investigation of the optimized average excited state. They are:

(1) To use this single optimized average excited state (OAES) as a calculational tool for evaluating scattering amplitudes. The optimization, in some sense insures, (within the two state approximation), that no prechosen state could better average the effect of the inelastic channels on the elastic scattering. (See Chapter Five).

(2) To attempt to assign some physical reality to such an optimized average excited state by considering what if any defining characteristics (e.g. its width and lifetime) we could associate with such a state. It could then be possible (e.g. depending on whether the lifetime of the state is small compared to its energy) to consider the OAES as a collective excited state of the atom. Under these circumstances the OAES could be interpreted as a state excited by the incident electron. This electron then escapes with some range of lowered energy (the incident energy minus the excitation energy of the OAES) and the OAES decays into eigenstates of the target.

We will also use the above mentioned scattering information to see if any structure appears in the scattering as a function of energy that could be attributed to a resonance type of behavior on the part of the projectile and in turn a collective excited mode of the atom.

An essential ingredient in both of these procedures is an approximation for the optimized excited state.

Chapter Two will present a discussion of the type of variational principle needed in (1.1) as well as the derivation of the coupled equations for F, G and ω.

In Chapter Three we present an analysis of the relationship of the parameter found in the ω (average excited state) equation and the ω equation itself. Chapter Four deals with an approximation scheme, valid for heavy atoms, for the average excited state. Also derived here are a practical set of criteria to determine the validity of the approximation for any particular atom. In Chapter Five, the average excited state, as approximated in Chapter Four, is used in the problem of electron-atom scattering. In particular, we are interested in this chapter, in the effect of the optimized average excited state on the process of elastic scattering. We analyze the eikonal approximation for the coupled equations of the coefficients (F and G) of the elastic and inelastic channels. We also present and investigate here the angular momentum decomposed F and G equations.

In Chapter Six, we use the theory of the previous several chapters in the specific case of electron-Argon scattering.

We show in this chapter that the criteria established in Chapter Four for the average excited state of an atom are satisfied in the case of Argon. Then having justified the approximate average excited state in this case, we use it in the angular momentum decomposed F and G equations to evaluate both elastic scattering and inelastic scattering into the average inelastic channel. We chose the latter method of Chapter Five because of the short range nature of the coupling potential (whose effect on elastic scattering we wish to establish). We also discuss in this chapter the width of our approximate OAES and suggest

how the effect of such a state could be detected experimentally.

Recent successes in intermediate energy scattering techniques[11] (e.g. the Eikonal-Born series) has changed the relative weight we should give to the two above mentioned justifications. It seems now that less of an emphasis on the search for an optimized average excited state for the sake of its use as an intermediate energy scattering technique is justified. Correspondingly, more weight should then be applied to the very active area of the reality of the optimized excited state and its possible interpretation as a collective mode.

These recent scattering techniques, however, were developed after we initiated this investigation and the weights we originally attributed to these factors would now be somewhat different.

Chapter One

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Chapter Two

(I) The Variational Principle, (II) Derivation of the Coupled Equation for F, G and ω . (III) Appendix on Lagrange Multipliers

(I) The Variational Principle:

As mentioned in Chapter 1, there are various criteria we could use to optimize the choice of ω . We choose here the Kohn formalism.

In this section, we investigate the Kohn principle for scattering off targets with internal degrees of freedom. We then proceed to see how the principle applies specifically to a trial function of the form (1.1).

Let H be the hamiltonian of the system: $H = H_T + T + V$ where H_T is the target hamiltonian, T is the kinetic energy operator of the projectile and V is the interaction potential energy of the projectile and the target.

Consider the integral:

$$\mathcal{A} = \int \psi_{k_f}^{(-)\times} (E - H) \psi_{k_i}^{(+)} d\tau$$

$\psi_{k_i}^{(+)}$ and $\psi_{k_f}^{(-)\times}$ are trial functions for a system of projectile (electron) and neutral atom (+ and − denote the usual outgoing and incoming wave boundary conditions, respectively). At the high energies to be considered the Pauli principle between the incident and target electrons lead to small corrections to the elastic scattering[1] and can consequently be neglected.

We define: (using Hartree's Atomic Units)

$\varphi_n =$ the target eigenfunctions where,

$$H_T \varphi_n = W_n \varphi_n$$

$\varphi_0 =$ the target ground state

$E = \frac{p^2}{2} + W_0 =$ the total energy of the target projectile system

$\frac{p^2}{2} =$ the incident electron's energy

$W_0 =$ the ground state of the target

$d\tau =$ the differential volume in the target and projectile coordinate system

$\vec{r} =$ position vector of the projectile

$\vec{X} = (\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_Z)$ is the position vector of the Z atomic electrons.

$\mathcal{L}$ would vanish identically if $\psi_{k_i}^{(+)}$ and $\psi_{k_i}^{(-)}$ were the exact eigenfunctions of H for eigenvalue E.

Expand these trial functions using as a basis set the target eigenfunctions :

$$\psi_{k_i}^{(+)} = \sum_n F_{n k_i}^{(+)}(\vec{r})\, \varphi_n(\vec{X}) \tag{2.1}$$

$$\psi_{k_f}^{(-)} = \sum_n F_{n,k_f}^{(-)}(\vec{r})\, \varphi_n(\vec{X}) \tag{2.2}$$

where the $F_n^{(\pm)}$ are the coefficients of the φ_n .

Asymptotically we have:

$$\psi_{k_i}^{(+)} \simeq \varphi_0 e^{i\vec{k}_i \cdot \vec{r}} + \sum_{n=0}^{\infty} \frac{f_n^{(+)}(\vec{k}_i \to \vec{k}_n) e^{i k_n r}}{r} \varphi_n \tag{2.3}$$

$$\psi_{k_f}^{(-)} \cong \varphi_0 e^{i\vec{k}_f\cdot\vec{r}} + \sum_{n=0}^{\infty} \frac{f_n^{(-)}(\vec{k}_f \to \vec{k}_n)}{r} e^{-ik_n r} \varphi_n \quad (2.4)$$

In terms of the coefficients $F_n^{(\pm)}$ the asymptotic conditions are:

$$F_{n,k_i}^{(+)} \cong \delta_{no} e^{i\vec{k}_i\cdot\vec{r}} + \frac{f_n^{(+)} e^{ik_n r}}{r} \quad (2.5)$$

$$F_{n,k_f}^{(-)} \cong \delta_{no} e^{i\vec{k}_f\cdot\vec{r}} + \frac{f_n^{(-)} e^{-ik_n r}}{r} \quad (2.6)$$

where $\vec{k}_n = k_n \hat{r}$ and $\frac{k_n^2}{2} + W_n = E$.

Consider a general variation of $\mathcal{A}$ in which:

$$\psi_{k_f\ \text{trial}}^{(-)\times} = \psi_{k_f\ \text{exact}}^{(-)\times} + \delta\psi_{k_f}^{(-)\times}$$

and

$$\psi_{k_i\ \text{trial}}^{(+)} = \psi_{k_i\ \text{exact}}^{(+)} + \delta\psi_{k_i}^{(+)}$$

By a general variation we mean that φ_n (for $n \neq 0$), $F_n^{\pm}$, $(F_n^{\pm})^{\times}$ are all allowed to vary, subject only to the restrictions on the asymptotic forms of $F_n^{\pm}$ (given by (2.5) and (2.6)) and φ_n (going to zero fast enough for large $\vec{r}$ to insure H_T is hermetian).

φ_0 the ground state wave function of the target, is assumed to be known exactly.

We can now write $\mathcal{A}_t$ as:

$$\mathcal{A}_t = \int \left(\psi^{(-)\times}_{k_f\,\text{exact}} + \delta\psi^{(-)\times}_{k_f} \right) (E-H) \left(\psi^{(+)}_{k_i\,\text{exact}} + \delta\psi^{(+)}_{k_i} \right)$$

or

$$\mathcal{A}_t = \int \psi^{(-)\times}_{k_f\,\text{exact}} (E-H)\, \delta\psi^{(+)}_{k_i}\, d\tau + O(\delta\psi^2) \tag{2.7}$$

or

$$\mathcal{A}_t = \int \psi^{(-)}_{k_f\,\text{trial}} (E-H)\, \delta\psi^{(+)}_{k_i}\, d\tau + O(\delta\psi^2) \tag{2.8}$$

where $(E-H)\,\psi^{(+)}_{k_i\,\text{exact}}$ equals zero has been used in deriving (2.7).

Therefore, to first order in the variation $\delta\psi$ we have: $\delta\mathcal{A}$

$$\equiv \mathcal{A}_t - \mathcal{A}_{\text{exact}} = \mathcal{A}_t = \int \psi^{(-)\times}_{k_f\,\text{trial}} (E-H)\, \delta\psi_{k_i}\, d\tau \tag{2.9}$$

In (2.7) let us write

$$(E-\overrightarrow{H}) = E-\overrightarrow{H_T} - \overrightarrow{T} - V = E - \overleftarrow{H_T} - \overleftarrow{T} - V + (\overleftarrow{T} - \overrightarrow{T}) \tag{2.10}$$

where ($\longrightarrow$ or $\longleftarrow$) means that the operator acts to the right or left respectively. H_T and V are hermetian whereas T is not, giving rise to the $\overleftarrow{T} - \overrightarrow{T}$ term in (2.10).

Using (2.7), (2.9) and (2.10) we have:

$$\delta\mathcal{A} = \int \psi^{(-)\times}_{k_f} \left(\overleftarrow{T} - \overrightarrow{T} \right) \delta\psi^{(+)}_{k_i}\, d\tau$$

$$= \frac{1}{2} \int d\vec{X} \int d\vec{r}\; \psi^{(-)\times}_{k_f} \left(-\overleftarrow{\nabla^2_{\vec{r}}} + \overrightarrow{\nabla^2_{\vec{r}}} \right) \delta\psi^{(+)}_{k_i}$$

Making use of Gauss's theorem we then have:

$$\delta\mathcal{L} = \int d\vec{X} \int d\Omega_{\hat{r}} \lim_{r\to\infty} r^2 \left[\psi_{k_f}^{(-)*} \frac{\partial}{\partial r} (\delta\psi_{k_i}^{(+)}) - \delta\psi_{k_i}^{(+)} \frac{\partial}{\partial r} (\psi_{k_f}^{(-)*}) \right] \tag{2.11}$$

where $d\Omega_{\hat{r}}$ is the differential solid angle in the projectiles coordinate space.

Now utilize the expansions (2.1) and (2.2) to write:

$$\delta\psi_{k_i}^{(+)} = \sum_{n=0}^{\infty} \left(\delta F_{n\,k_i}^{(+)} \varphi_n + F_{n\,k_i}^{(+)} \delta\varphi_n \right) \tag{2.12}$$

Equation (2.12) together with the asymptotic forms (2.3) and (2.4) leads to the asymptotic form of $\delta\psi_{k_i}^{(+)}$:

$$\delta\psi_{k_i}^{(+)} \cong \sum_{n=0}^{\infty} \frac{e^{ik_n r}}{r} \delta f_n^{(+)} \varphi_n + \sum_{n=1}^{\infty} \frac{e^{ik_n r}}{r} f_n^{(+)} \delta\varphi_n \tag{2.13}$$

In (2.13) we have made use of the fact that $\delta\varphi_0 = 0$. We also have a similar expression for $\delta\psi_{k_f}^{(-)*}$.

Substitution of these asymptotic forms in the $\delta\mathcal{L}$ of (2.11) we find:

$$\delta\mathcal{A} = \int d\vec{X} \lim_{r\to\infty} \int r^2 d\Omega_{\hat{r}} \Big[\Big\{ e^{-i\vec{k}_f\cdot\vec{r}}\varphi_0^{\times} + \sum_{n=0}^{\infty} \frac{e^{ik_n r}}{r} \varphi_n^{\times} f_n^{(-)\times} \Big\} \Big\{ \sum_{n'=0}^{\infty} \frac{d}{dr}\Big(\frac{e^{ik_{n'}r}}{r}\Big) \Big[\delta f_{n'}^{(+)}(\vec{k}_i\to\vec{k}_{n'})\varphi_{n'} + f_{n'}^{(+)}(\vec{k}_i\to\vec{k}_{n'})\delta\varphi_{n'} \Big] \Big\}$$
$$- \Big\{ \sum_{n=0}^{\infty} \frac{e^{ik_n r}}{r} \Big[\delta f_n^{(+)}(\vec{k}_i\to\vec{k}_n)\varphi_n + f_n^{(+)}\delta\varphi_n \Big] \Big\}$$
$$\Big\{ -i\vec{k}_f\cdot\hat{r}\, e^{-i\vec{k}_f\cdot\vec{r}}\varphi_0^{\times} + \sum_{n'=0}^{\infty} \frac{d}{dr}\Big(\frac{e^{ik_{n'}r}}{r}\Big)\varphi_{n'}^{\times} f_{n'}^{(-)\times} \Big\} \Big] \qquad (2.14)$$

The exact target eigenstates satisfy the orthonormality condition:

$$(\varphi_n, \varphi_{n'}) = \delta_{nn'} \qquad (2.15)$$

If we ask that the trial target states also satisfy this condition we have:

$$(\varphi_{n_t}, \varphi_{n'_t}) = \delta_{nn'} \qquad (2.15a)$$

These last two relations lead to (keeping terms of O $(\delta\varphi_n)$):

$$(\varphi_{n_t}, \delta\varphi_{n'}) = -(\delta\varphi_n, \varphi_{n'_t}) \tag{2.15b}$$

Using the fact that $\delta\varphi_0$ equals zero, (2.15b) becomes for $n = 0$:

$$(\varphi_0, \delta\varphi_n) = 0 \tag{2.16}$$

for all n.

Integrating over $\vec{X}$ in $\delta\mathcal{A}$ (2.14) using (2.15a) and (2.16) and the performing the angular integration we find:

$$\delta\mathcal{A} = -4\pi\, \delta f_0^{(+)}(\vec{k}_i \to \vec{k}_f) \tag{2.17}$$

The result (2.17) is the Kohn principle. This principle states that the wave function which extremizes $\delta\mathcal{A} = \mathcal{A}_t$ will in turn extremize the difference

$$f_0^{(+)}{}_{\text{trial}} - f_0^{(+)}{}_{\text{exact}}.$$

It also is a method to improve the evaluation of elastic scattering amplitudes found using trial wave functions. That is, the elastic scattering amplitude found using trial wave functions will be improved (as long as we can neglect) $O(\delta\psi^2)$ by adding I_t to $f_{0_t}^{(+)}$.

(II) Derivation of the Coupled Equations for F_1 G and ω

We now turn our attention to the problem of interest and consider the trial function (1. 1):

$$\psi_k^{\pm} = \varphi_0 F_k^{\pm} + \omega G_k^{\pm} \qquad (1.1),$$

where φ_0 is the ground state of the target and ω is the average excited state of the target.

Explicitly:

$$\psi_{k_i}^{(+)} = \varphi_0(\vec{x}) F_{k_i}^{(+)}(\vec{r}) + \omega(\vec{x}) G_{k_i}^{(+)}(\vec{r}) \qquad (2.18)$$

$$\psi_{k_f}^{(-)} = \varphi_0(x) F_{k_f}^{(-)}(\vec{r}) + \omega(\vec{x}) G_{k_f}^{(-)}(\vec{r}) \qquad (2.19)$$

and where $F_{k_i}^{(+)}$, $F_{k_f}^{(-)}$, $G_{k_i}^{(+)}$, $G_{k_f}^{(-)}$ and ω will be determined variationally.

Consider the integral,

$$\mathcal{A} = \mathcal{A}_1 + \mathcal{A}_1^{*} + \mathcal{A}_2 + \mathcal{A}_2^{*} \qquad (2.20)$$

where $$\mathcal{A}_1 = \int \psi_{k_f}^{(-)*} (E - H) \psi_{k_i}^{(+)} d\tau$$

and $$\mathcal{A}_2 = \int \psi_{k_i}^{(+)*} (E - H) \psi_{k_f}^{(-)} d\tau$$

The reasons for this choice of $\mathcal{A}$ will be discussed below.

From section (I) of this chapter it follows that for a general variation:

$$\delta \mathcal{L}_1 = -4\pi \delta f_0^{(+)}$$

$$\delta \mathcal{L}_1^{\times} = -4\pi \delta f_0^{(+)\times}$$

$$\delta \mathcal{L}_2 = -4\pi \delta f_0^{(-)}$$

$$\delta \mathcal{L}_2^{\times} = -4\pi \delta f_0^{(-)\times}$$

and therefore: $$\delta \mathcal{L} = -4\pi \left[2\, \text{Real} \left(\delta f_0^{(+)} + \delta f_0^{(-)} \right) \right]$$

However, now rather than the general variation, we will vary independently $F^{(+)}$, $F^{(-)}$, $F^{(+)\times}$, $F^{(-)\times}$, $G^{(+)}$, $G^{(-)}$, $G^{(+)\times}$, $G^{(-)\times}$, ω and $\omega^{\times}$. The results of these independent variations are:

$$\delta \mathcal{L}_{F^+} = -4\pi \delta f_0^{(+)} \tag{2.21}$$

$$\delta \mathcal{L}_{F^{+\times}} = -4\pi \delta f_0^{(+)\times} \tag{2.22}$$

$$\delta \mathcal{L}_{F^{(-)}} = -4\pi \delta f_0^{(-)} \tag{2.23}$$

$$\delta \mathcal{L}_{F^{(-)\times}} = -4\pi \delta f_0^{(-)\times} \tag{2.24}$$

where the right hand sides of equations (2.21), (2.22), (2.23), (2.24) come from the non zero contributions due to $(\delta \mathcal{L}_1)_{F^+}$, $(\delta \mathcal{L}_1^{\times})_{F^{+\times}}$, $(\delta \mathcal{L}_2)_{F^{(-)}}$ and $(\delta \mathcal{L}_2^{\times})_{F^{(-)\times}}$ respectively.

The other independent variations lead to:

$$\delta \mathcal{L}_{G^{(-)}} = 0 \tag{2.25}$$

$$\delta \mathcal{L}_{G^{(-)X}} = 0 \tag{2.26}$$

$$\delta \mathcal{L}_{G^{(+)}} = 0 \tag{2.27}$$

$$\delta \mathcal{L}_{G^{(+)X}} = 0 \tag{2.28}$$

$$\delta \mathcal{L}_{\omega} = 0 \tag{2.29}$$

$$\delta \mathcal{L}_{\omega X} = 0 \tag{2.30}$$

The reason for the asymmetric look (between the F and G's) in the above variational principles is that we are scattering off the ground state of the target. That is, the F and G's have different asymptotic forms, due to the fact that F is the coefficient of the target ground state and consequently has an incident plane wave component (absent in G).

This difference causes variations with respect to $F^{\pm}$ or $(F^{\pm *})$, (unlike $G^{\pm}$ and $G^{\pm *}$) to have non-zero contributions whenever these variations occur to the right of E - H in an integral. If we were scattering off an excited state of the target, the right hand sides of (2.21) - (2.24) would still correspond to an elastic scattering amplitude, (where in this elastic scattering amplitude the initial and final states of the target are the original excited target state).

These independent variations lead to coupled integro-differential equations for $F^{\pm}$, $G^{\pm}$ and ω .

Remarks on the Choice of $\mathcal{L}$

a) Including $\mathcal{L}_1^*$ with $\mathcal{L}_1$ leads to equations for ω^*, $F^{(+)*}$, $F^{(-)*}$, $G^{(+)*}$ and $G^{(-)*}$ which are the complex conjugates of the equations for ω, $F^{(+)}$, $F^{(-)}$, $G^{(+)}$ and $G^{(-)}$ respectively. (E.g. if $\mathcal{L}_1^*$ were left out the ω and ω^* equations would not be complex conjugates.) Also with $\mathcal{L}_1^*$ included $F_k^{(-)}$ and $G_k^{(-)}$ satisfy the same equation as $F_k^{(+)}$ and $G_k^{(+)}$ respectively (as they should).

b) Including $\mathcal{L}_2 + \mathcal{L}_2^*$ gives an integral $\mathcal{L}$ with asymmetric dependence on $+$ and $-$ states, i.e. $\mathcal{L}(\psi_{k_i}^{(+)}, \psi_{k_f}^{(-)}) = \mathcal{L}(\psi_{k_f}^{(-)}, \psi_{k_i}^{(+)})$. Physically ω should be derived from a variational principle symmetrically dependent on $+$ and $-$ states.

However, using (2.20) for $\mathcal{L}$ is essentially done for mathematical completeness and its clear aesthetic and physical appeal, since the inclusion of $\mathcal{L}_2 + \mathcal{L}_2^*$ leads to no new contributions beyond $\mathcal{L}_1 + \mathcal{L}_1^*$ to the equations for F , G and ω .

c) Because of Remark (b) we will henceforth deal with the mathematically equivalent (for the variations of interest to us) reduced $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_1^*$. With this new $\mathcal{L}$ the variations which produce the $F^{(+)}$, $G^{(+)}$ and ω equations respectively are:

$$\delta \mathcal{L}_{F^{(-)x}} = 0 \tag{2.31}$$

$$\delta \mathcal{L}_{G^{(-)x}} = 0 \tag{2.32}$$

$$\delta \mathcal{L}\, \omega^{x} = 0 \tag{2.33}$$

for $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_1^{x}$. Note the difference between equations (2.31) and (2.24). We have (2.31) because in $\mathcal{L}_1 + \mathcal{L}_1^{x}$, $F^{(-)x}$ never appears on the right hand side of E - H.

In the previous $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_1^{x} + \mathcal{L}_2 + \mathcal{L}_2^{x}$, $\mathcal{L}_2^{x}$ contributes a term $F^{(-)x}$ appearing on the right of E - H. This $\mathcal{L}_2^{x}$ in (2.20) leads to $\delta f_0^{(-)x}$ on the right hand side of (2.24).

Writing $\mathcal{L}_1 + \mathcal{L}_1^{x}$ in detail:

$$\begin{aligned}
\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_1^{x} = \\
&\int F_k^{(-)x} \underbrace{(E - W_0}_{P^2/2} - T - VS)\, F_k^{(+)}\, d\vec{r} \\
&+ \int \varphi_0^{x} F_k^{(-)x} (E - H_T - T - V)\, \omega\, G^{(+)}\, d\vec{r}\, d\vec{x} \\
&+ \int \omega^{x}\, G^{(-)x} (E - H_T - T - V)\, \varphi_0\, F^{+}\, d\vec{r}\, d\vec{x} \\
&+ \int \omega^{x}\, G^{(-)x} (E - H_T - T - V)\, \omega\, G^{+}\, d\vec{r}\, d\vec{x}
\end{aligned}$$

$$+ \quad \text{(Complex Conjugate)} \tag{2.34}$$

where $VS = (\varphi_0 V \varphi_0)$.

$\mathcal{A}$ will be varied with respect to $F^{(-)*}$, $G^{(-)*}$ and ω^* to give the three coupled equations for $F^{(+)}$, $G^{(+)}$ and ω.

Note that the T operator (the projectile's kinetic energy operator) can now go in either direction. The reason is that the contribution from this change of direction is either zero or what we set equal to zero in asking for stationary $f_0^{\pm}$ or $(f_0^{\pm})^*$ values. (I.e. $\delta f_0^{\pm}$ or $\delta(f_0^{\pm})^*$ are set equal to zero). The former situation occurs when we take $\delta G^{\pm}$, $(\delta G^{\pm})^*$, $\delta\omega$ or $\delta\omega^*$ as the variation and the latter when we take $\delta F^{\pm}$ or $(\delta F^{\pm})^*$ from the right to the left of E - H. If we vary $F^{\pm}$ or $(F^{\pm})^*$ in an integral in which this $F^{\pm}$ or $(F^{\pm})^*$ occurs on the left of E - H then we also have the former situation.

We want ω to be an average excited state of the target. We therefore impose the condition on ω of orthogonality to the single unexcited state to keep ω exclusively in the part of Hilbert space spanned by the excited states of the target. This will also insure that F contains all of the elastic scattering. For these two reasons we impose the constraint on :

$$(\varphi_0, \omega) = 0 \tag{2.35}$$

It is permissible to include this constraint directly in these independent variations of $\delta\mathcal{V}_{FT\to}$ and $\delta\mathcal{U}_{G^{(-)*}}$. (A discussion is given below explaining why terms like (φ_0, ω) must be kept when varying with respect to ω^*).

Using (2.35) in (2.34):

$$\delta \mathcal{L}_{F^{(-)x}} = \int \delta F^{(-)x}(\vec{r}) \left\{ \left(\frac{p^2}{2} - T - VS \right) F^{+} - v G^{+} \right\} d\vec{r}$$

where the coupling potential v is introduced:

$$v(\vec{r}) = \left(\phi_0(x) V(r,x) w(x) \right)$$

Noting that $\delta F^{(-)x}$ is an arbitrary function (within the restriction that all the $F^{(-)}$ trial have the same asymptotic form (2.5)) we have using (2.31) and (2.35):

$$\left(\frac{p^2}{2} - T - VS \right) F^{+} = v G^{+} \tag{2.36}$$

Now taking $\delta \mathcal{L}_{G^{(-)x}}$ and arguing as in the case of $\delta \mathcal{L}_{F^{(-)x}}$ we find:

$$\left(\frac{p'^2}{2} - T - \bar{V} \right) G^{(+)} = \frac{v^x}{(w,w)} F^{(+)} \tag{2.37}$$

where $$\frac{p'^2}{2} = E - \frac{(w, H_T w)}{(w,w)} = E - \varepsilon$$

and $$\bar{V} = \frac{(w V w)}{(w,w)}.$$

(2.36) and (2.37) are similar to the usual two state close coupling equations.

Now to find the equation for the average excited state w by varying w^x.

$$\delta I_{\omega^*} = \int \delta\omega^* G^{(-)*}(E - H_T - T - V)\varphi_0 F^+ d\tau$$
$$+ \int \delta\omega^* G^{(-)*}(E - H_T - T - V)\omega G^+ d\tau$$
$$+ \int \varphi_0 F^{(-)}(E - H_T - T - V)\delta\omega^* G^{(+)*} d\tau$$
$$+ \int \omega G^{(-)}(E - H_T - T - V)\delta\omega^* G^{(+)*} d\tau$$

(2.38)

In the first and third integrals of (2.38) we are going to keep terms that the constraints on (φ_0, ω) and $(\varphi_0, \delta\omega)$ would cause to vanish. These terms could be considered as a part of (or as it turns out, (see below) all of) a Lagrange multiplier whose presence will insure the orthonormality of φ_0 and ω in the ω equation.

We could have added a term $\lambda(\omega, \varphi_0)$ to $\mathcal{L}$, where λ is a Lagrange multiplier, and λ would appear on the inhomogeneous side of the ω equation. We show in the appendix to this chapter that λ must be equal to zero to have ω orthogonal to φ_0. Therefore, the terms that are kept with (φ_0, ω) in (2.38) constitute the entire Lagrange multiplier needed to insure $(\varphi_0, \omega) = 0$ in the ω equation.

Using: (1) the equations for $F^{(+)}$, $F^{(-)}$, $G^{(+)}$ and $G^{(-)}$ (2) the notation $\langle\ \rangle =$ integrate over $\vec{r}$, $(\ \ ) =$ integrate over $\vec{x}$, (3) the requirement that $\delta\omega^*$ be an arbitrary variation (within the restriction that ω is normalizable) we have using (2.33) the equation for ω :

$$\{\langle G^{(-)} \times G^{(+)} \rangle + \langle G^{(+)} \times G^{(-)} \rangle\} (\varepsilon - H_T)\omega$$

$$-[\langle G^{(+)} \times V G^{(-)} \rangle + \langle G^{(-)} \times V G^{(+)} \rangle]\omega$$

$$+[\langle G^{(+)} \times \bar{V} G^{(-)} \rangle + \langle G^{(-)} \times \bar{V} G^{(+)} \rangle]\omega$$

$$+\frac{1}{(\omega, \omega)}[\langle G^{(-)} \times v \times F^{+} \rangle + \langle G^{(+)} \times v \times F^{-} \rangle]\omega$$

$$+[\langle G^{(-)} \times VS\, F^{(+)} \rangle + \langle G^{(+)} \times VS\, F^{(-)} \rangle]\phi_0$$

$$-[\langle G^{(-)} \times V F^{(+)} \rangle + \langle G^{(+)} \times V F^{(-)} \rangle]\phi_0$$

$$+[\langle G^{(-)} \times v\, G^{(+)} \rangle + \langle G^{(+)} \times v\, G^{(-)} \rangle]\phi_0 = 0$$

(2.39)

Now define:

$$\varepsilon = \frac{(\omega H_T \omega)}{(\omega, \omega)} \tag{2.40}$$

$$N = \langle G^{(-)} \times G^{(+)} \rangle + \langle G^{(+)} \times G^{(-)} \rangle \tag{2.41}$$

$$\Omega(x) = \frac{1}{N}\{\langle G^{(+)} \times V G^{(-)} \rangle + \langle G^{(-)} \times V G^{(+)} \rangle\} \tag{2.42}$$

$$\Sigma(x) = \frac{1}{N}\{\langle G^{(-)} \times V F^{(+)} \rangle + \langle G^{(+)} \times V F^{(-)} \rangle\} \tag{2.43}$$

$$\varepsilon' = \varepsilon + \frac{1}{N}\left\{\langle G^{(+)} \times \bar{V} G^{(-)}\rangle + \langle G^{(-)} \times \bar{V} G^{(+)}\rangle + \frac{1}{(\omega,\omega)}\left[\langle G^{(-)} \times \bar{V} \times F^{(+)}\rangle + \langle G^{+} \times \bar{V} \times F^{(-)}\rangle\right]\right\} \quad (2.44)$$

$$\varepsilon' = \frac{(\omega, h\omega) + (\omega \Sigma \varphi_0)}{(\omega, \omega)} \quad (2.45)$$

$$h = H_T + \Omega \quad (2.46)$$

$$\Sigma' = \Sigma - (\varphi_0 \Sigma \varphi_0) \quad (2.47)$$

The ω equation with these definitions takes the form:

$$\left(\varepsilon + \frac{(\omega, \Omega\omega)}{(\omega,\omega)} + \frac{(\omega, \Sigma\varphi_0)}{(\omega,\omega)} - H_T - \Omega\right)\omega = \left[\Sigma - (\varphi_0 \Omega\omega) - (\varphi_0, \Sigma\varphi_0)\right]\varphi_0$$

or finally: $$(\varepsilon' - h)\omega = \left[\Sigma' - (\varphi_0, \Omega\omega)\right]\varphi_0 \quad (2.48)$$

which is the third of the coupled integro-differential equations with (2.36) and (2.37) for $F_1^{(+)}$ $G^{(+)}$ and ω .

(III) Appendix: The Lagrange Multipliers in the Variational Principle for ω .

If we take $\langle \varphi_0$ on both sides of equation (2.48) we find:

$$\mathcal{E}'(\varphi_0,\omega) - (\varphi_0, h\omega) = (\varphi_0 \Sigma' \varphi_0) - (\varphi_0 \Omega\omega)$$
$$(\mathcal{E}' - W_0)(\varphi_0,\omega) = 0$$

Therefore $(\varphi_0,\omega)=0$ if $\mathcal{E}' \neq W_0$ and (2.48) satisfies orthogonality. The inclusion of a Lagrange multiplier λ in,

$$\mathcal{L}' = \mathcal{L} + \lambda(\varphi_0,\omega) \tag{2.49}$$

would not change the $F^{(+)}$ and $G^{(+)}$ equations, but would appear in the ω equation:

$$(\mathcal{E}' - h)\omega = (\Sigma' - (\varphi_0,\Omega\omega) + \lambda)\varphi_0 \tag{2.50}$$

Now taking $\langle \varphi_0$ on both sides of (2.50) we find:

$$(\mathcal{E}' - W_0)(\varphi_0,\omega) = \lambda \tag{2.51}$$

Therefore (2.51) implies that if we want $(\varphi_0,\omega) \to 0$, λ must vanish.

If we use an additional Lagrange multiplier to insure the normalization of the average excited state as well as its orthogonality to the ground state we consider:

$$\mathcal{L}'' = \mathcal{L} + \lambda_1 (\omega, \varphi_0) + \lambda_2 (\omega, \omega) \tag{2.52}$$

$$\delta \mathcal{L}'' = \int \delta \omega^* \left[(\varepsilon' - h)\,\omega - \Sigma \varphi_0 + (\varphi_0 \Sigma \varphi_0)\varphi_0 + (\varphi_0 \Omega \omega)\varphi_0 \right] + \lambda_1 (\delta \omega^*, \varphi_0) + \lambda_2 (\delta \omega^*, \omega)$$

Now $\delta \mathcal{L}'' = 0$ (from (2.33) and the fact that we want ω^* to be varied such that (φ_0, ω) and (ω, ω) are stationary) gives:

$$(\varepsilon' + \lambda_2 - h)\,\omega = (\Sigma' - (\varphi_0 \Omega \omega) + \lambda_1)\,\varphi_0 \tag{2.53}$$

Taking $\langle \varphi_0 |$ on both sides of (2.53), assuming $\langle \varphi_0 | \varphi_0 \rangle = 1$ we have:

$$(\varepsilon' + \lambda_2 - W_0)\,(\varphi_0, \omega) = \lambda_1 \tag{2.54}$$

Taking $\langle \omega |$ on both sides of (2.53) leads to

$$\lambda_2 (\omega, \omega) = -(\omega, \varphi_0)\left[(\varphi_0 \Sigma \varphi_0) + (\varphi_0 \Omega \varphi_0) - \lambda_1 \right] \tag{2.55}$$

Equations (2.55) and (2.54) imply that if we want (ω, φ_0) to vanish, and retain a nonvanishing (ω, ω) then λ_1 and λ_2 must both equal zero.

We therefore choose λ_1 and λ_2 equal to zero in (2.53) and return to (2.48).

References for Chapter Two

1. Marvin H. Mittleman, Ann. Phys. 10 (268) 1960.

Chapter Three

(I) A Study of the Relationship between the Equation for ω and ε' .

(II) ε' and the Five Coupled Equations

It is the usual case that when a parameter appears in an equation for a state which is normalizable (bound): the equation itself determines the parameter. (E.g. the bound state eigenvalues of the Schroidinger equation are determined by the equation itself).

We are interested in this chapter in determining whether the equation for ω specifies its parameter ε' in a similar way.

As can be seen from (2.45) ε' is a complex functional of ω , $G^{\pm}$ and $F^{\pm}$. Note also that the ω equation is not an eigenvalue equation for ε'.

In the first section (Ia) we will examine the question of the specification of ε' in relation to the general ω equation. In sections (Ib, c, d) several special cases of the ω equation will also be analyzed. We will examine how each of these simplified models deals with the ω equation and the ε' determinacy question and then relate it to the general conclusion(s) of section (Ia). Section (Ie) will be a summary and overview of the ε' determinacy situation in relation to the equation.

In section (II) we take a different perspective on this situation and consider the relation of ε' to the five coupled equations for $F^{\pm}$, $G^{\pm}$ and ω . With this viewpoint the conclusion about ε''s determinacy is quite different from that of section (I). Comparing sections (I) and (II) gives us an insight into the nature of

the parameter found i n the equation for the OAES. In particular, the role played by the optimization (rather than prechoice) of the average excited state on the specification of its parameter is clarified.

(Ia) ε' and the General ω Equation:

Consider the ω equation:

$$(\varepsilon' - h)\,\omega = (\Sigma' - (\varphi_0 \Omega \omega))\,\varphi_0 \tag{2.48}$$

where $$\varepsilon' = \frac{(\omega h \omega) + (\omega \Sigma' \varphi_0)}{(\omega, \omega)}$$

Assume here that (ω, ω) equals one. At the end of this section (Ia) we comment on the role ω's normalization plays in the specification of ε'.

Define the operator $d = \varepsilon' - h$, and invert this operator to find an integral equation solution for ω:

$$\omega = \frac{1}{d}\left[\Sigma' - (\varphi_0 \Omega \omega)\right]\varphi_0 \tag{3.1}$$

Using (3.1) the orthogonality condition (2.35) ((φ_0, ω) equals zero) gives us:

$$(\varphi_0, \frac{1}{d}\Sigma'\varphi_0) = (\varphi_0 \Omega \omega)(\varphi_0 \frac{1}{d} \varphi_0) \tag{3.2}$$

Again using (3.1) in the normalization condition $(\omega, \omega) = 1$, we are lead to:

$$1 = (\omega, \frac{1}{d}\Sigma'\varphi_0) - (\varphi_0 \Omega \omega)(\omega \frac{1}{d} \varphi_0) \tag{3.3}$$

Substituting (3.1) for ω in this last equation (3.3) we find,

$$1 = \frac{1}{\varepsilon' - \varepsilon'^{\times}} \Big\{ (\varphi_0 \Sigma'^{\dagger} \tfrac{1}{d^+} \Sigma' \varphi_0) - (\varphi_0 \Sigma'^{\dagger} \tfrac{1}{d} \Sigma' \varphi_0)$$
$$- (\omega, \Omega \varphi_0) \left((\varphi_0 \tfrac{1}{d^+} \Sigma' \varphi_0) - (\varphi_0 \tfrac{1}{d} \Sigma' \varphi_0) \right)$$
$$- (\varphi_0 \Omega \omega) \left((\varphi_0 \Sigma'^{\dagger} \tfrac{1}{d^+} \varphi_0) - (\varphi_0 \Sigma'^{\dagger} \tfrac{1}{d} \varphi_0) \right)$$
$$+ |(\varphi_0 \Omega \omega)|^2 \left((\varphi_0 \tfrac{1}{d^+} \varphi_0) - (\varphi_0 \tfrac{1}{d} \varphi_0) \right) \Big\}$$

(3.4)

Now making use of (3.2) in (3.4):

$$1 = \frac{1}{\varepsilon' - \varepsilon} \Big\{ (\varphi_0 \Sigma'^{\dagger} [\tfrac{1}{d^+} - \tfrac{1}{d}] \Sigma' \varphi_0)$$
$$- \frac{(\varphi_0 \Sigma'^{\dagger} \frac{1}{d^+} \varphi_0)}{(\varphi_0 \frac{1}{d^+} \varphi_0)} (\varphi_0 (\tfrac{1}{d^+} - \tfrac{1}{d}) \Sigma' \varphi_0)$$
$$- \frac{(\varphi_0 \frac{1}{d} \Sigma' \varphi_0)}{(\varphi_0 \frac{1}{d} \varphi_0)} (\varphi_0 \Sigma'^{\dagger} (\tfrac{1}{d^+} - \tfrac{1}{d}) \varphi_0)$$
$$+ \frac{|(\varphi_0 \frac{1}{d} \Sigma' \varphi_0)|^2}{|(\varphi_0 \frac{1}{d} \varphi_0)|^2} (\varphi_0, (\tfrac{1}{d^+} - \tfrac{1}{d}) \varphi_0) \Big\} \qquad (3.5)$$

Equation (3.5) contains the information $(\omega, \omega) = 1$ and $(\omega, \varphi_0) = 0$.

To simplify the algebra, substitute:

$$A = (\varphi_0 \tfrac{1}{d} \varphi_0)$$
$$B = (\varphi_0 \tfrac{1}{d} \Sigma' \varphi_0)$$

$$C = (\varphi_0 \Sigma'^{+} \frac{1}{d} \Sigma' \varphi_0)$$

$$D = (\varphi_0 \Sigma'^{+} \frac{1}{d} \varphi_0)$$

where A B, C and D contain ω through ε'. Equation (3.5) in terms of A, B, C and D is:

$$I = \frac{1}{2i\varepsilon_I'} \left(C^* - C - \frac{B^*}{A^*} (D^* - B) - \frac{B}{A} (B^* - D) \right.$$

$$\left. + \frac{|B|^2}{|A|^2} (A^* - A) \right)$$

$$I = \frac{1}{\varepsilon_I'} \left\{ -C_I + \frac{Im(BDA^*)}{|A|^2} \right\}$$

and substituting back for A B, C, and D:

$$I = \frac{1}{\varepsilon_I'} \left[-(\varphi_0, \Sigma'^{+} \frac{1}{d} \Sigma' \varphi_0)_I + \right.$$

$$\left. \frac{\left[(\varphi_0 \frac{1}{d} \Sigma' \varphi_0)(\varphi_0 \Sigma'^{+} \frac{1}{d} \varphi_0)(\varphi_0 \frac{1}{d^*} \varphi_0) \right]_I}{|(\varphi_0 \frac{1}{d} \varphi_0)|^2} \right] \qquad (3.6)$$

The subscripts R and I denote respectively the real and imaginary parts of the expression. We would have lost equation (3.6) had we not specified ω's normalization.

Equation (3.6) is a single real algebraic equation relating ε_R' and ε_I' This is the only equation for ε' with (w,w) set equal to one. Therefore, the equation for w (with w normalized) doesn't specify ε'. With w normalized there is in this general situation a one dimensional freedom in ε'. If we had not specified the normalization of w, ε' would be completely undetermined.

(Ib, c, d) ε' and Three Particular Situations of the ω Equation

In this section we are going to investigate ε' and various special cases of the ω equation.

The first example is of genuine interest (e.g. see Chapter Four) whereas the others are academic exercises used to gain insight about the problem at hand.

b) The ω equation with peaked $G^{(\pm)}$.

We will now study the ω equation's relation to ε' in the practical situation of $G^{(\pm)}$ peaked about the origin (see Chapter Four).

In Chapter Four, we will show that when $G^{(\pm)}$ is a peaked function the following relations hold:

$$\Sigma' = \alpha \Omega$$

$$\alpha = \frac{F^{(+)}(0) \int G^{(-)\times}(\vec{r})\, d\vec{r} + F^{(-)}(0) \int G^{(+)\times}(\vec{r})\, d\vec{r}}{\int G^{(+)\times}(\vec{r})\, G^{(-)}(\vec{r})\, d\vec{r} + \int G^{(-)\times}(\vec{r})\, G^{(+)}(\vec{r})\, d\vec{r}}$$

where Σ' and Ω are given by (2.43) and (2.42) respectively.

The ω equation under these conditions becomes

$$(\varepsilon' - h^{(-)})\,\omega = \Big[\alpha \sum_j \frac{1}{\chi_j}\cdot - \alpha(\varphi_0 \sum_j \frac{1}{\chi_j}\cdot \varphi_0) - (\varphi_0 \sum_j \frac{1}{\chi_j}\cdot \omega)\Big]\varphi_0 \qquad (4.1')$$

$$\varepsilon' = \frac{(\omega, h^{(-)}\omega) + \alpha(\omega \sum_j \frac{1}{\chi_j}\cdot \varphi_0)}{(\omega, \omega)} \qquad (3.7)$$

A solution is then found for ω

$$\omega = \alpha \left(-\mathbb{1} + \frac{a^{-1}}{d}\right) \varphi_0 \tag{4.6}$$

where $d = \varepsilon' - h^{(-)}$ and $a = (\varphi_0 \frac{1}{d} \varphi_0)$

Equation (4.6) identically satisfies (4.1') and (3.7) as well as $(\varphi_0, \omega) = 0$

Choose $(\omega, \omega) = 1$. The evaluation of this normalization using (4.6) leads (see Chapter Four) to the single relation:

$$(\omega, \omega) = 1 = -|\alpha|^2 \left(1 + \frac{a_I}{\varepsilon_I' |a|^2}\right) \tag{4.7}$$

or

$$\varepsilon_I' = -\frac{|\alpha|^2}{1 + |\alpha|^2} \frac{a_I}{|a|^2} \tag{4.8}$$

Equation (4.8) is the special case of (3.6) for the situation in which $G^{(\pm)}$ is peaked. Keeping in mind that a and a_I are functions of ε' we see that (4.8) is a single real equation relating ε_R' and ε_I' in the $G^{(\pm)}$ peaked situation. With (ω, ω) specified there exists a one dimensional freedom in ε' in this model of the ω equation. If ω were not considered normalized (4.7), ε' would be completely unspecified. (I.e. no relation between ε_R' and ε_I' would exist).

(c) One Dimensional Delta Function Model

In this model, the $\varepsilon' - \omega$ equation situation is analyzed for the case of a single target electron in one dimension. For mathematical simplicity we replace all the potentials appearing in the ω equation by Dirac delta functions.

In particular: $$H_T = -\frac{d^2}{dx^2} - c^2\delta(x)$$

$$\Omega = \lambda\,\delta(x)$$

$$\Sigma' = \alpha\Omega = \alpha\lambda\,\delta(x)$$

Define $\mathcal{Z} = (\varphi_0 \Omega \varphi_0)$ and $\chi_1 = (\varphi_0 \Omega \omega)$.

With these approximations φ_0, W_0 and $\mathcal{Z}$ can be written:

$$H_T \varphi_0 = W_0 \varphi_0$$

$$\varphi_0 = \frac{c}{\sqrt{2}}\, e^{-(c^2/4)|x|}$$

$$W_0 = -c^4/4$$

$$\mathcal{Z} = (\varphi_0 \Omega \varphi_0) = \lambda\,\varphi_0^2(0) = \frac{\lambda c^2}{2}$$

The ω equation is then written:

$$(\varepsilon' - h)\omega = \alpha\left(\Omega - \mathcal{Z} - \frac{\chi_1}{\alpha}\right)\varphi_0 \qquad (3.8)$$

where $$h = -\frac{d^2}{dx^2} - c^2\delta(x) + \lambda\,\delta(x)$$

We now find A_1 and B_1 such that (3.9):

$$\omega = A_1 e^{-c^2/2\,|x|} + B_1 e^{-q\,|x|} \tag{3.9}$$

is a solution to (3.8).

Substitution of ω and φ_0 into (3.8) leads for $(x>0)$ to:

$$A_1 = -\frac{\alpha c}{\sqrt{2}} \frac{(z + \chi_1/\alpha)}{\varepsilon' + c^4/4}$$

and

$$\varepsilon' = -q^2 \quad , \quad B_1 \neq 0$$

Requiring $(\varphi_0, \omega) = 0$ leads to:

$$0 = \frac{A_1}{c^2} + \frac{B_1}{c^2/2 + q}$$

Finally substitution of χ_1 in terms of ε' we find:

$$A_1 = \frac{-\frac{\alpha}{2} \frac{\lambda c^3}{\sqrt{2}}}{\left[\sqrt{-\varepsilon'} + c^2/2\right]\left[\sqrt{-\varepsilon'} + \frac{c^2+\lambda}{2}\right]} \tag{3.10}$$

$$B_1 = \frac{\frac{\alpha \lambda c}{2\sqrt{2}} \left(\sqrt{-\varepsilon'} + c^2/2\right)}{\left(-\sqrt{-\varepsilon'} + c^2/2\right)\left(\sqrt{-\varepsilon'} + \frac{c^2+\lambda}{2}\right)} \tag{3.11}$$

Using this A_1 and B_1 and requiring ω to be normalized to 1 gives a single equation for q :

$$\frac{1}{2}\left(|q|^2+c^2q_R+\frac{c^4}{4}\right)\left(|q|^2+(c^2+\lambda)q_R+\frac{(c^2+\lambda)^2}{4}\right)$$

$$=\frac{|\alpha|^2\lambda^2c^2}{8}\left(\frac{|q|^2+c^2q_R+c^2/4}{4q_R}-c^2\right) \qquad (3.12)$$

Equation (3.12) is equation (3.6) for this particular situation.

(3.12) is a single real equation for q (q_R and q_I) and therefore cannot specify q. Consequently, q and therefore ε' ($\varepsilon' = -q^2$) are not determined. If we take $\varepsilon' = (\omega\hbar\omega) + \alpha\chi_1^x$ with

$$\omega = Ae^{-c^2/2|x|} + Be^{-q|x|}$$

and $$\chi_1 = -\frac{\alpha\lambda^2c^2/4}{q+[(c^2+\lambda)/2]}$$

A_1 and B_1 given by (3.10) and (3.12) we find $\varepsilon' = -q^2$ an identity: no additional information about q_I and q_R. Therefore once again a one dimensional freedom exists in ε'.

d) The Three State Calculation with Localized G.

A solution for ω could be found by expanding in an infinite sum and integral over the eigenstates of the target. This expansion would (when substituted into ω's equation) lead to an infinite set of coupled algebraic equations for the weights (coefficients) of this expansion.

For mathematical simplicity consider the case of ω confined to three eigenstates (2 excited states) of the target. We will not present the yet simpler two state situation (even though the same conclusion concerning the one dimensional freedom in ε' is true in this case). The reason is that ω would then be an exact eigenstate of the target and the interpretation of ω as, in some sense, an average excited state of the target is lost. For the three state calculation we can consider ω as the OAES of the part of Hilbert space spanned by the two included excited states of the target. Let $G^{(\pm)}$ be peaked functions.

Under these circumstances:

$$\varphi_0 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \omega = \begin{pmatrix} 0 \\ a \\ b \end{pmatrix} \tag{3.13}$$

$$H_T = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix} \qquad \Omega = \begin{pmatrix} 0 & \Omega_{12} & \Omega_{13} \\ \Omega_{21} & 0 & \Omega_{23} \\ \Omega_{31} & \Omega_{32} & 0 \end{pmatrix}$$

The diagonal terms of Ω have been incorporated into the E_1, E_2 and E_3 of H_T.

Now impose $(\omega,\omega)=1$:

$$|a|^2+|b|^2=1$$

$$a=e^{i\chi_1}\cos\theta$$
$$b=e^{i\chi_2}\sin\theta$$

(3.14)

$$\omega=\begin{pmatrix}0\\ e^{i\chi_1}\cos\theta\\ e^{i\chi_2}\sin\theta\end{pmatrix}=e^{i\nu}\begin{pmatrix}0\\ e^{i\chi/2}\cos\theta\\ e^{-i\chi/2}\sin\theta\end{pmatrix} \quad (3.15)$$

where $\nu=\frac{\chi_1+\chi_2}{2}$

and $\chi=\chi_1-\chi_2$

Substitution of ω and ϕ_0 into (4.1') leads to:

$$\begin{bmatrix}\varepsilon'-E_1 & -\Omega_{12} & -\Omega_{13}\\ -\Omega_{12}^* & \varepsilon'-E_2 & -\Omega_{23}\\ -\Omega_{13}^* & -\Omega_{23}^* & \varepsilon'-E_3\end{bmatrix}\begin{pmatrix}0\\ a\\ b\end{pmatrix}=\alpha\begin{pmatrix}0\\ \Omega_{12}^*\\ \Omega_{13}^*\end{pmatrix}-\begin{pmatrix}\Omega_{12}a+\Omega_{13}b\\ 0\\ 0\end{pmatrix}$$

This matrix equation is now written as three algebraic equations, one an identity:

$$-\Omega_{12}a-\Omega_{23}b=-\Omega_{12}a-\Omega_{13}b$$

$$(\varepsilon'-E_2)a-\Omega_{23}b=\alpha\Omega_{12}^* \quad (3.16)$$
$$(\varepsilon'-E_3)b-\Omega_{23}^*a=\alpha\Omega_{13}^* \quad (3.17)$$

where $\varepsilon'=(w\mathcal{H}^{(-)}w)+\alpha(w\Omega\phi_0)$ (3.18)

Using (3.15) and (3.13) in (3.18) we find:

$$\mathcal{E}' = E_2 |a|^2 + E_3 |b|^2 + 2\,\mathrm{Re}\,(\Omega_{23} a^* b) + \alpha (a^* \Omega_{12}^* + b^* \Omega_{13}^*) \tag{3.19}$$

Using (3.19) in (3.16) and (3.17).

From the two complex equations, (3.16) and (3.17) we arrive at two independent real equations. If we set ν equal to zero (for convenience) and assume that the Ω_{ij} are real (also for convenience) and that

$$\Omega_{12} = \Omega_{13} = \Omega \tag{3.20}$$

and write

$$\bar{\Omega} = \Omega_{23} \tag{3.21}$$

(where (3.20) assumes that the two components of the inelastic space are equally coupled to the ground state) we then find two real equations for θ and χ . The two equations, found after some algebra, (and also assuming α is real for convenience) with $\Delta = E_3 - E_2$ are:

$$\Delta + \frac{(\alpha\Omega)^2}{\bar{\Omega}} \cos 2\theta - 2\bar{\Omega} \cot 2\theta = 0 \tag{3.22}$$

$$\cos\frac{\chi}{2} = -\frac{\alpha\Omega}{2\bar{\Omega}} (\sin\theta + \cos\theta) \tag{3.23}$$

These two equations would determine θ and χ .

Remember, however, that γ, if not set equal to zero, would appear in these two equations giving us two real algebraic equations for three parameters. Therefore, one of the three parameters θ, χ and γ can be looked upon as unspecified.

ε' can be written in terms of the parameters which describe ω as:

$$\varepsilon' = E_2 \cos^2\theta + E_3 \sin^2\theta + 2\,\mathrm{Re}\left(\Omega_{23} e^{-\frac{i\chi}{2}} \cos\theta \sin\theta\right)$$
$$+ \alpha e^{-i\gamma}\left[e^{-i\chi/2}\cos\theta\,\Omega_{12}^{x} + e^{i\chi/2}\sin\theta\,\Omega_{13}^{x}\right]$$

(3.24)

Equation (3.24) demonstrates how ε' depends on γ, θ and χ. There are two algebraic equations relating γ, θ and χ. Thus we once again have a one dimensional freedom in ε'.

The assumptions (3.20), (3.21) and α being real will certainly affect the equations (3.22), (3.23) for θ and χ. The inclusion of the general Ω_{ij} and α complex would just complicate the algebra without gaining additional information concerning the parameters θ, χ and γ.

(Ie) Summary and Significance of Section (I)

We have seen in this section (I) that in both the general and particular models of the equation for ω: the ω equation with (ω,ω) equals one doesn't specify ε'.

There always exists a one dimensional freedom in ε'. The normalization of ω gives us information about ε', but it doesn't complete the picture.

We will now describe the most natural way of looking at the freedom in ε'. Let t be a real parameter describing the freedom in ε'. (I.e. with the ω equation and (ω,ω) equals one we have $\varepsilon'(t)$.)

The three state calculation gives us a hint about how we can look at this one dimensional parameter t. The two equations (3.22) and (3.23), had we not set ν equal to zero, could be looked at as having given a single freedom to through ν. This is saying, that in this case, the multiplicative factor $e^{i\nu}$ in ω leads to a freedom in ε': $\varepsilon'(\nu)$. This choice, obviously is not unique. We could have chosen θ or χ or a combination of θ, χ and ν as the freedom giving parameter in ε'.

With this last statement in mind, we look at the definition of ε':

$$\varepsilon' = \frac{(\omega, h\omega) + (\omega \Sigma \phi_0)}{(\omega,\omega)}$$

We notice that when ω undergoes a multiplicative phase shift ν

$$\omega \longrightarrow \omega e^{i\nu}$$

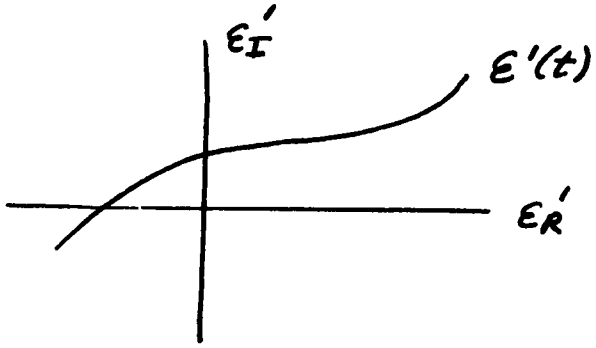
$$\varepsilon' \longrightarrow \hat{\varepsilon}'(\nu) = \frac{(w, h w) + e^{-i\nu}(w, \Sigma \phi_0)}{(w, w)} \neq \varepsilon'$$

We therefore have the following four statements and conclusion:

(1) As evidenced by the general ω equation and three particular examples: ε' always has a one dimensional freedom.

(2) ε' always has a one dimensional freedom due to the freedom of the phase of ω. This statement is justified by comparing the equations (3.25) and (3.26) for ε'.

(3) Look at the freedom in ε' as a parameter specifying ε_R' and ε_I' in a two dimensional complex ε' space.



$$\varepsilon_R' = f_1(t) \tag{3.27}$$

$$\varepsilon_I' = f_2(t) \tag{3.28}$$

Equations (3.27) and (3.28) represent a particular parametrization of the curve ε'.

(4) From statement (2) we also know that a way to specify this curve is given by:

$$\varepsilon_R' = g_1(\nu) \tag{3.29}$$

$$\varepsilon_I' = g_2(\nu) \tag{3.30}$$

where ν is the parameter corresponding to the phase of ω. If we believed that perhaps (3.29) and (3.30) correspond to a different curve than (3.27) and (3.28) then this would imply that ε' has a two dimensional freedom and contradict statement (1).

Conclusion:

Any one dimensional parameter t must be a function of ν, another one dimensional parameter describing this curve. Explicitly, $t = f_1^{-1}(g_1(\nu))$ or $t = f_2^{-1}(g_2(\nu))$.

Therefore the conclusion we reach is that the freedom in ε' can always be parametrized as a function of the phase of ω.

The first statement of this chapter is that it is usual for a bound state equation of motion to determine its parameter. ε' is not the usual parameter. ε' is not an eigenvalue and the ω equation is not an eigenvalue equation for ω. ε' is complex and is a sum of linear and bilinear ω terms. The usual conclusion, concerning parameters of bound state equations, is therefore not to be expected for ε'.

(II) We now take a look at the ε' determinacy question from a different perspective.

If we consider the five coupled equations together,

$$\left(\frac{p^2}{2} - T - VS\right) F^{(+)} = v\, G^{(+)} \tag{3.31}$$

$$\left(\frac{p^2}{2} - T - VS\right) F^{(-)} = v\, G^{(-)} \tag{3.32}$$

$$\left(\frac{p'^2}{2} - T - \bar{V}\right) G^{(+)} = \frac{v^*}{(w, w)} F^{(+)} \tag{3.33}$$

$$\left(\frac{p'^2}{2} - T - \bar{V}\right) G^{(-)} = \frac{v^*}{(w, w)} F^{(-)} \tag{3.34}$$

$$(\varepsilon' - h)\, w = (\Sigma' - (\rho_0 \Omega w))\, \phi_0 \tag{3.35}$$

and then inquire about the ε' determinacy situation, a different conclusion is reached.

An examination of equations (3.31-3.34) above shows that the relative phases of $F^{(\pm)}\phi_0$ and $G^{(\pm)}\, w$ must be fixed, i.e. determined by these five equations. For example, if $w\, G^{(\pm)}$ undergoes a phase shift γ then $\phi_0 F^{(\pm)}$ must undergo an equal phase shift or equations (3.31-3.34) will be changed. The above conclusion can also be seen from looking directly at the total trial wave function $\psi_t^{\pm} = \phi_0 F^{\pm} + w G^{\pm}$, where we notice that the relative phase of the elastic part $\phi_0 F^{\pm}$ and the inelastic part $w G^{\pm}$ must be fixed. The overall phase will have no effect on the above mentioned relative phase.

These remarks imply that when w undergoes a phase shift γ, then a possible overall phase shift in the total trial wave function of λ would lead to

the following (assuming for simplicity that φ_0 doesn't change its phase) general relative-phase-preserving transformation T :

$$\varphi_0 \to \varphi_0$$
$$F^{(\pm)} \to e^{i\lambda} F^{(\pm)}$$
$$G^{(\pm)} \to e^{i(\lambda-\gamma)} G^{(\pm)}$$
$$w \to e^{i\gamma} w$$
$$\psi_t^{(\pm)} \to e^{i\lambda} \psi_t^{(\pm)}$$

We now examine what happens to ε' under such a general relative-phase-preserving transformation.

From (2.43) and (2.45) we have:

$$\Sigma = \frac{\langle G^{(+)*} V F^{(-)} \rangle + \langle G^{(-)*} V F^{(+)} \rangle}{\langle G^{(+)*} G^{(-)} \rangle + \langle G^{(-)*} G^{(+)} \rangle} \tag{2.43}$$

$$\varepsilon' = \frac{(w, hw) + (w \Sigma \varphi_0)}{(w, w)} \tag{2.45}$$

and under T, Σ becomes.

$$\frac{\langle e^{-i(\lambda-\gamma)} G^{+*} V e^{i\lambda} F^{(-)} \rangle + \langle e^{-i(\lambda-\gamma)} G^{(-)*} V e^{i\lambda} F^{(+)} \rangle}{\langle e^{-i(\lambda-\gamma)} G^{(+)*} e^{i(\lambda-\gamma)} G^{(-)} \rangle + \langle e^{-i(\lambda-\gamma)} G^{(-)*} e^{i(\lambda-\gamma)} G^{(+)} \rangle}$$

and consequently under T, $\Sigma \to e^{i\gamma}\Sigma$. In the peaked $G^{(\pm)}$ approximation,

it is easy to see that α will go to $\alpha e^{i\delta}$. The conclusion that we draw, in the five coupled equations situation, is that when ω changes its phase consistent with the relative-phase-preserving transformation T : ε' does not change. That is, ε' is completely specified within the five coupled equation situation. That ε' has a one dimensional freedom attributable to an unspecified phase of ω is true only when we isolate and examine the ω equation (apart from the other four coupled equations).

This property of the parameter ε' that it is not specified by the ω equation alone, but rather by all five equations is ultimately attributable to ω being optimized rather than prechosen. (For example, if we prechose φ_0 and φ_1, where φ_0 and φ_1 are the ground and first excited states of the atom then the parameters W_0 and W_1 their respective energy eigenvalues are totally independent of the close coupling equations for their respective coefficients.) It is the optimization procedure on the average excited state which couples ω to $F^{(\pm)}$ and $G^{(\pm)}$, and demands that in order that ε' be well defined it is necessary that ε' also remain coupled to the $F^{(\pm)}$ and $G^{(\pm)}$ equations.

Chapter Four

Approximate Solution for the Optimized Average Excited State ω .

$$(\varepsilon' - h)\,\omega = [\Sigma' - (\phi_0, \Omega\,\omega)]\,\phi_0 \qquad (4.1)$$

Equation (4.1) is one of three non-linear coupled integro-differential equations and there is little hope of obtaining an exact solution to this set of equations.

The purpose of this chapter is to describe an approach to solving this equation (4.1) valid for heavy atoms.

A natural starting point in the investigation of equation (4.1) is to consider the nature of the hamiltonian h. It differs from H_T by a sum of single particle potentials:

$$\Omega = \sum_i \bar{\Omega}(x_i)$$

where $\bar{\Omega}(x_i) = \frac{1}{N}\left(\langle G^{(-)*}(\vec{r}) \frac{1}{|\vec{x}_i - \vec{r}|} G^{(+)}(\vec{r})\rangle \right.$

$$\left. + \langle G^{(+)*}(\vec{r}) \frac{1}{|\vec{x}_i - \vec{r}|} G^{(-)}(\vec{r})\rangle \right)$$

For large x , $\bar{\Omega}$ behaves like $1/x$ while for small x it is a finite constant. If $\bar{\Omega}$ were $1/x$ for all x , then h would be the hamiltonian of a singly negative ion isoelectronic with the target $h^{(-)}$:

$$\Omega \sim \sum_i 1/x_i$$

$$h \sim h^{(-)} = \sum_i T_i + \frac{1}{2} \sum_{i,j} \frac{1}{|x_i - x_j|} - \sum_i \frac{Z}{x_i} + \sum_i \frac{1}{x_i}$$

$$= \sum_i T_i + \frac{1}{2} \sum_{i,j} \frac{1}{|x_i - x_j|} - \sum_i \frac{(Z-1)}{x_i}$$

$T_i =$ kinetic energy of the i th electron.

An argument will now be given suggesting that for heavy atoms the low lying states of h do not depend in an important way on the short range behavior of $\bar{\Omega}$.

For heavy atoms the inner shell electrons experience an effective charge which is large. (See, e.g., Slater's screening rules[1].) Therefore the addition of a single particle potential $\bar{\Omega}$ will be a small perturbation on a large attractive central potential experienced by these inner-shell electrons. Therefore for heavy atoms the low lying states of h are not much perturbed from the eigenstates of H_T.

The valence shell electrons do not penetrate deeply into the atom and therefore the short range behavior of $\bar{\Omega}$ is of no great moment to them either. On the other hand, note that the valence electrons experience a small effective charge so that the addition of $\bar{\Omega}$ to H_T for these electrons reduces the effective charge by unity : a significant change.

The above argument indicates that the states of h for heavy atoms are closely related to the states of $h^{(-)}$: the hamiltonian of the singly negative ion isoelectronic with the target.[2]

Since for heavy atoms the eigenstates of h and $h^{(-)}$ should be closely related, the solution of equation (4.1) should, for these atoms, not be greatly affected by replacing h by $h^{(-)}$.

An examination of h shows that a way to have h approach $h^{(-)}$ is to have $G^{(\pm)}$ replaced by sharply peaked functions about the origin. Physically this last statement points out that a way to have h replaced by $h^{(-)}$ is to have $G^{(\pm)}$ replaced by a resonance type of behavior about the origin. (I.e. in the inelastic channel the projectile spends a long time in the vicinity of the nucleus.) In this $G^{(\pm)}$ peaked approximation:

$$\Sigma'(\chi) = \frac{\langle G^{(+)\chi}(r) \sum_i \frac{1}{|\chi_i - r|} F^{(-)}(r) \rangle + \langle G^{(-)\chi} \sum_i \frac{1}{|\chi_i - r|} F^{(+)} \rangle}{N}$$

becomes

$$\Sigma(\chi) = \alpha \sum_i 1/\chi_i$$

where $$\alpha = \frac{\left[F^{(-)}(0) \int G^{(+)\chi}(\vec{r}) d\vec{r} + F^{(+)}(0) \int G^{(-)\chi}(\vec{r}) d\vec{r} \right]}{N}$$

The replacement of h by $h^{(-)}$ in equation (4.1) behooves us to consider and compare the equation of a state of the isoelectronic negative ion orthogonalized to the ground state of the target.

For convenience let us consider the ground state of the isoelectronic negative ion:

$\varphi_0 =$ the ground state of the target

$$H_T \varphi_0 = W_0 \varphi_0$$

$\varphi_0^{(-)} =$ the ground state of the isoelectronic negative ion.

$$h^{(-)} \varphi_0^{(-)} = W_0^{(-)} \varphi_0^{(-)} \quad , \quad h^{(-)} = H_T + \sum_j \frac{1}{r_j}$$

$$w_0 = \frac{\varphi_0^{(-)} - (\varphi_0, \varphi_0^{(-)}) \varphi_0}{\sqrt{1 - |(\varphi_0, \varphi_0^{(-)})|^2}}$$

$w_0 =$ the ground state of the isoelectronic negative ion orthogonalized to φ_0 and normalized to one.

We ask for w (and any approximation for w) to be normalized since we want to be able to interpret w as a decaying state of the atom. The quantum mechanical postulate that the absolute value squared of the wave function of a state is the probability density of that state, requires the normalization of w. (I.e., the integrated probability that the atomic electrons are somewhere in space must be unity).

Using the last equations:

$$h^{(-)} w_0 = h^{(-)} \left[\frac{\varphi_0^{(-)} - (\varphi_0, \varphi_0^{(-)}) \varphi_0}{\sqrt{1 - |(\varphi_0, \varphi_0^{(-)})|^2}} \right]$$

$$= \frac{h^{(-)} \varphi_0^{(-)}}{\sqrt{1 - |(\varphi_0, \varphi_0^{(-)})|^2}} - \frac{(\varphi_0, \varphi_0^{(-)}) \left\{ W_0 + \sum_j \frac{1}{r_j} \right\} \varphi_0}{\sqrt{1 - |(\varphi_0, \varphi_0^{(-)})|^2}}$$

$$= \frac{W_0^{(-)} \varphi_0^{(-)} - (\varphi_0, \varphi_0^{(-)}) \left\{ W_0 + \sum_j \frac{1}{r_j} \right\} \varphi_0}{\sqrt{1 - |(\varphi_0, \varphi_0^{(-)})|^2}}$$

Now adding and subtracting $\frac{(\varphi_0, \varphi_0^{(-1)})\,\varphi_0}{\sqrt{1-|(\varphi_0, \varphi_0^{(-1)})|^2}}$ to the right hand side of this last equation leads directly to the equation satisfied by ω_0.

$$\left(W_0^{(-)} - h^{(-1)}\right)\omega_0 = \frac{(\varphi_0, \varphi_0^{(-1)})\left[\left(W_0 - W_0^{(-)}\right) + \sum_j \frac{1}{\chi_j}\cdot\right]\varphi_0}{\sqrt{1-|(\varphi_0, \varphi_0^{(-1)})|^2}} \tag{4.2}$$

Now equation (4.1) with $G^{(\pm)}$ peaked near the origin is:

$$\left(\varepsilon' - h^{(-1)}\right)\omega = \left[\alpha\left(\sum_j 1/\chi_j\cdot - \left(\varphi_0 \sum_j \frac{1}{\chi_j}\cdot \varphi_0\right)\right) - \left(\varphi_0 \sum_j \frac{1}{\chi_j}\cdot \omega\right)\right]\varphi_0 \tag{4.1'}$$

where $$\varepsilon' = \frac{(\omega\, h^{(-1)}\omega) + \alpha\left(\omega \sum_j 1/\chi_j\cdot \varphi_0\right)}{(\omega,\omega)}$$

At this point we are compelled to ask whether we can determine a set of conditions under which ω_0 would satisfy (4.1'). The answer to this question is remarkably simple.

Directly substitute ω_0 in (4.1'). First use equation (4.2) to determine $\varepsilon'(\omega_0)$:

$$\varepsilon'(\omega_0) = (\alpha - \beta)\left(\omega_0, \sum_j \frac{1}{\chi_j}\cdot \varphi_0\right) + W_0^{(-)} \tag{4.3}$$

where $$\beta = \frac{(\varphi_0, \varphi_0^{(-1)})}{\sqrt{1-|(\varphi_0, \varphi_0^{(-1)})|^2}}$$

Now using $\varepsilon'(w_0)$ and after some algebra equation (4.1') with w_0 substituted for w becomes:

$$\left[(\alpha-\beta)\left(w_0, \sum_j 1/x_j \cdot \varphi_0\right) + W_0^{(-1)} - h^{(-1)}\right] w$$
$$= \left[\beta\left[W_0 - W_0^{(-1)}\right] + (\beta-\alpha)\left(\varphi_0, \sum_j 1/x_j \cdot \varphi_0\right) + \alpha \sum_j 1/x_j\right] \varphi_0 \qquad (4.4)$$

Comparing equations (4.2) and (4.4) we notice that w_0 will indeed satisfy (4.1') exactly if $\alpha = \beta$. I.e. if

$$\frac{F^{(-1)}(0)\int G^{(+)*} d\vec{r} + F^{(+)}(0)\int G^{(-)*} d\vec{r}}{\int G^{(+)*} G^{(-)} d\vec{r} + \int G^{(-)*} G^{(+)} d\vec{r}} = \frac{(\varphi_0, \varphi_0^{(-)})}{\sqrt{1 - |(\varphi_0, \varphi_0^{(-)})|^2}} \qquad (4.5)$$

We also see that if the difference between α and β is such that

$(\alpha-\beta)\left(w_0 \sum_j 1/x_j \cdot \varphi_0\right)$ and $(\alpha-\beta)\left(\varphi_0 \sum_j 1/x_j \cdot \varphi_0\right)$

are small compared to the other terms on the l.h.s. and r.h.s. of equation (4.4) respectively; w_0 will to that extent approximate the solution to (4.1').

We now show under what circumstances equation (4.5) will be satisfied.

Equation (4.1') has an integral equation solution:

$$w = \alpha\left(-1 + \frac{a^{-1}}{d}\right)\varphi_0 \qquad (4.6)$$

where $d = \varepsilon' - h^{(-1)}$

and $a = \left(\varphi_0 \frac{1}{\varepsilon' - h^{(-1)}} \varphi_0\right)$

That (4.6) identically satisfies (4.1') and is orthogonal to φ_0 is seen by direct substitution.

Using (4.6) to evaluate the normalization of ω:

$$(\omega,\omega) = |\alpha|^2 \left(\left(-\mathbb{1} + \frac{a^{-1}}{d} \right) \varphi_0, \left(-\mathbb{1} + \frac{a^{-1}}{d} \right) \varphi_0 \right)$$

$$(\omega,\omega) = |\alpha|^2 \left(-1 + \frac{1}{a^* a} \left(\varphi_0 \frac{1}{d^* d} \varphi_0 \right) \right)$$

Making use of the identity $\frac{1}{d^* d} = \frac{1}{2i\varepsilon_I'} \left(\frac{1}{d^*} - \frac{1}{d} \right)$

where ε_I' is the imaginary part of ε', the normalization becomes:

$$(\omega,\omega) = -|\alpha|^2 \left(1 + \frac{1}{|a|^2} \frac{a_I}{\varepsilon_I'} \right) \qquad (4.7)$$

If we ask for $(\omega,\omega) = 1$ we have solving for ε_I':

$$\varepsilon_I' = -\frac{a_I}{|a|^2} \left(\frac{|\alpha|^2}{1+|\alpha|^2} \right) \qquad (4.8)$$

In the expression for $a = \left(\varphi_0 \frac{1}{\varepsilon' - h^{(-)}} \varphi_0 \right)$ insert a complete set of eigenstates of $h^{(-)}$:

$$a = \sum_n \frac{|\langle \varphi_0 | \varphi_n^{(-)} \rangle|^2}{\varepsilon' - W_n^{(-)}}$$

If

$$|\langle \varphi_0 | \varphi_0^{(-)} \rangle|^2 \gg |\langle \varphi_0 | \varphi_n^{(-)} \rangle|^2 \tag{4.9a}$$

and $\varepsilon' - W_n^{(-)}$ is not small for all $n \geq 1$ (4.9b)

we have:

$$a \cong \frac{|\langle \varphi_0 | \varphi_0^{(-)} \rangle|^2}{\varepsilon' - W_0^{(-)}} \tag{4.10}$$

Now $h^{(-)}$ and H_T can be written:

$$h^{(-)} = -\sum_{j'} \frac{Z}{x_{j'}} \left(1 - 1/Z\right) + \frac{1}{2} \sum_{i'j'} \frac{1}{|x_{i'} - x_{j'}|} + T$$

$$H_T = -\sum_{j'} \frac{Z}{x_{j'}} + \frac{1}{2} \sum_{i'j'} \frac{1}{|x_{i'} - x_{j'}|} + T$$

$h^{(-)}$ and H_T describe isoelectronic atoms. As argued previously for large Z, $h^{(-)}$ and H_T and their respective eigenstates are "closely related." Therefore, for heavy atoms φ_0 and $\varphi_0^{(-)}$ should have an appreciable overlap and for such atoms condition (4.9a) is reasonable.

Equation (4.10) can be written as:

$$\varepsilon' - W_0^{(-)} = \frac{|\langle \varphi_0 | \varphi_0^{(-)} \rangle|^2}{a} \tag{4.11}$$

Taking the imaginary part of both sides of (4.11)

$$\varepsilon_I' = -\frac{|\langle \varphi_0 | \varphi_0^{(-)} \rangle|^2 a_I}{|a|^2} \tag{4.12}$$

$$\varepsilon_I' = -\frac{|\beta|^2}{1+|\beta|^2}\frac{a_I}{|a|^2} \qquad (4.13)$$

where β is given by (4.3).

Now when we compare (4.8) with (4.13) we notice that $|\alpha|$ will equal $|\beta|$ as long as condition (4.9a) is satisfied.

We want to be able to say that (4.9) implies $\alpha = \beta$. With this in mind, we will now show that the phase of α can always be chosen, consistent with the transformation T, referred to in Chapter Three, such that α and β have the same phase.

In general β will be a complex number:

$$\beta = \frac{(\varphi_0, \varphi_0^{(-1)})}{\sqrt{1-|(\varphi_0, \varphi_0^{(-1)})|^2}} = |\beta| e^{i\mu}$$

where μ will be determined by $(\varphi_0, \varphi_0^{(-1)})$.

We have shown in detail at the end of Chapter Three, how, (within the five coupled equation viewpoint) when ω undergoes a phase shift δ , that Σ and α also must undergo a phase shift of δ to be consistent with the mandatory relative-phase-preserving transformation T. The phase of ω is allowed to change freely as long as we are consistent with T. We have shown that consistent with T, α 's phase change must equal ω 's phase change. We can infer from these last two statements that consistent with T, ω 's phase can be made to change by such an amount that α's new phase will become β 's phase. This conclusion also follows from looking at equation (4.6):

$$w = \alpha\left(-1 + \frac{a^{-1}}{\alpha}\right)\phi_0 \qquad (4.6)$$

where $\frac{a^{-1}}{\alpha}$ is only a function of w through ε'. Since ε' is determined within the five coupled equation picture (see Chapter Three) and does not vary with the free phase shift of w (consistent with T) we see that (4.6) implies that when w undergoes a phase shift of γ so must α. Therefore by changing w's free phase we can change α's phase until it becomes β's phase.

With this understanding concerning the relative phases of α and β (that we can choose α's phase, consistent with T to equal β's phase) we will henceforth consider (4.9) as implying $\alpha = \beta$ rather than $|\alpha| = |\beta|$.

Consequently we can now say that w_0 will be a solution to (4.1') as long as condition (4.9a) is satisfied.

If condition (4.9a) is approximately satisfied, α will be approximately β and w_0 will be approximately the solution to (4.1').

The claim is that for large atoms (4.9a) is approximately satisfied and for such atoms w_0 is an approximate average excited state.

There is a consistency in the above argument in that if (4.9) is satisfied and α is in turn near β we see that comparing (4.2) and (4.4) $\varepsilon' - W_0^{(-)}$ will then be small satisfying (4.9b).

References for Chapter Four

1. See, for example, J. O. Hirshfelder, C. F. Curtis and R. B. Bird, Molecular Theory of Gases and Liquids (Wiley, New York, 1954), p. 952.

2. M. H. Mittleman, Phys. Rev. A6 3 (879) 1972.

Chapter Five

(I) Use of the Optimized Average Excited State to Calculate Scattering Amplitudes

(II) Appendix

(I) In Chapter One we discussed the two basic and related reasons that justify this investigation. The purpose of this Chapter is the use of the optimized average excited state (OAES) to extract electron-atom scattering information. For example, to use the optimized average excited state to optimally average (within the two state approximation) the effect of the inelastic channels on the elastic scattering. That is, assuming the approximation scheme for ω (of Chapter Four) holds for a given heavy atom, we will focus our attention on the two remaining coupled equations for F and G (2.36) and (2.38):

$$\left(\frac{p^2}{2} - T - V_S\right) F = v\, G \tag{2.36}$$

$$\left(\frac{p'^2}{2} - T - \bar{V}\right) G = \frac{v^*}{(\omega,\omega)} F \tag{2.38}$$

We want to extract scattering information from these two equations. Keeping this goal in mind, the two methods we will investigate are:

1) the angular momentum decomposed F and G equations (partial wave analysis) and 2) the eikonal approximation for the elastic scattering coefficient, F.

We will also study (in an appendix) the relationship of the WKB method to the eikonal approximation to justify a procedure used in our eikonal technique.

(I) The Angular Momentum Decomposed F and G Equations

Consider VS, V and v as defined in Chapter Two. If VS, V and v are spherically symmetric, it is then possible to angular momentum decompose (2.36) and (2.38) for F and G. For the following discussion, assume we are dealing with states φ_0 and ω_0 such that VS, V and v are spherically symmetric.

We then expand F and G in Legendre Polynomials:

$$F = \frac{1}{pr}\sum_{\ell=0}^{\infty} (2\ell+1)\, F_\ell(pr)\, P_\ell(\omega\theta) \tag{5.1}$$

$$G = \frac{1}{pr}\sum_{\ell=0}^{\infty} (2\ell+1)\, G_\ell(p'r)\, P_\ell(\omega\theta) \tag{5.2}$$

Substitute (5.1) and (5.2) into (2.36) and (2.38). Multiply both sides by $P_\ell(x)$ and integrate from -1 to 1.

This procedure leaves us with the angular decomposed F and G equations:

$$\left(\frac{1}{2}\frac{d^2}{dr^2} + \frac{p^2}{2} - VS - \frac{\ell(\ell+1)}{2r^2}\right) F_\ell = v\, G_\ell \tag{5.3}$$

$$\left(\frac{1}{2}\frac{d^2}{dr^2} + \frac{p'^2}{2} - \bar{V} - \frac{\ell(\ell+1)}{2r^2}\right) G_\ell = v^* F_\ell \tag{5.4}$$

We have $(\omega,\omega)=1$ from our ω_0 of Chapter Four. We want F and G to asymptotically satisfy the conditions:

$$F \sim e^{i\vec{p}\cdot\vec{r}} + \frac{e^{ipr}}{r} f_0 \tag{5.5}$$

$$G \sim \frac{e^{ip'r}}{r} f_1 \tag{5.6}$$

where f_0 is the elastic scattering amplitude and f_1 is the inelastic scattering amplitude into the average inelastic channel.

To insure (5.5) and (5.6) F_ℓ and G_ℓ must asymptotically satisfy:

$$F_\ell \sim i^\ell \sin(pr - \ell\pi/2) + \alpha_\ell e^{ipr} \tag{5.7}$$

$$G_\ell \sim \beta_\ell e^{ip'r} \tag{5.8}$$

The first term in (5.7) comes from the angular momentum decomposed plane wave:

$$e^{i\bar{p}\cdot\bar{r}} = \sum_{\ell=0}^{\infty} j_\ell(pr)\, i^\ell (2\ell+1) P_\ell(\cos\theta)$$

$$\sim \sum_{\ell=0}^{\infty} \frac{\sin(pr - \ell\pi/2)}{pr}\, i^\ell (2\ell+1) P_\ell(\cos\theta) \tag{5.9}$$

F_ℓ and G_ℓ must satisfy,

$$F_\ell(0) = G_\ell(0) = 0 \tag{5.10}$$

in order to have F and G finite at $r = 0$.

We now derive a Wronskian condition for the pair of equations (5.3) and (5.4). If (F_ℓ^a, G_ℓ^a) and (F_ℓ^b, G_ℓ^b) are two pairs of solutions to (5.3) and (5.4):

$$\frac{1}{2}\frac{d^2}{dr^2} F_\ell^a + \left[\frac{p^2}{2} - VS - \frac{\ell(\ell+1)}{2r^2}\right] F_\ell^a = v\, G_\ell^a \tag{5.11}$$

$$\frac{1}{2}\frac{d^2}{dr^2} G_\ell^a + \left[\frac{p'^2}{2} - VS - \frac{\ell(\ell+1)}{2r^2}\right] G_\ell^a = v\, F_\ell^a \tag{5.12}$$

$$\frac{1}{2}\frac{d^2}{dr^2}F_\ell^b + \left(\frac{p^2}{2} - VS - \frac{\ell(\ell+1)}{2r^2}\right)F_\ell^b = v\,G_\ell^b \tag{5.13}$$

$$\frac{1}{2}\frac{d^2}{dr^2}G_\ell^b + \left(\frac{p'^2}{2} - \bar{V} - \frac{\ell(\ell+1)}{2r^2}\right)G_\ell^b = v^*F_\ell^b \tag{5.14}$$

Multiply (5.11), (5.12), (5.13) and (5.14) by F_ℓ^b, G_ℓ^b, F_ℓ^a and G_ℓ^a respectively. After the multiplication, subtracting (5.13) from (5.11) leads to

$$\frac{1}{2}\left(F_\ell^b\frac{d^2}{dr^2}F_\ell^a - F_\ell^a\frac{d^2}{dr^2}F_\ell^b\right) = v\left\{G_\ell^aF_\ell^b - G_\ell^bF_\ell^a\right\} \tag{5.15}$$

Repeating this operation on (5.14) and (5.12) we find:

$$\frac{1}{2}\left(G_\ell^b\frac{d^2}{dr^2}G_\ell^a - G_\ell^a\frac{d^2G_\ell^b}{dr^2}\right) = v\left(G_\ell^bF_\ell^a - G_\ell^aF_\ell^b\right) \tag{5.16}$$

Adding (5.15) and (5.16) we find:

$$F_\ell^b\frac{d^2F_\ell^a}{dr^2} - F_\ell^a\frac{d^2F_\ell^b}{dr^2} + G_\ell^b\frac{d^2G_\ell^a}{dr^2} - G_\ell^a\frac{d^2G_\ell^b}{dr^2} = 0 \tag{5.17}$$

Equation (5.17) can now be written:

$$\left[F_\ell^b(F_\ell^a)' - F_\ell^a(F_\ell^b)'\right]' + \left[G_\ell^b(G_\ell^a)' - G_\ell^a(G_\ell^b)'\right]' = 0$$

or

$$F_\ell^b(F_\ell^a)' - F_\ell^a(F_\ell^b)' + G_\ell^b(G_\ell^a)' - G_\ell^a(G_\ell^b)' = \text{constant}$$

Utilizing equation (5.10) we have:

$$F_\ell^b (F_\ell^a)' - F_\ell^a (F_\ell^b)' + G_\ell^b (G_\ell^a)' - G_\ell^a (G_\ell^b)' = 0 \tag{5.18}$$

This equation (5.18) is the Wronskian condition for a pair of solutions to (5.3) and (5.4). We now investigate the Wronskian condition (5.18) as applied to the asymptotic forms of a pair of solutions to (5.3) and (5.4).

Assuming VS, V and v go to zero faster than $\frac{1}{r}$ for large r, any pair of solutions which vanish at r equals zero have asymptotic forms such that phase shifts can be defined.

$$F_\ell^a \sim \sin(pr - \ell\pi/2 + \delta_\ell') \tag{5.19}$$

$$G_\ell^a \sim \chi_\ell \sin(p'r - \ell\pi/2 + \delta_\ell^2) \tag{5.20}$$

$$F_\ell^b \sim Z_\ell \sin(pr - \ell\pi/2 + \delta_\ell^3) \tag{5.21}$$

$$G_\ell^b \sim \sin(p'r - \ell\pi/2 + \delta_\ell^4) \tag{5.22}$$

where χ_ℓ and Z_ℓ are mixing parameters which go to zero in the limit of small coupling (v = 0).

Applying the Wronskian condition (5.18) to these asymptotic forms leads to the condition:

$$Z_\ell p \sin(\delta_\ell^3 - \delta_\ell') + \chi_\ell p' \sin(\delta_\ell^4 - \delta_\ell^2) = 0 \tag{5.23}$$

This relationship (5.23) will provide a check on machine calculated values of $Z_\ell, \chi_\ell, \delta_\ell^1, \delta_\ell^2, \delta_\ell^3$, and δ_ℓ^4.

We next find the proper linear combination of solutions (F_ℓ^a, G_ℓ^a), (F_ℓ^b, G_ℓ^b) such that the boundary conditions (5.7) and (5.8) are satisfied. That is, we want A and B such that:

$$F_\ell = A F_\ell^a + B F_\ell^b \tag{5.24}$$

$$G_\ell = A G_\ell^a + B G_\ell^b \tag{5.25}$$

satisfy (5.7) and (5.8).

Substituting (5.19), (5.20), (5.21) and (5.22) into (5.24) and (5.25) we have:

$$i^\ell \sin(pr - \ell\pi/2) + \alpha_\ell e^{ipr}$$

$$= A \sin(pr - \ell\pi/2 + \delta_\ell^1) + B Z_\ell \sin(kr - \tfrac{\ell\pi}{2} + \delta_\ell^3) \tag{5.26}$$

$$\beta_\ell e^{ip'r} = A \chi_\ell \sin(p'r - \ell\pi/2 + \delta_\ell^2) + B \sin(p'r - \tfrac{\ell\pi}{2} + \delta_\ell^4) \tag{5.27}$$

If we want to only have outgoing spherical waves, A and B must satisfy:

$$A = \frac{i^\ell e^{-i(\delta_\ell^4 - \delta_\ell^2)}}{e^{-i(\delta_\ell^4 - \delta_\ell^2 + \delta_\ell^1)} - \chi_\ell Z_\ell e^{-i\delta_\ell^3}}$$

$$B = \frac{-i^{\ell}\chi_\ell}{e^{-i(\delta_\ell^4-\delta_\ell^2+\delta_\ell')} - \chi_\ell z_\ell e^{-i\delta_\ell^3}}$$

Substituting these A and B values back into (5.26) and (5.27) we find:

$$\alpha_\ell = \frac{1}{2i}\left\{-1 + \frac{e^{i(\delta_\ell'+\delta_\ell^2)} - \chi_\ell z_\ell e^{i(\delta_\ell^3+\delta_\ell^4)}}{e^{i(\delta_\ell^2-\delta_\ell')} - \chi_\ell z_\ell e^{i(\delta_\ell^4-\delta_\ell^3)}}\right\} \tag{5.28}$$

$$|\alpha_\ell|^2 = \frac{1}{2}\left\{1 + (\chi_\ell z_\ell)^2\left\{1-\cos(2\delta_\ell^3)\right\}\right.$$

$$-\chi_\ell z_\ell\left\{\cos(\delta_\ell^3+\delta_\ell^4-\delta_\ell'-\delta_\ell^2)+\cos(\delta_\ell^4-\delta_\ell^3+\delta_\ell'-\delta_\ell^2)\right.$$

$$\left.-\cos(\delta_\ell^4-\delta_\ell^3-\delta_\ell'-\delta_\ell^2)-\cos(\delta_\ell^2-\delta_\ell'-\delta_\ell^3-\delta_\ell^4)\right\}$$

$$\left.-\cos(2\delta_\ell')\right\} \Big/ \left\{1+(\chi_\ell z_\ell)^2 - 2\chi_\ell z_\ell\cos(\delta_\ell^4-\delta_\ell^3-\delta_\ell^2+\delta_\ell')\right\} \tag{5.29}$$

$$\beta_\ell = \frac{\chi_\ell}{2i}\,\frac{\left(e^{2i\delta_\ell^2}-e^{2i\delta_\ell^4}\right)}{\left(e^{-i(\delta_\ell^4-\delta_\ell^2)} - \chi_\ell z_\ell e^{-i(\delta_\ell^3-\delta_\ell^4)}\right)} \tag{5.30}$$

$$|\beta_\ell|^2 = \chi_\ell^2\,\frac{\sin^2(\delta_\ell^4-\delta_\ell^2)}{\left\{1+(\chi_\ell z_\ell)^2 - 2\chi_\ell z_\ell\cos(\delta_\ell'-\delta_\ell^2+\delta_\ell^4-\delta_\ell^3)\right\}} \tag{5.31}$$

The partial elastic cross section (Q_ℓ^{00}) is defined as the flux of elastically scattered projectiles of angular momentum ℓ divided by the total incident flux. The partial inelastic cross section (Q_ℓ^{01}) is defined as the quotient of the flux of inelastically scattered projectiles of angular momentum (which have excited the OAES w and left with a lowered (range of) energy corresponding to the incident energy minus the excitation energy of the OAES) to the total incident flux.

The partial elastic and inelastic cross sections Q_ℓ^{00} and Q_ℓ^{01} are then found in terms of $|\alpha_\ell|^2$ and $|\beta_\ell|^2$,

$$Q_\ell^{00} = \frac{4\pi}{p^2}(2\ell+1)|\alpha_\ell|^2$$

$$Q_\ell^{01} = 4\pi\frac{p'}{p^3}(2\ell+1)|\beta_\ell|^2$$

where p and p' are the projectiles' momenta in the elastic and inelastic channels respectively. We see that if $\delta_\ell^4 = \delta_\ell^2$ the inelastic scattering vanishes. Also if χ_ℓ (or using (5.23), Z_ℓ) vanishes the inelastic scattering vanishes. I.e., in the limit of small coupling (v or χ_ℓ and Z_ℓ small) we have

$$\alpha_\ell = \frac{1}{2i}\left(-1 + e^{2i\delta_\ell'}\right)$$

and

$$\beta_\ell = 0$$

as we expect for ordinary potential scattering in which all the scattering is elastic.

The above results for α_ℓ, β_ℓ, $|\alpha_\ell|^2$ and $|\beta_\ell|^2$ agree with Mott and Massey[1] where they treat the special case,

$$\delta_\ell' = \delta_\ell^2 \,, \quad \delta_\ell^3 = \delta_\ell^4 \tag{5.32}$$

$$Z_\ell = - \frac{\chi_\ell \rho'}{\rho} \tag{5.33}$$

Equation (5.33) is the Wronkian condition for the special case of (5.32).

The reason we are presenting this general result is that the specialized result with (5.32) is harder to use in practice. That is, to attempt to impose (5.32) by manipulating the small r boundary conditions on the F_ℓ and G_ℓ is not simple in practice.

The method outlined above will be particularly useful when only a small number of angular momenta describe the process under investigation. For short range potentials and low energy projectiles the number of angular momentum appreciably affected by the potential is small. (I.e. $\ell_{max} \sim \rho$. range). The great advantages of this method are (1) the replacement of a pair of coupled partial differential equations by a set of N (if N angular momenta are to be considered) pairs of total differential equations and (2) allowing us to follow the scattering of projectiles of a given angular momenta.

(II) The Eikonal Approximation to Calculate Elastic Scattering

We present in this section another formulation, the eikonal method, for the extraction of elastic scattering information within our two state model.

The eikonal technique gives good results for fast projectiles scattered near the forward direction.

Consider again the coupled equations

$$\left(\frac{p^2}{2} - T - VS\right) F^+ = v\, G^+ \tag{2.36}$$

$$\left(\frac{p'^2}{2} - T - \bar{V}\right) G^+ = v^x F^+ \tag{2.38}$$

We now eliminate $G^{(+)}$ from (2.36) by inverting the operator $\frac{p'^2}{2} - T - \bar{V}$ in (2.38) and substitute the $G^{(+)}$ thus found into (2.36).

We find:

$$\left(\frac{p^2}{2} - T - VS - v\, \mathcal{G}_{p';\bar{V}}\, v^x\right) F^+ = 0 \tag{5.34}$$

where $\mathcal{G}_{p';\bar{V}} = \left(\frac{p'^2}{2} - T - \bar{V}\right)^{-1}$

(5.34) is an equation for $F^{(+)}$ in terms of a non-local operator. After multiplying the non-local term of (5.34) by $F^{(+)}(\vec{r})\left[F^{(+)}(\vec{r})\right]^{-1}$ we find:

$$\left[\frac{p^2}{2} - T - VS - F^{-1}(\vec{r})\, v(r) \int \mathcal{G}_{p';\bar{V}}(\vec{r},\vec{r}')\, v^x(\vec{r}')\, F(\vec{r}')\right] F(\vec{r}) = 0 \tag{5.35}$$

where we replaced the non-local potential of (5.34) by a "local potential" dependent on F.

We will carry out the eikonal technique on equation (5.35). First, however, consider the eikonal technique in ordinary potential scattering.

The eikonal wave function, taken as:

$$\psi_{eik} = e^{i(\bar{p}\cdot\bar{r}+\Lambda)} \tag{5.36}$$

when substituted into equation (5.37) for ordinary potential scattering

$$\left(\frac{p^2}{2} - T - V\right)\psi = 0 \tag{5.37}$$

becomes

$$-\vec{p}\cdot\nabla\Lambda - \frac{1}{2}|\nabla\Lambda|^2 + \frac{i}{2}\nabla^2\Lambda - V = 0 \tag{5.38}$$

(5.38) is an exact equation. That is, no approximations have been made and if we could solve (5.38) for Λ, (5.36) would be the exact solution to (5.37). However, (5.38) is as difficult an equation to solve exactly as the original (5.37).

As in the case of light waves entering a region of smoothly varying index of refraction, an electron wave will not experience an appreciable distortion in a region where the potential doesn't change appreciably in a wavelength. E.g. such phenomena as interference and reflection will be small).

To be able to say that our incident plane wave is not much distorted in some region and therefore we can approximate Λ, we ask that the fractional change of the potential in a wavelength be small, i.e. $\lambda \frac{\Delta V}{V} \ll 1$

or $\lambda \ll \frac{V}{\Delta V} p$.

This condition will be easier to satisfy (for a smoothly varying potential) the smaller the incident particles wavelength or equivalently the higher the incident particles energy.

For a smoothly varying potential, we therefore seek a high energy approximation for Λ . The hope is therefore to be able to expand Λ as a power series in $1/p$,

$$\Lambda = \frac{\Lambda_1}{p} + \frac{\Lambda_2}{p^2} + \frac{\Lambda_3}{p^3} + \cdots \tag{5.39}$$

and thus, in the high energy limit, Λ will be a small correction to a plane wave solution. With (5.39) substituted into (5.38), the terms of (5.38) will have the following p dependence:

$$\bar{p}\cdot\nabla\Lambda \sim O(p^0)$$
$$|\nabla\Lambda|^2 \sim O(p^{-2})$$
$$\nabla^2\Lambda \sim O(p^{-1})$$
$$V \sim O(p^0)$$

Keeping terms of $O(p^0)$, (5.38) becomes

$$-\bar{p}\cdot\nabla\Lambda - V = 0 \tag{5.40}$$

$$\Lambda(\vec{b},z) = -\frac{1}{p}\int_{-\infty}^{z} V(\vec{b},z')\,dz' \tag{5.41}$$

where $\vec{P}$ is chosen in the $+Z$ direction (and $\vec{b}$ is perpendicular to $\vec{P}$). The limits of integration insure the incoming plane wave boundary condition at $Z = -\infty$. There are problems (notably, time reversal invariance) involved in (5.36) with Λ given by (5.41) but these have been studied extensively[2] and will consequently not concern us here. (E.g. we can avoid the time reversal problem by changing our path of integration). At this point it should be noted that there are alternate but equivalent ways to arrive at (5.40) from (5.38).[3]

We concern ourselves here with how this eikonal formalism could be applied to (5.35). The obvious difference is that (5.35) includes an essentially non-local potential.

In our presenting this multichannel eikonal approximation MEA we recognize that other improved MEA techniques exist (e.g. the curvature of the path has been included[4]). In fact, it turns out (see Chapter Six) that in the problem we are interested in, the criteria for the eikonal technique are not satisfied. The main reason we are presenting this MEA is to provide a simple but instructive comparison of the elastic scattering in the MEA found using an optimized rather than prechosen average excited state in the optical potential method[5].

Consistent with the approximations we have of (1) high $P^2/2$ (2) small distortion of the wave function from the plane wave, we can linearize the kinetic energy operator in the bilinear form of this non-local potential's greens function. A factor of $1/P'$, arises from this procedure (see later on in this chapter for details) of linearization.

That is, the potential of (5.35):

$$V = VS + F^{-1} v \mathcal{G}_{p';\bar{v}} v^{x} F \tag{5.42}$$

will have a factor of $1/p'$ in the second term when $\mathcal{G}_{p';\bar{v}}$ is linearized.

Now $\frac{p'^2}{2} = \frac{p^2}{2} + W_0 - \epsilon$ as defined in Chapter Two. For high p, $p' \sim p$ and the second term in the potential has an essentially $1/p$ dependence.

Now if we want to keep the entire V (5.42) in the eikonal approximation, we should (looking back at equation (5.38)) also keep the $\nabla^2 \Lambda$ term since it has a $1/p$ dependence. (I.e., we are keeping terms up to Λ_2 in the $1/p$ expansion). The problem with this is that $\nabla^2 \Lambda$ can be shown to diverge. We believe that a natural solution to this problem lies in looking at the eikonal expansion as a special case of the WKB approximation (an expansion in $\hbar$). This is discussed in an appendix. In this $\hbar$ expansion, $\nabla^2 \Lambda$ is of a higher order in $\hbar$ than the non-local term in our potential and can consequently be ignored to the order in $\hbar$ we are considering.

We will therefore proceed to eikonalize equation (5.25) with the non-local potential included in the generalization of (5.40). The generalization of (5.40) in our two state model is:

$$-p \cdot \nabla \Lambda - VS - F^{-1} v \mathcal{G}_{p';\bar{v}} v^{x} F = 0 \tag{5.43}$$

Write the bilinear form of $\mathcal{G}_{p';\bar{v}}$:

$$\mathcal{G}_{p';\bar{v}} = \int \frac{d\vec{k}\ \psi_{\vec{k}}(\vec{r})\, \psi^{*}_{\vec{k}}(\vec{r}')}{p'^2 - k^2 + i\epsilon} \tag{5.44}$$

(The terms of the bound state part of $\mathcal{G}_{p';\bar{V}}$ are $O\left(\frac{1}{p^2}\right)$ [6] and therefore will not be considered) where $\psi_{\vec{k}}$ satisfies:

$$\left(\frac{k^2}{2} - T - \bar{V}\right)\psi_{\vec{k}} = 0 \tag{5.45}$$

Let q (the momentum transfer) be defined as:

$$\vec{q} = \vec{k} - \vec{p}'$$

Now make the following approximations (consistent with the eikonal approximations):

(1) $$k^2 = q^2 + 2\vec{q}\cdot\vec{p}' + p'^2 \cong 2\vec{q}\cdot\vec{p}' + (p')^2$$

where q^2 is small for high p and scattering near the forward direction. This last process linearizes the denominator of (5.44).

(2) Take for ψ_k its eikonal approximation:

$$\psi_k = e^{i\vec{k}\cdot\vec{r} - \frac{1}{k}\int \bar{V} dz} \tag{5.46}$$

Changing the integration variable in (5.44) we find using the above approximations:

$$\mathcal{G}_{p';\bar{V}} = e^{i\vec{p}'\cdot(\vec{r}-\vec{r}')}\left[e^{\frac{i}{p'}\left[\int_{-\infty}^{z'} \bar{V}(b,z'')dz'' - \int_{-\infty}^{z} \bar{V}(b,\tilde{\tilde{z}})d\tilde{\tilde{z}}\right]}\right] \cdot \left[\frac{-i}{2p'}\,\delta^{(2)}(\vec{b}-\vec{b}')\,\Theta(z-z')\right] \tag{5.47}$$

Similarly, eikonalize F and F^{-1}, inside the non-local potential (keeping only the VS term in their eikonals here; the non-local part has a $1/p$ factor and is smaller

than VS for large p^2).

Using (5.47) and the eikonalized forms for F, F^{-1}, ψ , ψ^x we have:

(again choosing the z axis as the incident momentum direction)

$$\Lambda(\vec{b},z) = -\frac{1}{p}\left[\int_{-\infty}^{z} VS(\vec{b},\tilde{z})\,d\tilde{z} - \frac{i}{p'}\int_{-\infty}^{z} d\tilde{z}\, v(\vec{b},\tilde{z})\cdot\right.$$

$$\cdot e^{\left[i/p\int_{-\infty}^{\tilde{z}} VS(b,\tilde{\tilde{z}})d\tilde{\tilde{z}} - i/p'\int_{-\infty}^{\tilde{z}} \bar{V}(b,\tilde{\tilde{z}})d\tilde{\tilde{z}}\right]}$$

$$\cdot \int_{-\infty}^{\tilde{z}} dz'\, e^{-i\xi(\tilde{z}-z')} \cdot e^{i\left[1/p'\int_{-\infty}^{z'} \bar{V}(b,\hat{z})d\hat{z} - \frac{1}{p}\int_{-\infty}^{z'} VS(b,\hat{z})d\hat{z}\right]}$$

$$\cdot \psi^x(\vec{b},z')$$

(5.48)

where $\xi = \Delta/p$ and $\Delta = \frac{p^2}{2} - \frac{p'^2}{2}$ is the excitation energy.

To evaluate the elastic scattering amplitude in the eikonal approximation:

$$f^{\text{elastic}}_{\text{eikonal}} = \langle e^{i\vec{k}_f\cdot\vec{r}} | V | \psi^{\text{eikonal}}_{k_i} \rangle$$

Now in the eikonal approximation choosing the z axis as the incident direction (5.40) and (5.43) gives us

$$V = -p\frac{\partial \Lambda}{\partial z}$$

and

$$f^{\text{elastic}}_{\text{eikonal}} = \int e^{i(\vec{p}_i - \vec{p}_f)\cdot\vec{r}} - p\frac{\partial \Lambda}{\partial z} e^{i\Lambda(\vec{b},z)}$$

Again for scattering near the forward direction (with high p) we have q almost perpendicular to the incident direction.

$$\vec{q}\cdot\vec{r} = \vec{q}\cdot\vec{b} + \vec{q}\cdot z\hat{z} \cong \vec{q}\cdot\vec{b}$$

Therefore the z integration is always double in the eikonal approximation (as long as we can write $-\rho\cdot\nabla\Lambda = V$) and

$$f^{\text{elastic}}_{\text{eikonal}} = -\rho\int e^{i\vec{q}\cdot\vec{b}}\, d^2b\left[e^{i\Lambda(\vec{b},\infty)} - 1\right]$$

where Λ is given by (5.48). We see that a great advantage of the eikonal technique is that the z integration of the elastic scattering amplitude is always immediately done.

We will now compare these results with the eikonalized optical potential method (EOPM)[5]. In the EOPM the technique is to expand the optical potential and keep one term beyond the static potential[5]. In the context of the optical potential method to consider a single average inelastic channel the following approximations are made:[5]

(1) The replacement of the excitation energies to the intermediate states of the target by an average excitation energy Δ , enabling a completeness sum to be carried out.

(2) With approximation (1) the term beyond the static term in the optical potential contains A($\vec{r}, \vec{r}'$) defined as:[7]

$$A(\vec{r},\vec{r}') = \int d\vec{x}\, d\vec{x}'\ \varphi_0^*(\vec{x})\, V(\vec{r},\vec{x})$$
$$\left[\delta(\vec{x},\vec{x}') - \varphi_0(\vec{x})\varphi_0^*(\vec{x}')\right] V(\vec{x}',\vec{x}')\,\varphi_0(\vec{x}')$$

(where V is the interaction of the projectile with all the target particles). The second approximation consists of replacing A($\vec{r}, \vec{r}'$) by a separable approximation, namely: $A(\vec{r},\vec{r}') = v(\vec{r})v(\vec{r}')$

which replaces all the inelastic channels by a single average inelastic one.

If we compare the equations for the eikonal found by this technique (equation (3.6) of Reference (5)) with equation (5.48) we find that the former has a $\overline{V}$ term missing throughout.

This is due to the fact that the single inelastic channel has been imposed on the optical potential method, rather than in some way optimizing the choice of average inelastic channel within the optical potential framework.

The simple close coupling equations, for any two state problem, can be derived from a Kohn variational principle. Therefore, no matter what the two states are (either optimized or prechosen) the best way to find their coefficients is by using:

$$\left(\frac{p^2}{2} - T - VS\right) F = v G \qquad (5.49)$$

$$\left(\frac{p'^2}{2} - T - \overline{V}\right) G = v^* F \qquad (5.50)$$

i.e. an extremized choice (within the two state problem) contains VS and V in a symmetric way.

In the choosing of an average inelastic channel in the optical potential method, we are in effect solving (5.49) and (5.50) with $\overline{V}$ set equal to zero, i.e.

$$\left(\frac{p^2}{2} - T - VS\right) F = v\, G \tag{5.51}$$

$$\left(\frac{p'^2}{2} - T \quad\right) G = v F \tag{5.52}$$

Since (5.49) and (5.50) are the optimum choice for coefficients in the two state method they must be an improvement on (5.51) and (5.52).

We see here how imposing, rather than optimizing, the average excited state at a point in a given method can lead to coefficients F and G for the scattering which are in error. This example in itself is another justification of the optimization rather than prechoice of the average inelastic channel.

Note should be made of the fact that although $\overline{V}$ doesn't appear in the first term beyond VS, (in imposing the average inelastic channel on the optical potential) $\overline{V}$ will appear in the second term beyond VS (in the imposed average inelastic channel on the optical potential).

We are claiming here that the work here with ω optimized is an improvement for elastic scattering on the average inelastic channel imposed on the optical potential, keeping one term beyond VS.

However, we are not making any claims about the relative merits of the two methods if $A(\vec{F}, \vec{F}')$ is not separated.

Appendix - Chapter Five

A Relationship between the WKB and Eikonal Technique

The already mentioned (Chapter Five) conditions for the eikonal approximation on the smoothness of the potential and the incident energy imply that the specifically quantum mechanical features arising from the wave properties of matter will not be important and a semi-classical description will be adequate. The purpose of this appendix is to discuss this viewpoint and thereby compare the WKB and eikonal techniques.

The WKB approximation is a technique valid when quantum mechanical effects are not of very great moment. We can see from the high energy smooth potential condition:

$$\lambda \frac{\Delta V}{V} \ll 1 \tag{5.53}$$

with $\lambda = \frac{\hbar}{p}$ that

$$\hbar \ll \frac{V}{\Delta V} p$$ and

therefore h being small compared to $\frac{V}{\Delta V} p$ is equivalent to (5.53). The WKB method is an expansion of the wave function in powers of $\hbar$. We therefore would expect a close relationship between the WKB and eikonal techniques.

Consider the Schroidinger equation:

$$\left[E + \frac{\hbar^2}{2m} \nabla^2 - V\right] \psi = 0 \tag{5.54}$$

(We are not using atomic units here.) The fact that the potential is slowly varying implies that the wave function will take a form not changed much from what it would be with a constant potential, i.e. with a constant V,

$$\psi = e^{i\vec{p}\cdot\vec{r}/\hbar} \qquad \text{where} \quad |\vec{p}| = \sqrt{2m(E-V)}$$

and guided by this form we try

$$\psi = e^{iS} \qquad \text{where} \tag{5.55}$$

we will expand $$S = \frac{S_0}{\hbar} + S_1 + S_2\hbar + \cdots \tag{5.56}$$

Substituting (5.55) into (5.54)

$$E - V + \frac{\hbar^2}{2m}\left\{ i\nabla^2 S - |\nabla S|^2 \right\} = 0 \tag{5.57}$$

Now substituting (5.56) into (5.57) we find:

$$E - V + \frac{\hbar^2}{2m}\left\{ i\left(\frac{\nabla^2 S_0}{\hbar} + \nabla^2 S_1 + \cdots \right) - \left| \frac{\nabla S_0}{\hbar} + \nabla S_1 + \cdots \right|^2 \right\} = 0 \tag{5.58}$$

To $O(\hbar^0)$ then we have:

$$(E - V) = \frac{|\nabla S_0|^2}{2m} \tag{5.59}$$

An obvious solution to (5.59) is then:

$$\vec{p}(\vec{r}) = \nabla S_0 \tag{5.60}$$

and we write:

$$S_0(\vec{r}) = \int_{\vec{R}_0}^{\vec{r}} \vec{p} \cdot d\vec{r} \tag{5.61}$$

where $\vec{R}_0$ is an arbitrary constant vector (i.e. to any point outside the distorting potential). Now to $O(\hbar)$ we have from (5.58)

$$\left\{E - V + \frac{i\hbar}{2m}\nabla^2 S_0 - |\nabla S_0|^2 - \hbar\frac{\nabla S_0 \cdot \nabla S_1}{2m}\right\} = 0 \tag{5.62}$$

Using (5.60) in (5.62) we have

$$i\nabla^2 S_0 - 2\nabla S_0 \cdot \nabla S_1 = 0 \tag{5.63}$$

(5.60) will make (5.63) become

$$i\nabla\cdot\vec{p} - 2\vec{p}\cdot\nabla S_1 = 0 \tag{5.64}$$

The complicating factor in the three dimensional WKB form (5.63) (which doesn't appear in the one dimensional case) is that $\vec{p}$'s direction is not in general constant.

However, consistent with the other assumption in the WKB approximation consider the direction of $\vec{p}$ as close to the forward direction (i.e. $\hat{p} \approx \hat{p}_i$). Choosing z as the direction of $\vec{p}_i$, we are assuming

$$p_x, p_y \ll p_z$$

$$p_z \approx p$$

and (5.63) becomes:

$$2p\frac{\partial S_1}{\partial z} = i\frac{\partial p}{\partial z}$$

$$S_1 = \frac{i}{2}\ln p + f(x,y)$$

$f(x,y)$ has $\frac{\partial f}{\partial z}$ equal to zero and therefore f doesn't depend on p (since if f depended on p, $\frac{\partial f}{\partial z} = \frac{\partial f}{\partial p}\frac{\partial p}{\partial z} \neq 0$). Therefore, in the small p^2 limit (with constant V) the wave function would have the form $e^{i f(x,y)}$ an unphysical limit. We therefore choose f to be a constant and for convenience and without loss of generality set it equal to zero.

We therefore have:

$$S_1 = \frac{i}{2}\ln p \tag{5.65}$$

We therefore have using (5.61) and (5.65) ψ_{WKB} to $O(\hbar)$ as:

$$\psi_{WKB} = \frac{1}{\sqrt{|\vec{p}|}}\, e^{i\int_{\vec{R}_0}^{\vec{r}} \frac{\vec{p}\cdot d\vec{r}}{\hbar}}$$

In the usual eikonal method we take ψ_{eik} equal to $e^{i(k\cdot r+\Lambda)}$ which is particularly well suited for the specific scattering type of problem in which an incident plane wave enters a region of a slowly varying potential, and Λ describes its distortion.

The equation for Λ , (5.38) (with $\hbar$ not set equal to one)

$$\left(-2\vec{k}\cdot\nabla\Lambda - |\nabla\Lambda|^2 + i\nabla^2\Lambda - \frac{2mV}{\hbar^2}\right) = 0 \tag{5.67}$$

If now guiding ourselves by the WKB example (whose criteria are identical to those of the eikonal method; the difference being that in the eikonal technique an incident plane wave boundary condition, (useful for scattering problems) is imposed on the wave function) we set out to expand Λ in powers of $\hbar$ rather than 1/p:

$$\Lambda = \frac{\Lambda_0}{\hbar} + \Lambda_1 + \Lambda_2 \hbar + \cdots$$

we then find to $O(\hbar^{-2})$ equation (5.67) becomes:

$$-2\vec{p}_i \cdot \nabla\Lambda_0 - |\nabla\Lambda_0|^2 - 2mV = 0 \tag{5.68}$$

and the Λ_0 is found to be:

$$\Lambda_0 = \int_{\vec{r}_0}^{\vec{r}} \vec{p} \cdot d\vec{r} - \vec{p}_i \cdot (\vec{r} - \vec{r}_0) \tag{5.69}$$

where $\vec{r}_0$ is the point the incident particle enters the force field: ensuring us that $\Lambda(\vec{r}_0) = 0$.

Equation (5.69) for $\hat{p} \approx \hat{p}_i$ and $\frac{p_i^2}{2m} \gg V$ becomes (with $\hat{p}_i = \hat{z}$):

$$\Lambda_0(\vec{r}) = -\frac{1}{v_i} \int_{z_0}^{z} V(b, z')\, dz' \tag{5.70}$$

where $v_i = p_i/m$, our usual eikonal result.

In the eikonal expansion of Chapter Five for the case of the coupled F and G equations the potential:

$$V = VS + F^{-1} v \, \mathcal{S}_{p_i} \bar{v} \, v^* F \tag{5.71}$$

appears. The second term which is non-local (as discussed in detail in Chapter Five) when linearized has a $1/p$ factor, which led us to believe that we should include the term $i\nabla^2\Lambda$ (which diverges). It is now clear however, that a more fundamental viewpoint would be to consider the eikonal expansion as an $\hbar$ expansion for $\frac{p_i^2}{2m} \gg V(r)$ and $\hat{p} \approx \hat{p}_i$. In fact we will now demonstrate that for $\frac{p_i^2}{2m} \gg V(r)$ and $\hat{p} \approx \hat{p}_i$, the WKB solution (to lowest order in $\hbar$) yields the eikonal result.

Equation (5.68) is the eikonal equivalent of (5.59). That is,

$$E - V = \frac{|\nabla S_0|^2}{2m} \tag{5.59}$$

is the WKB generalization of:

$$-2\vec{p}_i \cdot \nabla\Lambda_0 - |\nabla\Lambda_0|^2 = 2mV = 0 \tag{5.68}$$

The WKB method is more general in that nothing is assumed about the form of the wave before the distortion due to the potential takes place. If we impose (the convenient scattering initial condition) that the undistorted form is a plane wave and look at the direction of $\vec{p}$ as close to $\vec{p}_i$ (consistent with p^2 large and V slowly varying) we should get the eikonal approximation from (5.72) below:

$$\psi^0_{WKB} = e^{iS_0/\hbar} = e^{i\int_{\vec{r}_0}^{\vec{r}} \vec{p}\cdot d\vec{r}/\hbar} \tag{5.72}$$

$$\psi_{eikonal} = e^{\frac{i}{\hbar}\left[\vec{p}_i \cdot \vec{r} - \frac{1}{v_i}\int_{-\infty}^{z} V\, dz\right]} \tag{5.73}$$

For $\hat{p}$ near $\hat{p}_i$ (taken as $\hat{z}$) we can write the WKB S_0 as:

$$S_0 = \int_{\vec{R}_0}^{\vec{\Lambda}} \vec{p} \cdot d\vec{r} \cong \int_{z_0}^{z} p_z \, dz \simeq \int_{z_0}^{z} p \, dz$$

For

$$\frac{p_i^2}{2m} \gg V(\Lambda)$$

$$p = [2m(E-V)]^{1/2} = (2mE)^{\frac{1}{2}} \left(1 - \frac{V}{E}\right)^{\frac{1}{2}}$$

$$\simeq p_i \left(1 - \frac{V}{2E}\right) = p_i - \frac{1}{v_i} V$$

(where $v_i = p_i/m$)

and the result is essentially the eikonal form (5.73).

Note that the usual eikonal form (as written in (5.73)) has

(i.e. the possibility of the potential having an infinite range is considered), and that under these circumstances the WKB form:

$$S_0 = \int_{\vec{R}_0}^{\vec{R}} \vec{p} \cdot d\vec{\Lambda} = p(z - z_0) - \frac{1}{v_i} \int_{z_0}^{z} V(\vec{b}, z') \, dz'$$

should have its constant z_0 chosen so that $p z_0 - \frac{1}{v_i} \int_{-\infty}^{z_0} V \, dz$ equals zero, to insure the eikonal boundary conditions.

With this viewpoint (that the eikonal expansion is a special case of the WKB method) we note that the second term in the potential (5.71) (although having a $1/p$ when linearized) is along with VS of order $O(k^{-2})$ in (5.67) whereas the $i\nabla^2\Lambda$ is $O(k^{-1})$. Therefore, with this view, the entire V of (5.71) can be taken (linearized or not) consistently without the inclusion of the divergent $i\nabla^2\Lambda$ term.

In conclusion, we note that the ultimate (if we went higher in $\hbar$ terms) inclusion of divergent terms is attributable to the semi-convergent[8] nature of the WKB expansion. However, we have shown here, that to the order needed to include the entire potential no divergent term appears.

References for Chapter Five

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Chapter Six

The Use of the Results of Chapters Four and Five in the Particular Case of e - Argon Scattering

There are several related purposes of this chapter. The first is to check the orthogonalized negative isoelectronic ion approximation (of Chapter Four) for a specific heavy atom: Argon. We then calculate VS, $\overline{V}$ and v for this atom using Hartree-Fock wave functions and determine an appropriate method to extract electron atom scattering information. Finding that v is a short range potential, we then pay particular attention to the effect that the OAES plays in large angle elastic scattering.

In this chapter, we also try to give some physical reality to the OAES. Two methods will be attempted in this assignment: (1) calculate the width (spread in energy) of the OAES. This width might (depending on its size compared to the energy) allow us to interpret (in the case of electron - Argon scattering) the ground state of the orthogonalized negative isoelectronic ion $Cl^{(-)}$ as a decaying state excited by the projectile and having a lifetime determined by this spread in energy and the uncertainty principle. The projectile would then leave with a (spread of) lowered energy and the target decays into eigenstates of Argon.

(2) To look for structure in the scattering cross sections as a function of energy. If, for example, around a particular incident energy there is a bump in the elastic scattering we could associate this structure with a resonance. At this energy the projectile has an appreciable time delay (i.e. time spent in the potential

of the target) associated with this rapid variation of the scattering. To somehow associate this resonance with the OAES we must compare this scattering with that produced solely by the static potential (VS). The non-local operator (and the OAES) could affect the elastic scattering directly (e.g. via a resonance) or through the interference of its scattering with that of VS and produce an appreciable effect even though v itself could be small. In the summary we mention how these effects might be experimentally determined.

(I) Check of the Negative Isoelectronic Approximation for the Optimized Average Excited State in the Case of the Argon Atom

Taking for the atomic wave functions the Slater determinant:

$$\frac{1}{\sqrt{N!}} \left| \{ \varphi_{n\ell m} \} \right|$$

where $\varphi_{n\ell m}$ is an orbital.

In the Clementi tables[1] these orbitals are expanded in terms of basis functions according to:

$$\varphi_{n\ell m} = \sum_{p} \chi_{p\ell m} C_{n\ell_p}$$

The subscript p refers to the p^{th} basis function. The basis functions χ are Slater-type orbitals with integer quantum numbers, namely

$$\chi_{p\ell m} = R_{\ell p}(r) Y_{\ell m}(\theta, \varphi)$$

where

$$R_{\ell p} = \left[(2n_{\ell p})! \right]^{-\frac{1}{2}} (2\zeta_{\ell p})^{n_{\ell p} + \frac{1}{2}} \cdot r^{n_{\ell p} - 1} e^{-\zeta_{\ell p} r}$$

and $Y_{\ell m}(\theta, \phi)$ are normalized spherical harmonics in complex form. Note that $n_{\ell p} \geq \ell + 1$ (the $n_{\ell p}$ are chosen, it seems, from experience) and the exponents $\zeta_{\ell p}$ are then determined via an optimization process to give the best energy. This analytic fit to numerical Hartree-Fock solutions is accurate to at least four significant figures.

Using these tables[1] for Argon and its negative-isoelectronic-ion $Cl^{(-)}$ (ground state) we find with:

$\varphi_0 =$ The Ar ground state

$\varphi_0^{(-)} =$ The $Cl^{(-)}$ ground state

that $(\varphi_0, \varphi_0^{(-)}) = .80865$

and $|(\varphi_0, \varphi_0^{(-)})|^2 = .65391$

Therefore we see that for the case of Ar and $Cl^{(-)}$ the ground state overlap is a significant fraction of one. From the completeness relation:

$$\sum_{n=0}^{\infty} |\langle \varphi_0 | \varphi_n^{(-)} \rangle|^2 = 1$$

we see that $$\sum_{n\neq 0}^{\infty} |\langle \varphi_0 | \varphi_n^{(-)} \rangle|^2 = .34609$$

For $\varphi_n^{(-)}$ corresponding to an excited state in the continuum $|\langle \varphi_0 | \varphi_n^{(-)} \rangle|^2$ will be a very small fraction of one. Since the lowest excited state of $Cl^{(-)}$ easily autodetaches to neutral Cl plus a free electron[2], the lowest excited state of $Cl^{(-)}$ is not strongly bound. Therefore no excited state of $Cl^{(-)}$ will have a significant overlap with φ_0 . In fact, since all the contributions in the sum are positive and their sum is .34609 no single term will be a significant fraction of .34609 and (4.9a) is satisfied. Consequently, $\alpha \approx \beta$ (see Chapter Four) and the ground state of $Cl^{(-)}$ orthogonalized to the ground state of Ar, should be a good approximation for ω the optimized average excited state of Ar.

Having justified the use of the negative ion approximation in the case of Argon, the next step is to calculate the potentials VS, $\bar{V}$ and v (as defined in Chapter Two).

The results of these calculations are listed in Tables (1, 2, 3) and graphed in Figures (1, 2, 3). Figure 4 is a comparison of these three potentials.

We note that: (1) For all r the magnitude of v is much smaller than VS or $\overline{V}$, (2) the range of v (the distance v becomes $e^{-1} v(0)$) is approximately .25a_0, (3) $\overline{V}$ always has a magnitude greater than VS due to $\phi_0^{(-)}$ being less tightly bound than ϕ_0.

Note also that the orthogonality of φ_0 and w_0 determines that the nuclear part of the potential plays no role in v. This point is critical, since it makes v a bounded potential for all r, unlike VS and $\overline{V}$ which are unbounded for small r.

The small r limit of v is determined by $\langle \phi_0 | \sum_{i=1}^{18} 1/r_i | w_0 \rangle$ a finite small constant. Its smallness is due to the fact that $1/r_i$ has its major contribution for small r_i where the inner orbitals of ϕ_0 and $\phi_0^{(-)}$ play a major role. The inner orbitals of ϕ_0 and $\phi_0^{(-)}$ are the most similar and consequently ϕ_0 and w_0 are the most dissimilar in this region. Further out in r_i where ϕ_0 and w_0 might be expected to have a somewhat more significant contribution the $\frac{1}{r_i}$ gets small wiping this out. Thus, for both large and small r_i the contributions to v(0) are small. This is marked contrast to VS and $\overline{V}$ which are both dominated by a large nuclear attraction (and unbounded) for small r.

For large r the leading terms in VS, $\overline{V}$ and v are:

$$VS \cong \langle \varphi_0 | \sum_{i=1}^{18} \vec{r}_i \cdot \hat{r} | \varphi_0 \rangle \frac{1}{r^2}$$

$$\overline{V} \cong \langle w_0 | \sum_{i=1}^{18} \vec{r}_i \cdot \hat{r} | w_0 \rangle \frac{1}{r^2}$$

$$v \cong \langle \varphi_0 | \sum_{i=1}^{18} \vec{r}_i \cdot \hat{r} | w_0 \rangle \frac{1}{r^2}$$

In deriving these last expressions we assume $r > \chi_i$. It seems reasonable that this point (at which $r > \chi_i$) will occur in these integrals for VS and $\overline{V}$ "outside the atom" in the state ϕ_o and w_o respectively.

However, in v, the coupling potential between orthogonal states, this point is likely to occur at a smaller r value. Consequently, we can understand that this $1/r^2$ behavior occurs sooner for v than for VS or $\overline{V}$ contributing to v falling off more rapidly than either VS or $\overline{V}$.

v(o) is 3.36 a.u. a very small number compared to VS(.1) (which is -128.7 a.u.) and v approaches v(o) smoothly as r goes to zero.

(II) The Use of VS, $\overline{V}$ and v to Calculate Electron Argon Scattering Information

One of the things we are interested in is the effect the average inelastic channel has on the elastic scattering.

The smallness of the size and range of v for the case of A $-Cl^{(-)}$ implies that the incident electron must get close in to feel the effect of the OAES. We therefore want to deal with a situation in which the electron comes in with a very small impact

parameter and where backscattering will be the principle process. The closer in the electron gets, however, the larger VS and V get in comparison to v. Consequently, the effect of v on the elastic scattering will not be expected to be particularly large. In our situation, the optimized average inelastic channel plays a role in the elastic scattering only at very large angles.

Note that even though v is small, once the projectile is in the range of v a major contribution from the OAES to the large angle elastic scattering could occur due to: (1) a resonance from $(p'^2 - T - V)^{-1}$ in the non-local part of the potential or (2) the interference of the scattering from the local and non-local parts of this potential.

For this type of problem, of the two methods mentioned in Chapter Five, one (the eikonal) is particularly ill-suited while the other (the partial wave analysis) is ideal. The reasons that a partial wave analysis is considered well suited for our problem are:

(1) VS, $\overline{V}$ and v are spherically symmetric, (for the closed shell ground states of Ar and $Cl^{(-)}$) enabling us to simply angular momentum decompose the F and G equations.

(2) Within the spherically symmetric two state problem then the projectile's angular momentum will be a good quantum number and it becomes interesting to watch the scattering of particles of specific angular momenta.

(3) The smallness of v's range tells us that only a small number of angular momenta play a role in the process of interest ($\ell_{max} \sim p \cdot range$).

(4) The resulting coupled equations for F_ℓ and G_ℓ can be rewritten as four

coupled first order differential equations and there are prepackaged machine programs to handle this situation.

The condition for the eikonal method requiring $\hat{p} \approx \hat{p}_i$ is certainly not satisfied for large angle scattering, making this method unapplicable. There are other methods, which could subsequently be carried out (e.g. the distorted Born method; or weak coupling approximations[3]), but the features (3) and (4) above convinced us to proceed with these angular momentum decomposed equations.

The results carried out by the method detailed in Chapter Five are listed for Q_ℓ^{00} (the partial elastic scattering amplitude), Q_ℓ^{01} (the partial inelastic scattering amplitude) for e - Argon scattering (see Tables (5, 6, 7, 8) and Figures (5 - 10)) with l equals zero, one and two and incident energy from 7.45071 a.u. to 31.45071 a.u. (7.45071 a.u. is the excitation energy $\epsilon - W_0$).

Tables (5 , 6 , 7) and Figures (5 , 6 , 7) show the effect of the inclusion of the optimized average inelastic channel on the elastic scattering (for angular momentum quantum numbers 0, 1 and 2). This is done by comparing (see Figures (5, 6 , 7)) the results of elastic scattering with and without the coupling to the inelastic channel. The difference of these curves (see Figs. (5 , 6, 7)) indicates the magnitude of the optimized average excited state's effect on the elastic scattering. Since the coupling to the OAES has an absorptive part, we might expect that at any given incident energy the elastic scattering with the coupling included will be smaller than with VS alone.

However, we notice for l equals one a crossing of these curves. The crossing could be explained by a possible interference effect of the scattering off VS and $v^x/\beta_{p;\bar{v}}\ v$ in the backward direction.

Neither of the above mentioned ways that the OAES can have (in the case of small v) a large influence on the large angle elastic scattering occur in our situation. Then as expected, there is not much of an effect with the inclusion of v since as previously mentioned v $\ll$ VS and the form of the scattering follows VS closely.

Looking at the inelastic partial cross sections (Table (8) and Figures (8, 9, 10)) we note first that Q_0^{01} is always less than Q_1^{01} for all energies. At first this might seem surprising since the particle with l equals zero feels the innermost portion of v (where v reaches its maximum value). This innermost region is essentially excluded from the range of the l equals one particle. However we can explain this result by looking at the classical turning point (CTP) for l equals one (and the energies under consideration) and at the shape of v itself. (The CTP is taken here to be the value of r for which $\frac{p^2}{\Sigma} - \frac{l(l+1)}{2r^2} - VS$ itse vanishes.)
van

For projectiles with l equal to one the CTP is $\approx .05\ a_0$ for the lowest
For projectiles with l equal to one the CTP is $\approx .05\ a_0$ for the lowest energy here considered. Consequently, a very small region is being excluded from the l equals one situation. Secondly, the potential v is very slowly varying in this innermost region. This makes the effective force for the "push" (scattering) of particles from ρ_0 to ω_0 small in the innermost region. v rises sharply, as we

move out of this innermost region, leading to an increase in the inelastic scattering for ℓ equals one, (i.e. the projectile with ℓ equals zero spends a smaller time(compared to the projectile with ℓ equals one) in this region where v has this rapid rise.)

The CTP for ℓ equals two essentially restricts the projectile from entering the region in which v has its greatest slope and therefore accounts for the smallness of Q_2^{01} .

(III) Attempt to Calculate the Width and Lifetime of the Optimized Average Excited State; Summary

The width of the optimized average excited state $\frac{\Gamma}{2}$ is given approximately by[4]:

$$\left(\frac{\Gamma}{2}\right)^2 \approx (\omega H_T^2 \omega) - (\omega H_T \omega)^2$$

where H_T is the target hamiltonian. This result can be understood from the uncertainty principle. $\frac{\Gamma}{2}$ is the uncertainty in energy (dispersion) and $1/\Gamma/2$ is $\sim$ the lifetime of the state.

From the Clementi Tables[1]:

$$W_0 = -526.817 \text{ a.u.}$$

$$W_0^{(-)} = -459.580 \text{ a.u.}$$

ε is calculated as $\approx$ -519.4 a.u. $\left(\varepsilon = \frac{(\omega, H_T \omega)}{(\omega, \omega)}\right)$

$$p^2 = p'^2 + 7.45071 \text{ a.u.}$$

$\varepsilon - W_0$ the excitation energy of the OAES is 7.45071 a.u. There are different ways to calculate ε, $(\omega H_T^2 \omega)$, etc. and consequently $\left(\frac{\Gamma}{2}\right)^2$. This arises from applying H_T to the right or left in the various inner products. These different directions of applying H_T would not give different results if the wave functions we used for ϕ_0 and $\phi_0^{(-)}$ were exact eigenfunctions of their respective hamiltonians. The use of our approximate wave functions (whose most serious error is in omitting

electron correlation effects) will lead to an uncertainty in the width (measured by the difference in $\Gamma/2$) found by applying to the left or right.

In our case $\mathcal{E}_L = -519.3671$ a.u.

$\mathcal{E}_R = -519.4770$ a.u.

where the subscript L and R correspond to taking H_T to the left or right respectively.

Take $\bar{\mathcal{E}} = \frac{\mathcal{E}_L + \mathcal{E}_R}{2}$, if we now consider the magnitude of the numbers under consideration:

a typical $(\omega, H_T^2 \omega) =$ 269,827.55 a.u.

$(\bar{\mathcal{E}})^2 =$ 269,799.27 a.u.

So a typical $\left(\frac{\Gamma}{2}\right)^2$ is:

$$\left(\frac{\Gamma}{2}\right)^2 \cong (\omega H_T^2 \omega) - (\bar{\mathcal{E}})^2 \approx \quad 28 \text{ a.u.}$$

a very small difference between very large numbers.

The error in $\mathcal{E}$ due essentially to leaving out electron correlation effects in the wave function is:

$$\delta\mathcal{E} \approx \mathcal{E}_L - \mathcal{E}_R = \quad .11 \text{ a.u.}$$

The error in $\mathcal{E}^2$ is then found using

$$\mathcal{E} = \mathcal{E}_{exact} + \delta\mathcal{E}$$

We have:

$$\mathcal{E}^2 = \mathcal{E}^2_{exact} + 2\mathcal{E}_{exact} \cdot \delta\mathcal{E} + (\delta\mathcal{E})^2$$

$$\mathcal{E}^2 = \mathcal{E}^2_{exact} + \delta(\mathcal{E}^2)$$

The error in ε^2 is $\delta(\varepsilon^2)$ and equals 2 $\varepsilon_{\text{exact}} \cdot \delta\varepsilon + (\delta\varepsilon)^2 \simeq$ 2(.11)(519)

$=$ 114 a.u.

Therefore the error in the numbers we are subtracting (due to leaving out correlation effects) is greater than the difference between them making the difference highly unreliable. We therefore conclude that with these wave functions the information about the width and lifetime of ω is lost in the omission of correlation in the wave functions.

Summary

There are several ways we might experimentally observe the OAES[5] of Argon (and other atoms).

(1) Send a monochromatic electron beam on Argon and look at the flux of electrons inelastically scattered through large angles with a kinetic energy loss equal to the excitation energy of our OAES. Compare this with our curves. We understand that this might be difficult due to the small flux at large angles.

(2) Detection of secondary electrons whose kinetic energy would be characteristic of the OAES and its decay modes.

(3) Measurement of the large angle electron-Argon elastic scattering as a function of incident energy to determine if any structure appears which might be associated with a time delay on the part of the projectile (i.e. a resonance). If for a different atom v were found to have a longer range we could not confine ourselves to investigate only large angle scattering.

We plan in the future to examine the perhaps more fruitful example of $e - K^+$ scattering. The reason we believe this to be a potentially more fruitful situation is the multiplicity of bound states in what would be the isoelectronic atom with one less proton : the neutral Argon atom. We could also consider linear combinations of such states so as to approximate the optimized excited state. Taking linear combinations is complicated by the non-linear character of the w equation and of ε''s linear and bilinear dependence on w .

A future inclusion of the electronic correlation in the atomic description could allow us to speak about the width and lifetime of such a state and in turn improve our ability to comment on the interpretation of ω as a collective mode of the atom. The inclusion of correlation could also improve our v and its influence on the elastic scattering and help bring any possible structure into focus.

References for Chapter Six

1. E. Clementi, IBM J. Res. Develop. Suppl. 9, 2 (1965).

2. J. J. Matese, S. P. Rountree and R. J. W. Henry, Phys. Rev. A 8, 2965 (1973); D. L. Cunningham and A. K. Edwards, Phys. Rev. A 8, 2960 (1973).

3. See, e.g., N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions, 3rd Edition (Oxford U.P., London, England, 1965) p. 349.

4. M. H. Mittleman, Phys. Rev. A 6, 879, (1972).

5. See, e.g. A. A. Lamola, Creation and Detection of the Excited State, (M. Dekker, Inc., New York 1971) Vol. 1, Part B.

Figures and Tables for Chapter Six

$R(a_o)$	VS (a.u.)
0.010000	-1730.947940
0.020000	-832.549507
0.030000	-534.622093
0.040000	-386.883991
0.050000	-303.189724
0.060000	-241.363819
0.070000	-200.576088
0.080000	-170.350084
0.090000	-147.110447
0.100000	-128.720333
0.300000	-25.888550
0.500000	-10.754801
0.700000	-5.727356
0.900000	-3.287080
1.100000	-1.925017
1.300000	-1.135704
1.500000	-0.636680
1.700000	-0.401955
1.900000	-0.241354
2.100000	-0.145838
2.300000	-0.088627
2.500000	-0.054130
2.700000	-0.033187
2.900000	-0.020717
3.100000	-0.012592
3.300000	-0.007776
3.500000	-0.004817
3.700000	-0.003005
3.900000	-0.001875
4.100000	-0.001184
4.300000	-0.000747
4.500000	-0.000470
4.700000	-0.000317
4.900000	-0.000209
5.100000	-0.000142
5.300000	-0.000107
5.500000	-0.000077
5.700000	-0.000055
5.900000	-0.000048
6.100000	-0.000036
6.300000	-0.000031
6.500000	-0.000030
6.700000	-0.000025
6.900000	-0.000023
7.100000	-0.000025
7.300000	-0.000024
7.500000	-0.000021
7.700000	-0.000020
7.900000	-0.000021

Table 1. VS versus R

$R(a_o)$	$\overline{V}$ (a.u)
0.010000	-1735.972210
0.020000	-837.356545
0.030000	-539.164246
0.040000	-391.159054
0.050000	-360.000004
0.060000	-245.169504
0.070000	-204.191752
0.080000	-173.803942
0.090000	-150.428322
0.100000	-131.922752
0.300000	-27.860361
0.500000	-12.015630
0.700000	-6.740076
0.900000	-4.184840
1.100000	-2.712726
1.300000	-1.805314
1.500000	-1.228070
1.700000	-0.853095
1.900000	-0.605034
2.100000	-0.438058
2.300000	-0.324117
2.500000	-0.210360
2.700000	-0.187517
2.900000	-0.146967
3.100000	-0.117392
3.300000	-0.095516
3.500000	-0.079147
3.700000	-0.066755
3.900000	-0.057245
4.100000	-0.049904
4.300000	-0.044157
4.500000	-0.039610
4.700000	-0.035987
4.900000	-0.033039
5.100000	-0.030652
5.300000	-0.028687
5.500000	-0.027027
5.700000	-0.025605
5.900000	-0.024398
6.100000	-0.023344
6.300000	-0.022415
6.500000	-0.021599
6.700000	-0.020851
6.900000	-0.020174
7.100000	-0.019553
7.300000	-0.018982
7.500000	-0.018443
7.700000	-0.017938
7.900000	-0.017475

Table 2. $\overline{V}$ versus R

$R(a_o)$	v (a.u.)
0.010000	-3.290000
0.020000	-3.130000
0.030000	-2.940000
0.040000	-2.750000
0.050000	-2.580000
0.060000	-2.430000
0.070000	-2.302000
0.080000	-2.193000
0.090000	-2.102000
0.100000	-2.024430
0.300000	-1.122860
0.500000	-0.641040
0.700000	-0.490950
0.900000	-0.416390
1.100000	-0.341860
1.300000	-0.266030
1.500000	-0.197920
1.700000	-0.142010
1.900000	-0.098690
2.100000	-0.066370
2.300000	-0.042690
2.500000	-0.038290
2.700000	-0.014230
2.900000	-0.005980
3.100000	-0.000300
3.300000	0.000000
3.500000	0.000000
3.700000	0.000000
3.900000	0.000000
4.100000	0.000000
4.300000	0.000000
4.500000	0.000000
4.700000	0.000000
4.900000	0.000000
5.100000	0.000000
5.300000	0.000000
5.500000	0.000000
5.700000	0.000000
5.900000	0.000000
6.100000	0.000000
6.300000	0.000000
6.500000	0.000000
6.700000	0.000000
6.900000	0.000000
7.100000	0.000000
7.300000	0.000000
7.500000	0.000000
7.700000	0.000000
7.900000	0.000000

Table 3. v versus R

$R(a_o)$	VS	$\overline{V}$	v
0.010000	-1730.947940	-1735.972210	-3.290000
0.020000	-832.549507	-837.356545	-3.130000
0.030000	-534.622093	-539.164246	-2.940000
0.040000	-386.883991	-391.159054	-2.750000
0.050000	-303.189724	-360.000004	-2.580000
0.060000	-241.363819	-245.169504	-2.430000
0.070000	-200.576088	-204.191752	-2.302000
0.080000	-170.350084	-173.803942	-2.193000
0.090000	-147.110447	-150.428322	-2.102000
0.100000	-128.720333	-131.922752	-2.024430
0.300000	-25.888550	-27.860361	-1.122860
0.500000	-10.754801	-12.015630	-0.641040
0.700000	-5.727356	-6.740076	-0.490950
0.900000	-3.287080	-4.184840	-0.416390
1.100000	-1.925017	-2.712726	-0.341860
1.300000	-1.135704	-1.805314	-0.266030
1.500000	-0.636680	-1.228070	-0.197920
1.700000	-0.401955	-0.853095	-0.142010
1.900000	-0.241354	-0.605034	-0.098690
2.100000	-0.145838	-0.438058	-0.066370
2.300000	-0.088627	-0.324117	-0.042690
2.500000	-0.054130	-0.210360	-0.038290
2.700000	-0.033187	-0.187517	-0.014230
2.900000	-0.020717	-0.146967	-0.005980
3.100000	-0.012592	-0.117392	-0.000300
3.300000	-0.007776	-0.095516	0.000000
3.500000	-0.004817	-0.079147	0.000000
3.700000	-0.003005	-0.066755	0.000000
3.900000	-0.001875	-0.057245	0.000000
4.100000	-0.001184	-0.049904	0.000000
4.300000	-0.000747	-0.044157	0.000000
4.500000	-0.000470	-0.039610	0.000000
4.700000	-0.000317	-0.035987	0.000000
4.900000	-0.000209	-0.033039	0.000000
5.100000	-0.000142	-0.030652	0.000000
5.300000	-0.000107	-0.028687	0.000000
5.500000	-0.000077	-0.027027	0.000000
5.700000	-0.000055	-0.025605	0.000000
5.900000	-0.000048	-0.024398	0.000000
6.100000	-0.000036	-0.023344	0.000000
6.300000	-0.000031	-0.022415	0.000000
6.500000	-0.000030	-0.021599	0.000000
6.700000	-0.000025	-0.020851	0.000000
6.900000	-0.000023	-0.020174	0.000000
7.100000	-0.000025	-0.019553	0.000000
7.300000	-0.000024	-0.018982	0.000000
7.500000	-0.000021	-0.018443	0.000000
7.700000	-0.000020	-0.017938	0.000000
7.900000	-0.000021	-0.017475	0.000000

Table 4. $v, \overline{V}, VS$ versus R

E(a.u.)	$Q_0^{00}(a_0^2)$ v	$Q_0^{00}(a_0^2)$ v=0	$Q_0^{00}(v=0) - Q_0^{00}(v)$
7.550710	0.552336	0.569953	0.017617
7.650710	0.553265	0.571416	0.018151
7.850710	0.554935	0.573650	0.018715
8.050710	0.556641	0.575032	0.018391
8.250710	0.557566	0.575636	0.018070
8.450710	0.557593	0.575529	0.017936
8.650710	0.557014	0.574778	0.017765
8.850710	0.556017	0.573440	0.017424
9.050710	0.554589	0.571572	0.016983
9.250710	0.552671	0.569219	0.016547
9.450710	0.550266	0.566428	0.016162
9.550710	0.549191	0.564882	0.015691
9.650710	0.547452	0.563243	0.015792
9.850710	0.544301	0.559704	0.015403
10.050710	0.540867	0.555839	0.014972
10.250710	0.537171	0.551688	0.014517
10.450710	0.533212	0.547280	0.014068
10.650710	0.528993	0.542642	0.013649
10.850710	0.524531	0.537800	0.013269
11.050710	0.519861	0.532776	0.012916
11.250710	0.515017	0.527592	0.012576
11.450710	0.510029	0.522268	0.012239
11.550710	0.507643	0.519558	0.011915
11.650710	0.504917	0.516820	0.011903
11.850710	0.499695	0.511266	0.011570
12.050710	0.494371	0.505619	0.011248
12.250710	0.488952	0.499896	0.010944
12.450710	0.483449	0.494107	0.010659
13.550710	0.452339	0.461579	0.009240
15.550710	0.395473	0.402599	0.007127
17.550710	0.342068	0.347484	0.005415
19.550710	0.293964	0.298122	0.004158
21.550710	0.251675	0.254918	0.003243
23.550710	0.215031	0.217575	0.002545
25.550710	0.183508	0.185487	0.001980
27.550710	0.156433	0.157972	0.001539
29.550710	0.133195	0.134392	0.001198

Table 5. $Q_0^{00}(v)$ and $Q_0^{00}(v=0)$ vs. incident energy .

E(a.u.)	$Q_1^{00}(a_0^2)$
7.550710	
7.650710	0.250451
7.850710	0.224491
8.050710	0.199190
8.250710	0.176141
8.450710	0.155587
8.650710	0.136966
8.850710	0.119981
9.050710	0.104634
9.250710	0.090893
9.450710	0.078637
9.550710	0.073004
9.650710	0.067677
9.850710	0.057886
10.050710	0.049142
10.450710	0.034556
10.650710	0.028562
10.850710	0.023331
11.050710	0.018788
11.250710	0.014865
11.450710	0.011512
11.550710	0.010030
11.650710	0.008679
11.850710	0.006321
12.050710	0.004405
12.250710	0.002892
12.450710	0.00 1745
13.550710	0.000748
15.550710	0.013500
17.550710	0.034480
19.550710	0.057128
21.550710	0.078554
23.550710	0.097751
25.550710	0.114523
27.550710	0.128962
29.550710	0.141299

E(a.u.)	$Q_1^{00}(a_0^2)$
7.550710	0.245742
9.550710	0.061214
11.550710	0.006229
13.550710	0.001768
15.550710	0.017465
17.550710	0.040196
19.550710	0.063882
21.550710	0.085864
23.550710	0.105269
25.550710	0.122033
27.550710	0.136375
29.550710	0.148567

Table 6. $Q_1^{00}(v)$ and $Q_1^{00}(v=0)$ vs. incident energy.

	v		v=0
E(a.u.)	$Q_2^{00}(a_0^2)$	E(a.u.)	$Q_2^{00}(a_0^2)$
7.550710	3.934866	7.550710	3.976217
7.650710	3.878051	9.550710	3.147807
7.850710	3.753170	11.550710	2.612700
8.050710	3.668560	13.550710	2.238433
8.250710	3.583073	15.550710	1.915358
8.450710	3.499280	17.550710	1.745466
8.650710	3.418728	19.550710	1.573243
8.850710	3.340947	21.550710	1.432314
9.050710	3.266143	23.550710	1.314891
9.250710	3.194694	25.550710	1.215495
9.450710	3.126608	27.550710	1.130166
9.550710	3.093731	29.550710	1.056007
9.650710	3.061554		
9.850710	2.999180		
10.050710	2.939335		
10.250710	2.882000		
10.450710	2.827105		
10.650710	2.774509		
10.850710	2.723955		
11.050710	2.675284		
11.250710	2.628309		
11.450710	2.582959		
11.550710	2.560890		
11.650710	2.539202		
11.850710	2.496972		
12.050710	2.456209		
12.250710	2.416813		
12.450710	2.378701		
13.550710	2.189091		
15.550710	1.915358		
17.550710	1.704779		
19.550710	1.536421		
21.550710	1.399033		
23.550710	1.285062		
25.550710	1.188797		
27.550710	1.106035		
29.550710	1.034046		

Table 7 . $Q_2^{00}(v)$ and $Q_2^{00}(v=0)$ vs. incident energy .

E(a.u.)	$Q_0^{01}(a_0^2)$
7.550710	0.004628
9.550710	0.005431
11.550710	0.004721
13.550710	0.004239
15.550710	0.003779
17.550710	0.003329
19.550710	0.002966
21.550710	0.002678
23.550710	0.002423
25.550710	0.002185
27.550710	0.001979
29.550710	0.001805

E(a.u.)	$Q_1^{01}(a_0^2)$
7.550710	0.016905
9.550710	0.021219
11.550710	0.018420
13.550710	0.016330
15.550710	0.014543
17.550710	0.012748
19.550710	0.011293
21.550710	0.010163
23.550710	0.009147
25.550710	0.008210
27.550710	0.007414
29.550710	0.006747

E(a.u.)	$Q_2^{01}(a_0^2)$
7.550710	0.000379
9.550710	0.014245
11.550710	0.016481
13.550710	0.017674
15.550710	0.017588
17.550710	0.016517
19.550710	0.015505
21.550710	0.014439
23.550710	0.013232
25.550710	0.012044
27.550710	0.011054
29.550710	0.010207

Table 8. Q_0^{01}, Q_1^{01}, Q_2^{01} vs. incident energy.

PLEASE NOTE:

The figures on pages 118 - 127 are very bad print. Filmed as received - best available copy.

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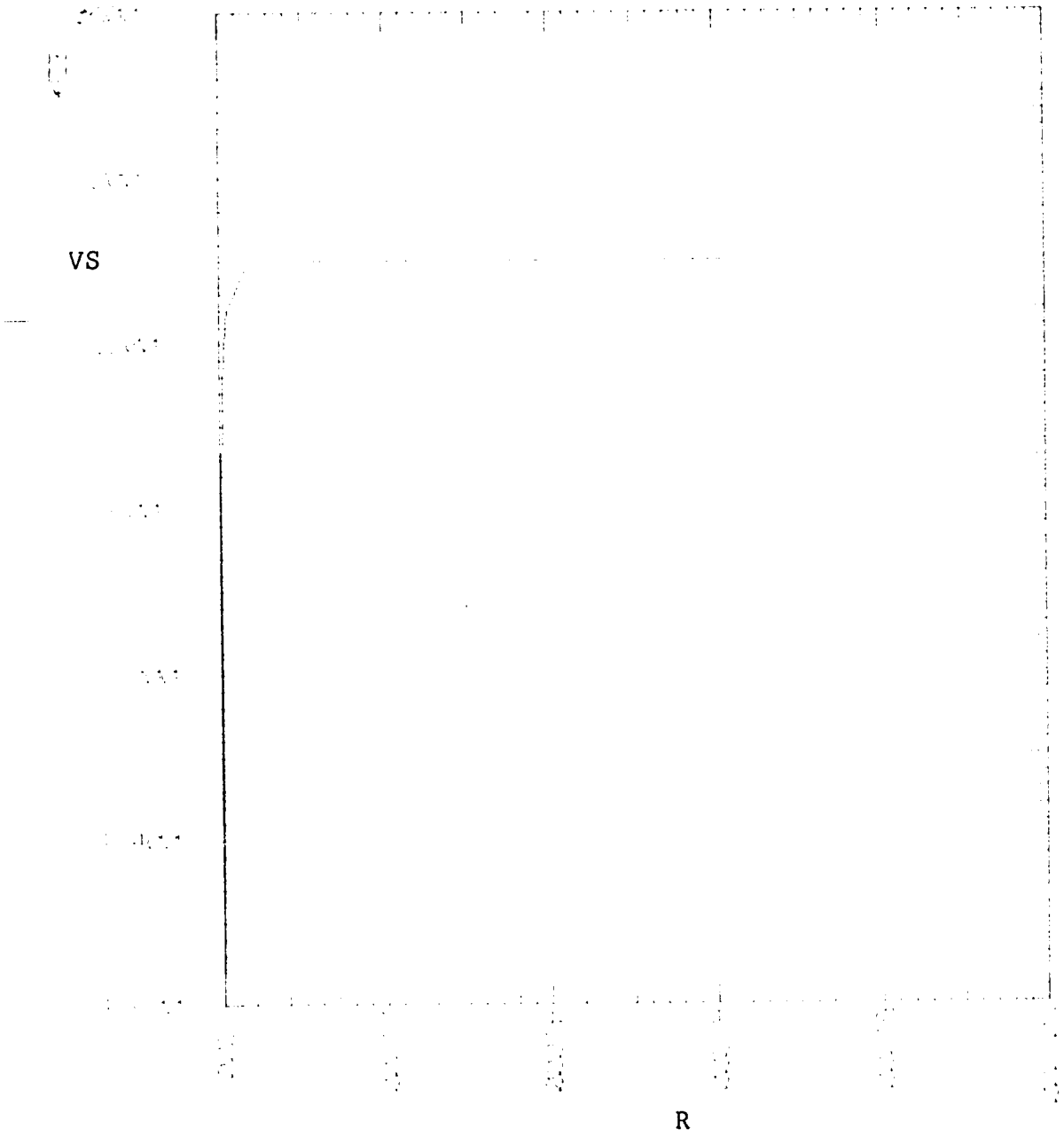

Fig.1. VS (10^3 a.u.) versus R (a_o)

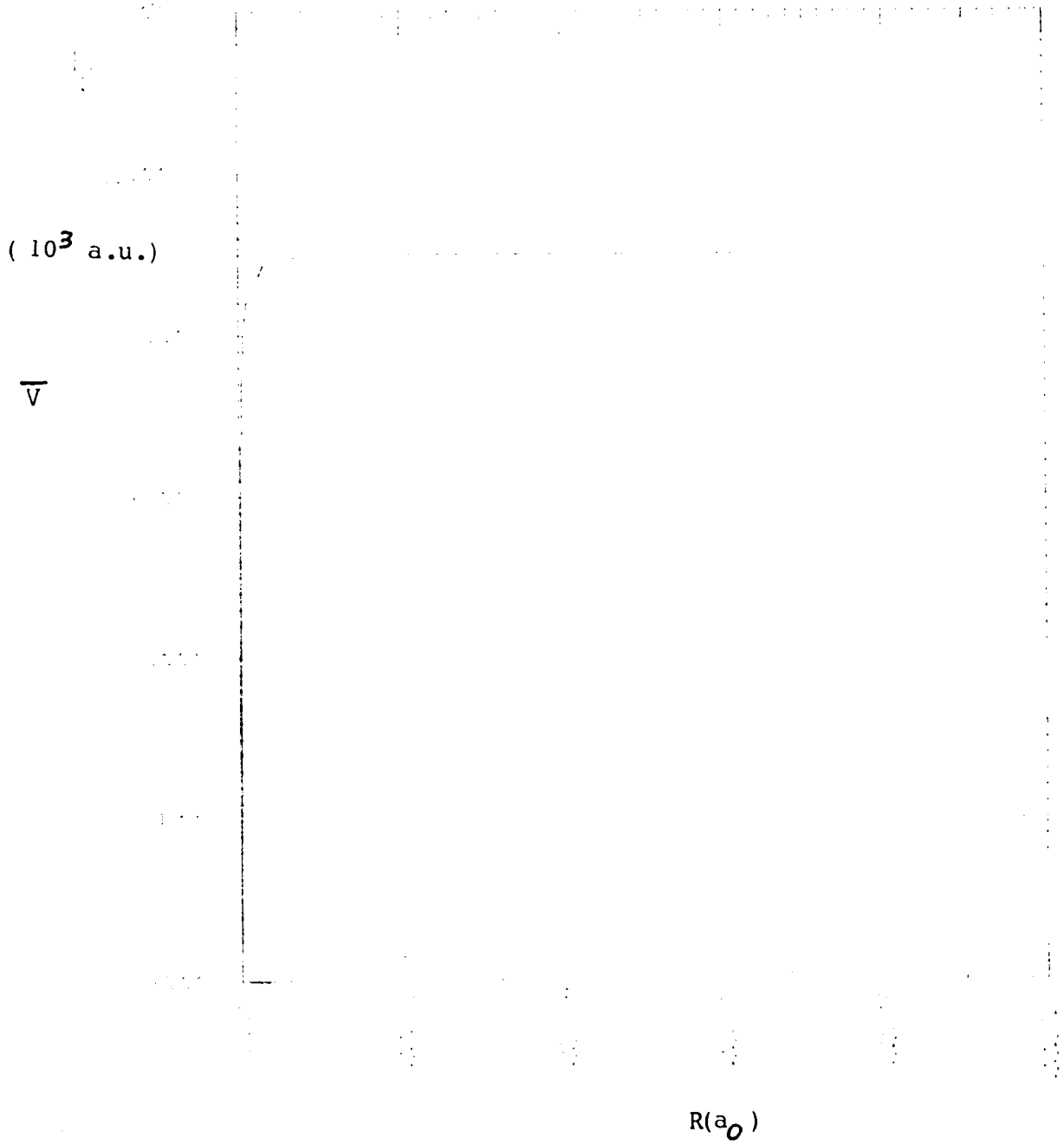

Fig.2. $\overline{V}$ versus R

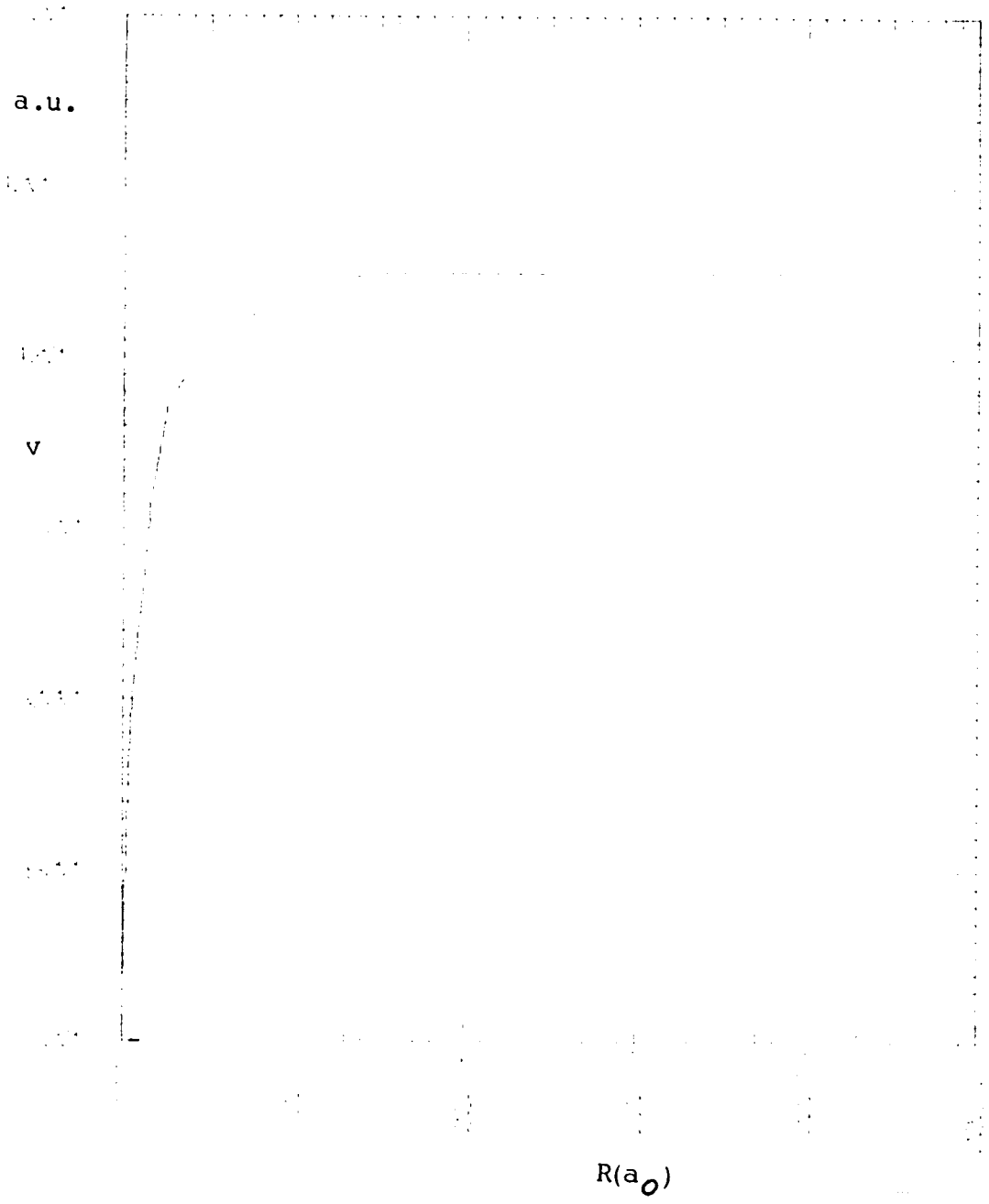

Fig.3. v versus R

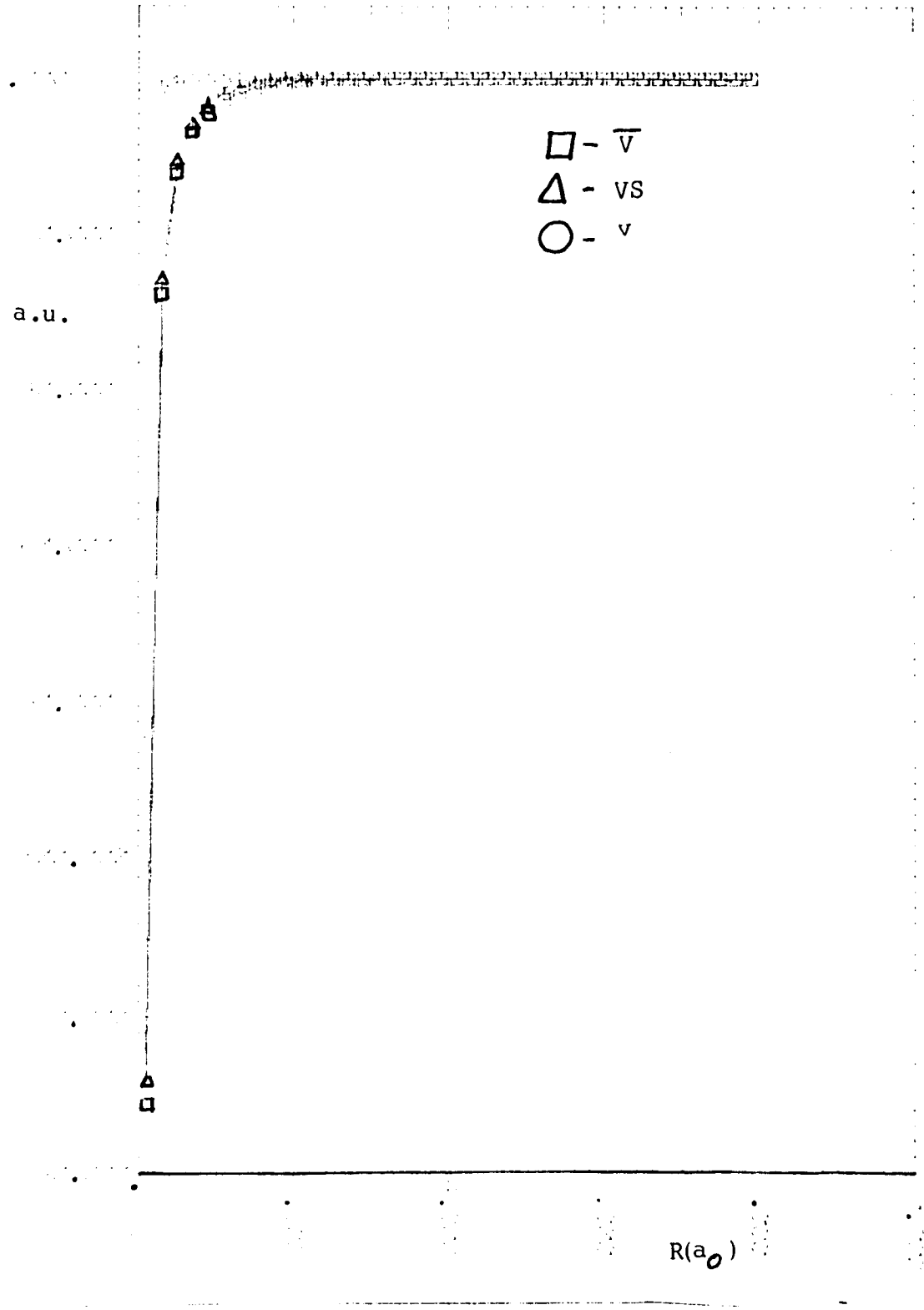

Fig.4. VS, $\overline{V}$ and v versus R

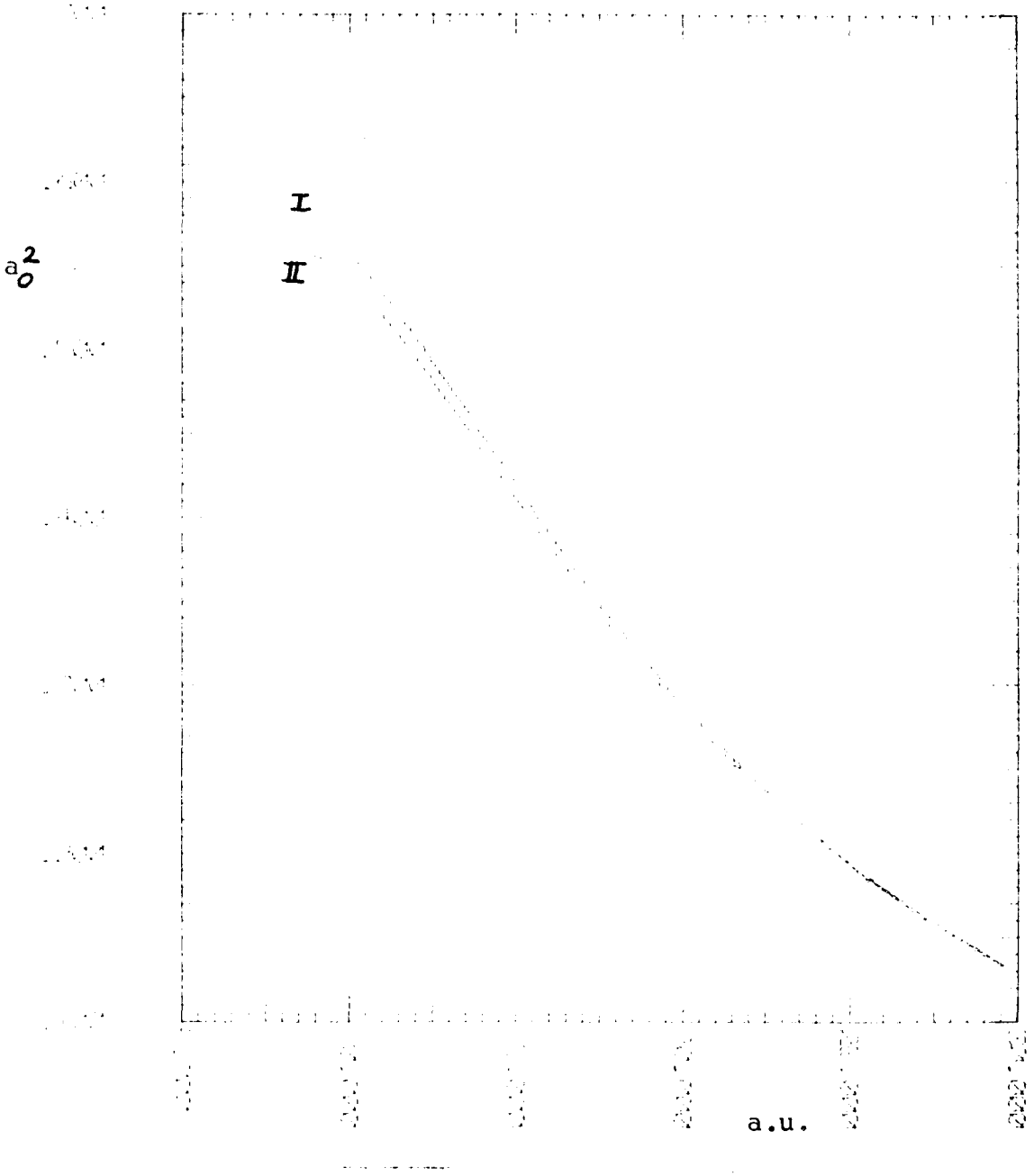

Fig.5. Q_0^{00} versus incident energy.

(Ⅰ) v=0 , (Ⅱ) v included

Fig.6. Q_1^{00} versus incident energy.

(Δ) v=0 , (O) v included

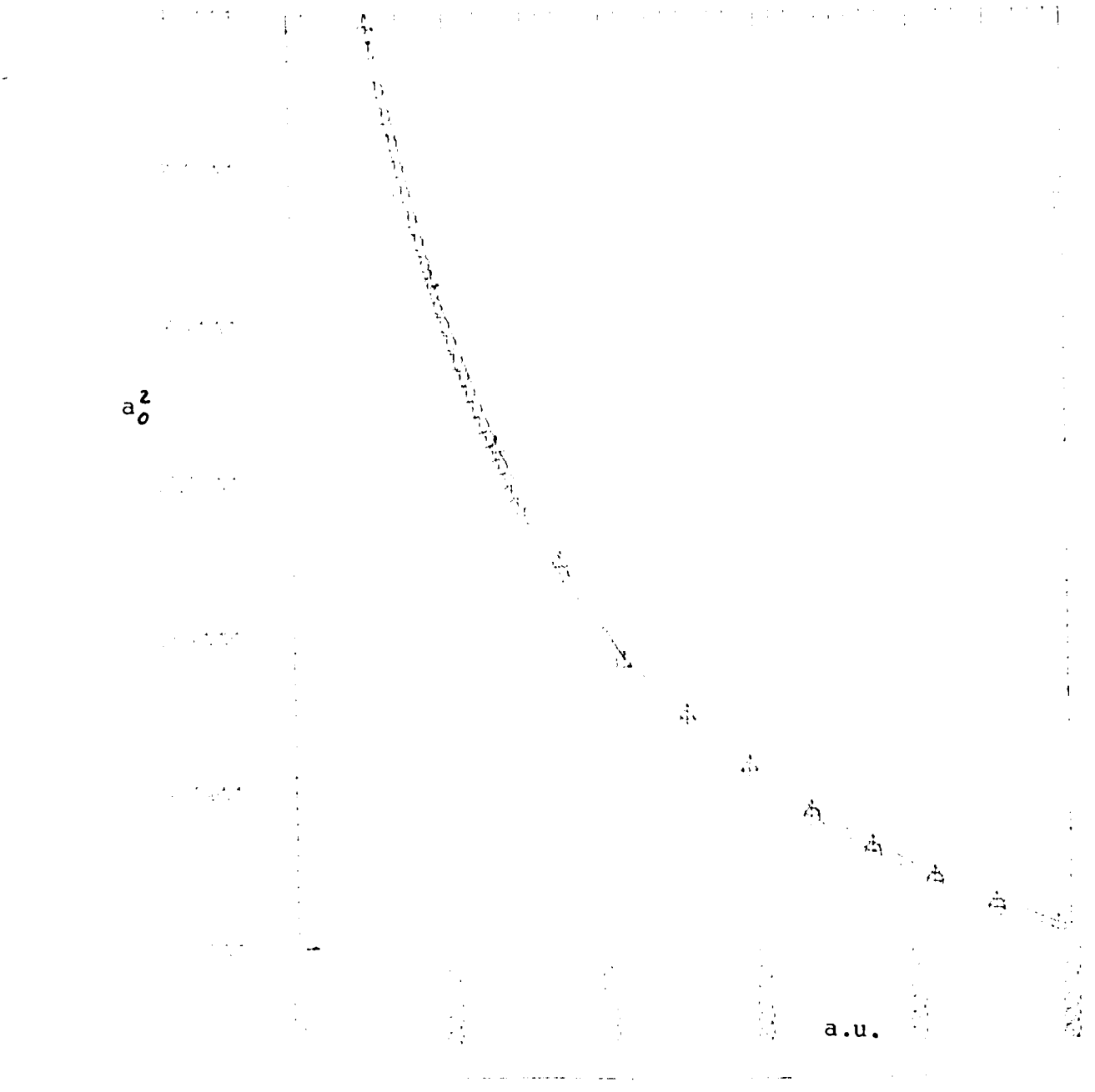

Fig.7. Q_2^{00} versus incident energy.

(Δ) v=0 , (O) v included

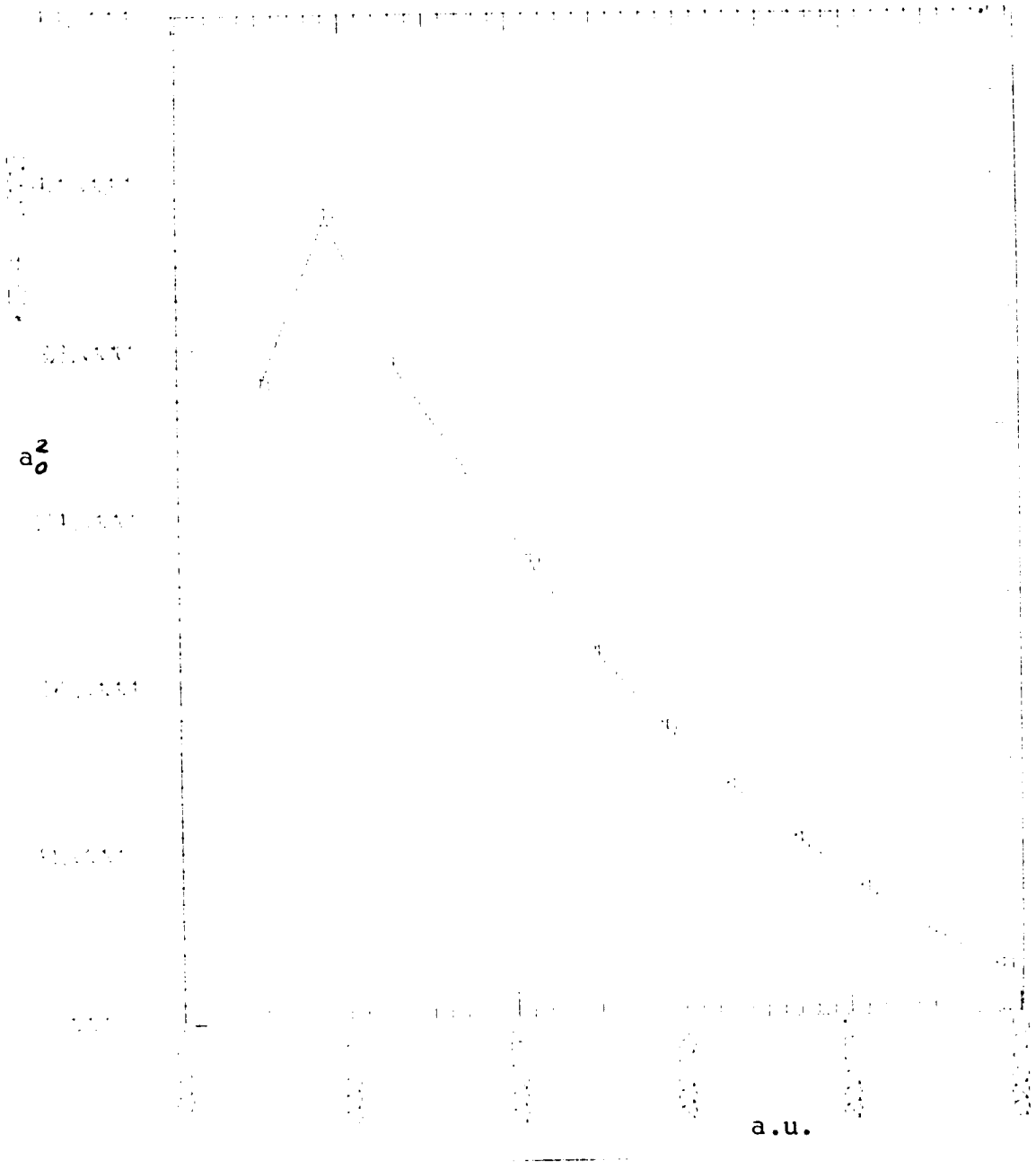

Fig. 8. Q_0^{01} versus incident energy

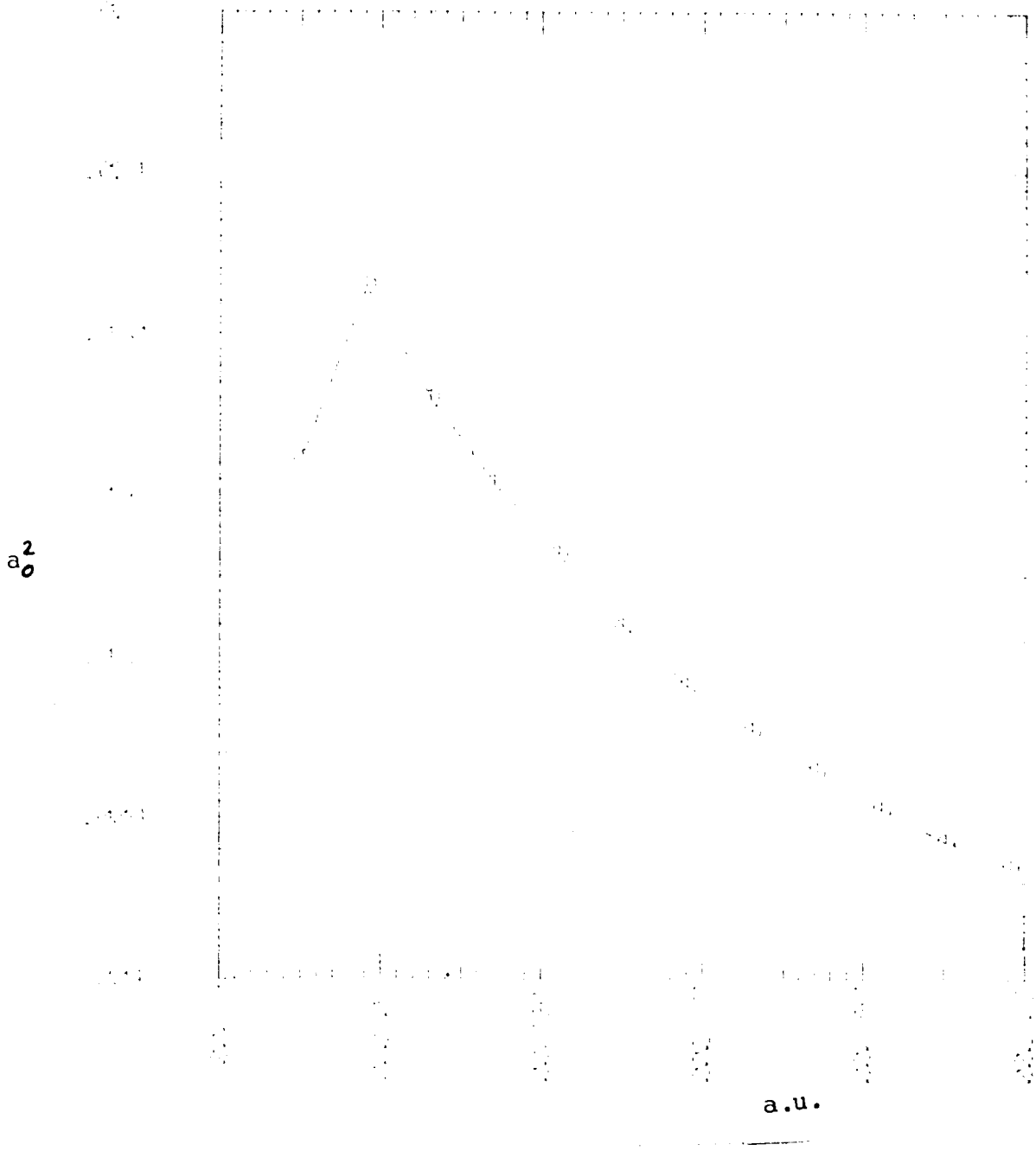

Fig.9. Q_1^{01} versus incident energy

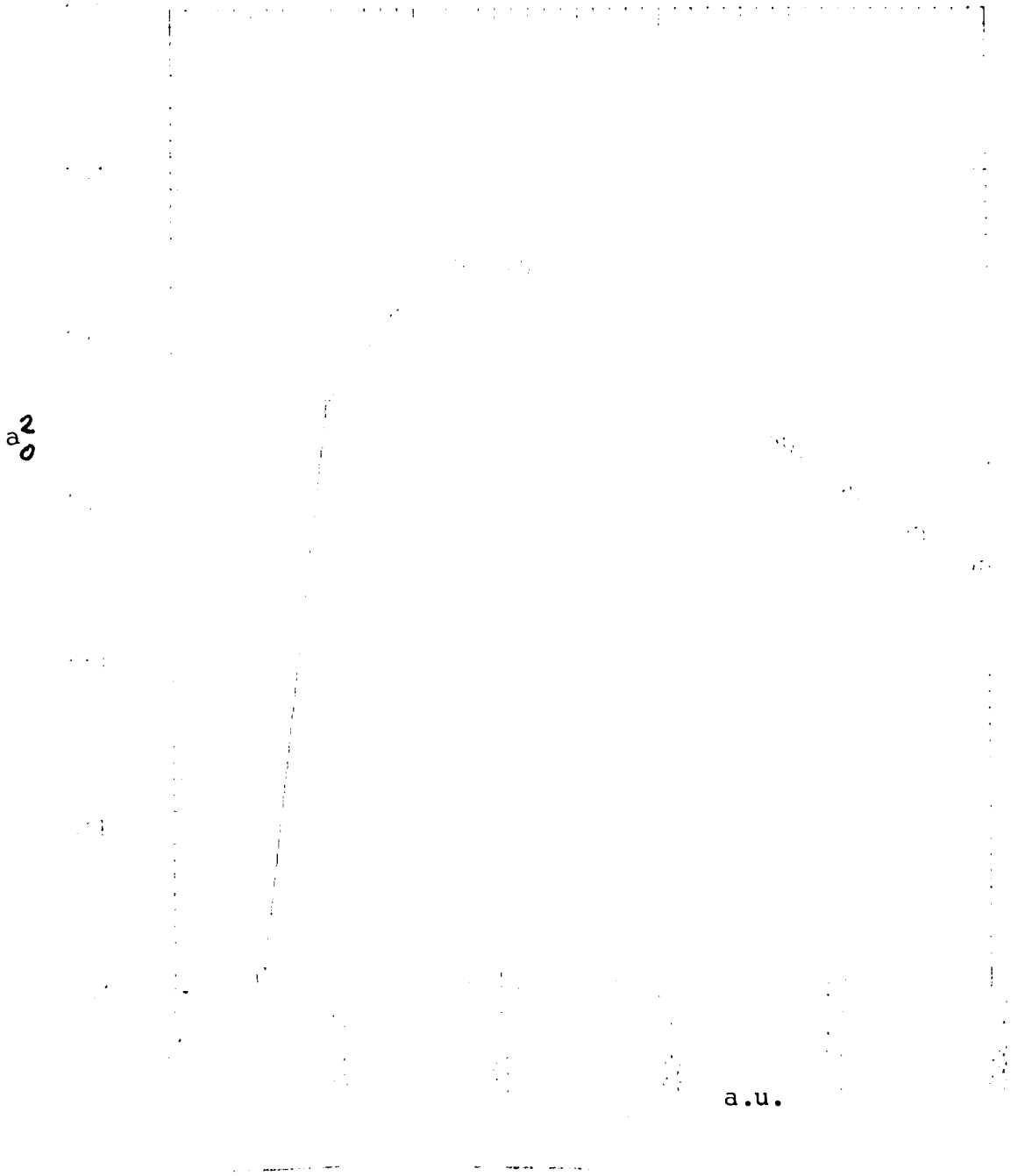

Fig.10. Q_2^{01} versus incident energy.