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THE ATOMIC PHYSICS OF HYDROGEN-LIKE ATOMS CHANNELING IN SINGLE THIN CRYSTALS

by

GERALD J. KUTCHER

A dissertation submitted to the
Graduate Faculty in Physics in
partial fulfillment of require-
ments for the degree of Doctor
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1973

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date

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Executive Officer

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Professor Joel Gersten
Professor Kenneth Rubin
Supervisory Committee

The City University of New York

"'How long do you live?' said the Sirian.

'Oh, a very short time,' replied the little man of Saturn.

'That is just as with us,' said the Sirian, 'we always complain how short. That must be a universal law of nature.'

'Alas! ' said the Saturnian, 'we live for only five hundred great revolutions of the sun.' (That comes to fifteen thousand years or thereabouts, counting in our way.) 'You can readily see that that is dying almost at the moment we are born; our existence is a point, our duration an instant, our globe an atom.'..."

Voltaire

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Introduction

The channeling of heavy ions in single thin crystals has received much attention in recent years. This effect deals with the penetration of energetic particles along low index directions. Further, it manifests itself in the attenuation of processes strongly dependent upon the impact parameter of the incident ion relative to the atoms (cores) of the solid. This lack of hard collisions is characteristic of channeling particles. This should be contrasted with penetrations in random directions. The characteristics of the processes are quite different in the two cases. For example, the transmitted energy spectra for channeled particles has a shoulder at the high energy end rather than being Gaussian as it is for the random (normal) case.

In this thesis, we are interested in studying the internal states of channeling atoms. Since channeling implies diminuation of hard collisions we might expect the charge of the atom to be lower than normal. In particular, consider an electron proton pair channeling through a single crystal. Imagine that the electronic density for an internal state of the pair decays as the pair penetrates into the crystal. We can then attempt to calculate the lifetime of states that live longest. Such a program which is attempted in this thesis is described briefly below. We must remark, however, that the spirit of this work is one of an exploratory study. This means that we have been most interested in stating the problem, characterizing the important processes and obtaining numerical results for simple models.

Chapter 1 discusses the main characteristics of channeling for heavy ions. Some experimental results are discussed and the important concept of a string potential is introduced.

Chapter 2 contains a derivation of the equation of motion for the internal state of an electron proton pair. This essentially entails studying the propagation of an arbitrary state in a subspace of the Hilbert space of the solid states. The amplitude for the electron in this channeling space is an average over a dense set of amplitudes for this subspace. The justification for this averaging is discussed at some length. Suffice it to say our average amplitude is shown to propagate according to a one body Schroedinger equation with a complex potential (optical potential). It is further shown that in an appropriate approximation states of maximum lifetime satisfy the equation.

Chapter 3 discusses in detail the various potential energy terms contained in the one body Schroedinger equation. This entails, in part, a study of the single particle excitation (of the solid) contributions to the potential. Further collective effects are discussed and the polarization potential for an electron gas is considered. Lastly, the rate of ionization of the incident pair is derived in an impulse approximation. This rate is interpreted as being proportional to the imaginary part of the optical potential.

Chapter 4 discusses the explicit detailed solution to the above discussed Schroedinger equation in a hydrogen basis for the channeling of an electron and proton in sodium. Further, the concept of string potential is applied. A self consistent procedure is outlined for this solution. The calculation involves numerical double integration for the matrix elements of the potentials and then numerical diagnolization of the Hamiltonian of the Schroedinger equation is effected. At this point energy levels and ionization rates have been obtained for long lived channeling hydrogen. To obtain the lifetimes of the internal states we also need capture rates.

Chapter 5 discusses the formal theory of capture of an electron by a proton from a sea of electrons. Some interesting formal results are obtained. The problem of capture from valence bands in a metal is then discussed. Finally, the capture of electrons from the sodium cores is derived in an impact parameter treatment.

Chapter 6 concludes the thesis. The work of the previous chapters is brought together and the numerical results are discussed. The particular computation techniques are briefly described. Finally, possible further theoretical work is proposed as well as possible experiments.

A word about notation is in order here. All equations are numbered anew in each section or subsection by which the chapters are divided. However, figures and an occasional table is numbered consecutively through the thesis. Equations in the same section as the text are referred to by number, for example equation 6. Equations in sections outside the immediate text are referred to by section followed by equation number in parenthesis. So equation 6 in section 3.2.1 is written thus 3.2.1(6).

Standard Dirac bra-ket notation is used interchangeably with amplitude notation, for example, $|n>$ and $\psi_n(x)$. The constant $\hbar$ is almost invariably taken to be one although whether atomic units[†] are used depends upon the context.

[†] $\hbar = e = m = 1$

Chapter 1

Channeling Effect in Single Thin Crystals

1.1 Introduction

Theoretical and experimental work on the motion of energetic charged particles in matter has a long and distinguished history. The early work which began with N. Bohr in 1912 and continues with Bethe, Fermi, Lamb and Wigner, to mention a few researchers, concentrates on motion in random media. For example, the slowing down (stopping) of fission fragments, and the related question of capture and loss of electrons by ions, is a problem that receives considerable attention in the 1940's. However, whether the medium through which the particle penetrates is gaseous or crystalline, the calculations themselves are independent of this difference except for polarization effects in condensed media.[†] That is, the medium is treated as randomly distributed with respect to the incident beam. To put it more precisely, there is no correlation between the scatterings a particle suffers in its motion through a gas or even a solid insofar as the above calculations are concerned. The total cross section is the sum of cross sections for the scattering from each atomic site in the medium each of which is treated as if the other centers did not exist.

Except for the papers of Stark[1,2], the fact that particle motion in crystals can reveal anisotropic effects is not discovered until 1963 by Robinson and Oen[3] in a computer experiment. They show that charged

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[†] Actually for a beam penetrating a crystal in a random direction the structure would reveal itself in fluctuations about an average result.

particles can be guided along low index directions with low energy losses and long penetrations relative to penetrations in random directions. This work has been followed by much experimental and some theoretical work. In this regard, the theoretical work of Lindhard[4] should be mentioned. It is not our wish here to discuss this recent history or go into the many interesting ramifications. The reader should consult references 4, 5 and 6 for the pertinent discussions and complete bibliographies. What we want to make clear is that a crystal under certain conditions does not behave as a gas with respect to the scattering of energetic particles. Further, this realization marks a shift in both experiment and theory.

In this chapter, we wish to describe briefly (and with an eye towards our own work) the basic properties of ion channeling. The reader should not be misled by the brevity of the presentation into believing that the subject is barren. On the contrary, it reveals a richness of phenomena that is rather startling.

1.2 Some Experimental Results

Robinson and Oen[3] at the Oak Ridge National Laboratories programmed binary encounter trajectories for atoms moving in solids along low index directions. Shown in Figures 1 are the projections of the motion of copper atoms in copper for two incident directions. The figures reveal one of the major characteristics of channeling; that the penetrating particle moves in regions of low electronic density. In Figure 1a, the particle is further confined in remaining along one axis. The more general case is shown in Figure 1b where transverse motion (wandering) between channels is possible. It should be noted that particles can also be confined to move along low index planes. The latter motion is called planar channeling to distinguish it from axial proper channeling in Figure 1a and axial channeling shown in Figure 1b.

In Figure 2[7] the transmitted energy spectra for 9 MeV protons penetrating in random and axial directions is shown. It is clear that a large fraction (in fact approximately 80 percent) of the protons transmitted along an axial direction have a smaller than normal (random) energy loss. This is shown again in Figure 3a[7] for planar channeling. The curves marked I and II are obtained by subtracting out the non-channeled counts since the beam transmitted along the $\{1,1,1\}$ planes contains both groups. Curve I corresponds to those channeling particles with higher than normal energy loss and Curve II for lower than normal. In Figure 4[7] subsets I and II of the set of channeled particles are shown labeled appropriately high loss and low loss components respectively. This figure shows the transmitted energy distributions for the low and high loss components as a function of the angle of incidence of the beam relative to the planes mentioned. Figure 3b also shows variations with incidence angle. We shall discuss these curves more fully in the next section. Finally, we might point out that in Figures 2, 3, and 4 channeling characteristics are displayed through transmission experiments. Equally compelling are experiments which reveal anisotropy in say Rutherford back scattering, nuclear reaction yields, blocking etc. The reader should consult 5 and 6 for these details.

1.3 String Effect

In the next few sections we shall attempt to characterize further particle channeling without giving a precise definition. The use of the term string effect to denote channeling will become clear as we proceed. Further, we shall assume that classical mechanics applies to the motion of the penetrating particle. We shall return to its justification later. If we attempt to understand the motion shown in say Figure 1 we might conjecture that the explanation of channeling is a geometrical one. This, however, is not correct. The angle of acceptance for motion through an open channel is approximately 10^{-5} radians (for a thin crystal) which is of the order of the incident beam divergence. Particles in the beam would then be scattered out of the channel in this billiard ball model. This is particularly convincing in playing a game of snooker. Rather, the explanation lies in the steering of the particles by the atomic rows of the solid.

1.3.1 Steering and Correlation

In Figure 5, the motion of a channeled particle is shown. For simplicity we can assume that the plane of the figure is a symmetry plane of the solid and that the particles velocity vector lies entirely in this plane. Then the two dimensional motion shown would in fact be correct. The particle shown is being gently guided along a low index direction through interaction with the atomic rows. Their core density is shown by the cross hatched circles. In the figure, ψ is the angle between the axis and the momentum vector of the particle, when the particle is far from the atomic sites. ρ_M is the distance of closest approach. From the figure it is clear that correlated motion favors larger impact parameters than random motion would. Thus, the energy loss should be less for governed motion since ionization rates are strongly impact parameter dependent. The higher energies of the emerging particles in channeling are shown in Figures 2 and 3. We must point out that Figure 5 is misleading in a few respects. First, the motion is often not along a single axis but wandering occurs around the atomic sites as is shown in Figure 1b. Second, a single period in the channel is of the order of a few hundred lattice spacing and so appears as in Figure 6, Curve II.

1.3.2 Critical Angle

It is clear that the motion typified by Curve III in Figure 6 ensues with increasing angle ψ between the momentum vector and crystal axis. Lindhard[4] shows that for high energies[†] channeling exists if the following inequality holds.

$$\psi < C\psi_1 = C\sqrt{E_1/E} \quad ; \quad E_1 = 2Z_1Z_2e^2/d \qquad (1)$$

Here E is the particle's energy, Z_1 and Z_2 the particle and solid's atomic numbers respectively, d the lattice spacing and C is a constant close to unity. This criteria expresses the notion that for stable channeling to occur the transverse energy of motion $E\psi^2$[††] must be less than the potential barrier that confines the particle $(Z_1Z_2e^2)/(d/2)$.

[†] Energies large relative to E_1.
[††] ψ is at most a few degrees.

potential $\Sigma'_i V(\mathbf{r}-\mathbf{R}_i)$ and the averaging prescription would be

$$\sum_i{}' V(\mathbf{r}-\mathbf{R}_i) \longrightarrow \frac{1}{d}\int_{-\infty}^{+\infty} dZ\, V(\mathbf{r}-\mathbf{R}) \equiv \overline{V}$$

where Z is the longitudinal component of R, i.e. along the string and $\overline{V}$ expresses the average nature of the potential. In fact, this average potential appears quite naturally in the impulse approximation for the scattering φ in the collision of a particle with momentum Mv with a potential V.

$$\varphi = -\frac{1}{Mv^2}\frac{\partial}{\partial\rho}\int_{-\infty}^{+\infty} dZ\, V(\sqrt{\rho^2+Z^2})$$

$$\varphi = \frac{-d}{Mv^2}\frac{\partial}{\partial\rho}\overline{V(\rho)}$$

The condition for the averaging procedure is that the longitudinal frequency of motion parallel to a string be large relative to the transverse frequency of oscillation of the particle. That is, the particle should sample many atomic sites without appreciable change in transverse position. A crute estimate follows when we write

$$\omega_L = v/d \qquad (2)$$

where $v = v \cos \psi$ is the longitudinal velocity and d is the lattice spacing. If we make an harmonic approximation to the transverse motion, then the effective spring constant follows from

$$\frac{1}{2} k_{eff} (d/2)^2 = \frac{2\cdot Z_1 Z_2 e^2}{d} \qquad (3)$$

from which we obtain the transverse frequency.

$$\omega_T = k_{eff}/M = \sqrt{\frac{2}{M}\cdot\frac{2Z_1 Z_2 e^2}{d}}\cdot\left(\frac{2}{d}\right) \qquad (4)$$

where M is the particle's mass. Then

$$\frac{\omega_T}{\omega_L} = 2\cdot\sqrt{\frac{2Z_1 Z_2 e^2}{d\cdot E}} \qquad (5)$$

Equation 5 shows that ω_T is very much smaller than ω_L for high energy encounters. For example, for an MeV proton channeling in sodium we find

$$\frac{\omega_T}{\omega_L} \sim 10^2 \text{ to } 10^3$$

This clearly implies that the particle samples many rows (of the order of a few hundred) before any appreciable change in direction ensues. Lindhard[4] obtains a similar result and notes that the criteria is independent of the mass of the channeling particle depending only on the energy and charge per unit length $(Z_1 e)/d$ of the solid. In fact, Lindhard[4] shows further that we can make the approximation of averaging the potential when $\psi < \psi_1$ where ψ_1 is given by 1.3.2(1), that is channeling and the average potential are not independent concepts.

1.3.4 Other Important Parameters

In Figure 7, we show the results of a computer simulation quoted by Gibson[8] for the penetration of 5 MeV protons in silicon along ⟨1,1,0⟩ rows. What concerns us most in this figure is the period for longitudinal motion and the distance of closest approach. We see that the proton can maintain, for small angles relative to the axis, a distance of closest approach of the order of a Bohr radius. Further, we see that it samples a few hundred atoms in one transverse oscillation. We shall return to these results directly in the following chapter.

1.3.5 Classical or Quantum Description?

Earlier we mentioned that we would assume that the trajectory of the incident charged particle would be described correctly by Newtonian mechanics. To justify this we point out that a necessary condition for classical mechanics to apply is that the potential experienced by the particle vary slowly over the wave packet characterizing the particle. If this were not true, the concept of classical particle would have no meaning. For heavy particle channeling this condition is always met, although for electrons in the KeV range quantum considerations begin to take an importance. This is so since the electron's wavelength becomes of the order of the range of the potentials. Reference 4 shows also that the above considerations are sufficient for classical mechanics to hold. So the channeling of an MeV proton is strictly a classical phenomenon and quantum calculations are unnecessary.

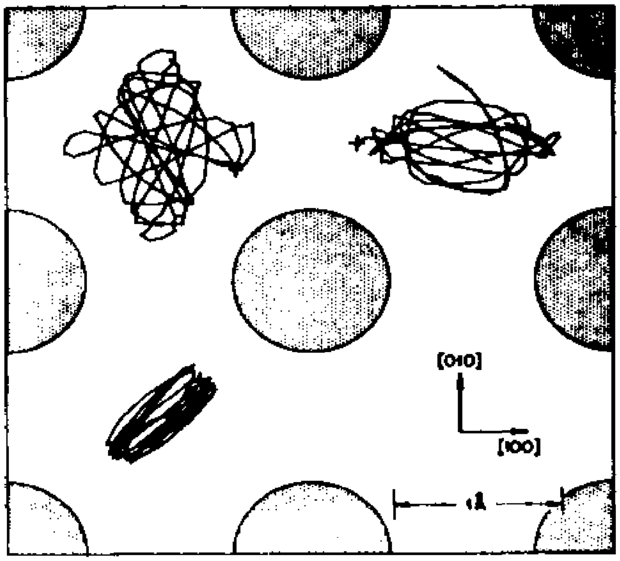


Fig. 1a

Projection of some ⟨001⟩ channel trajectories onto the (001) surface of f.c.c. Cu 1-keV Cu slowing down.[1]

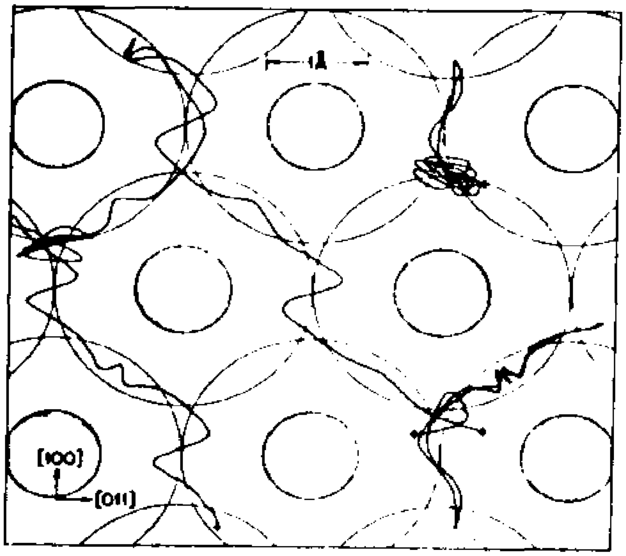


Fig. 1b

Projection of some ⟨001⟩ channel trajectories onto the (011) surface of f.c.c. Cu. 1-keV Cu slowing down.[1]

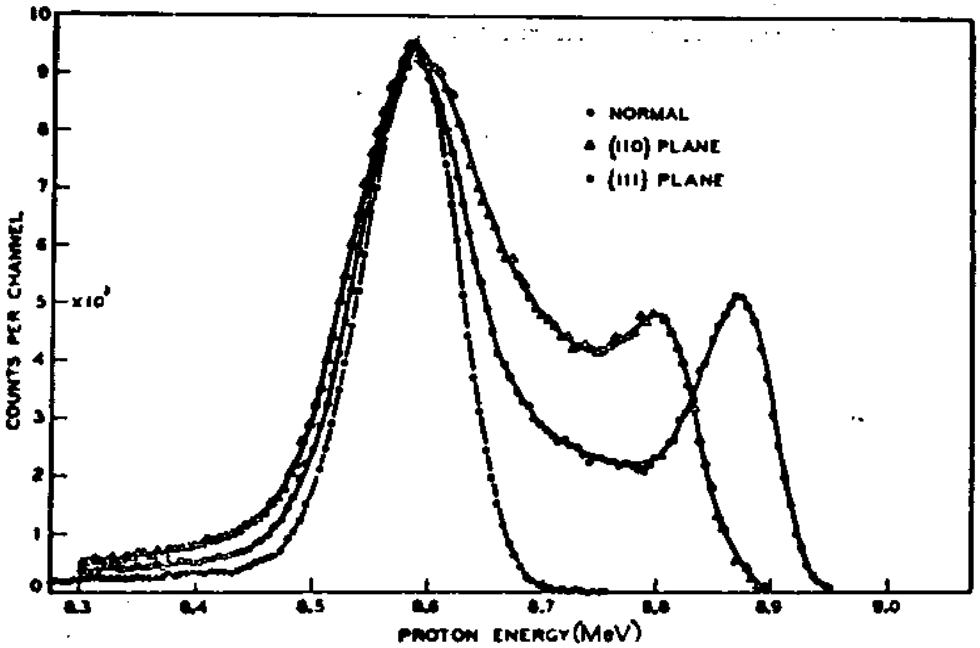


Fig. 2

Transmitted energy spectra for 9.0 MeV protons incident parallel to {111}, {110} planes and in a normal direction of a 25μ thick germanium crystal.[7]

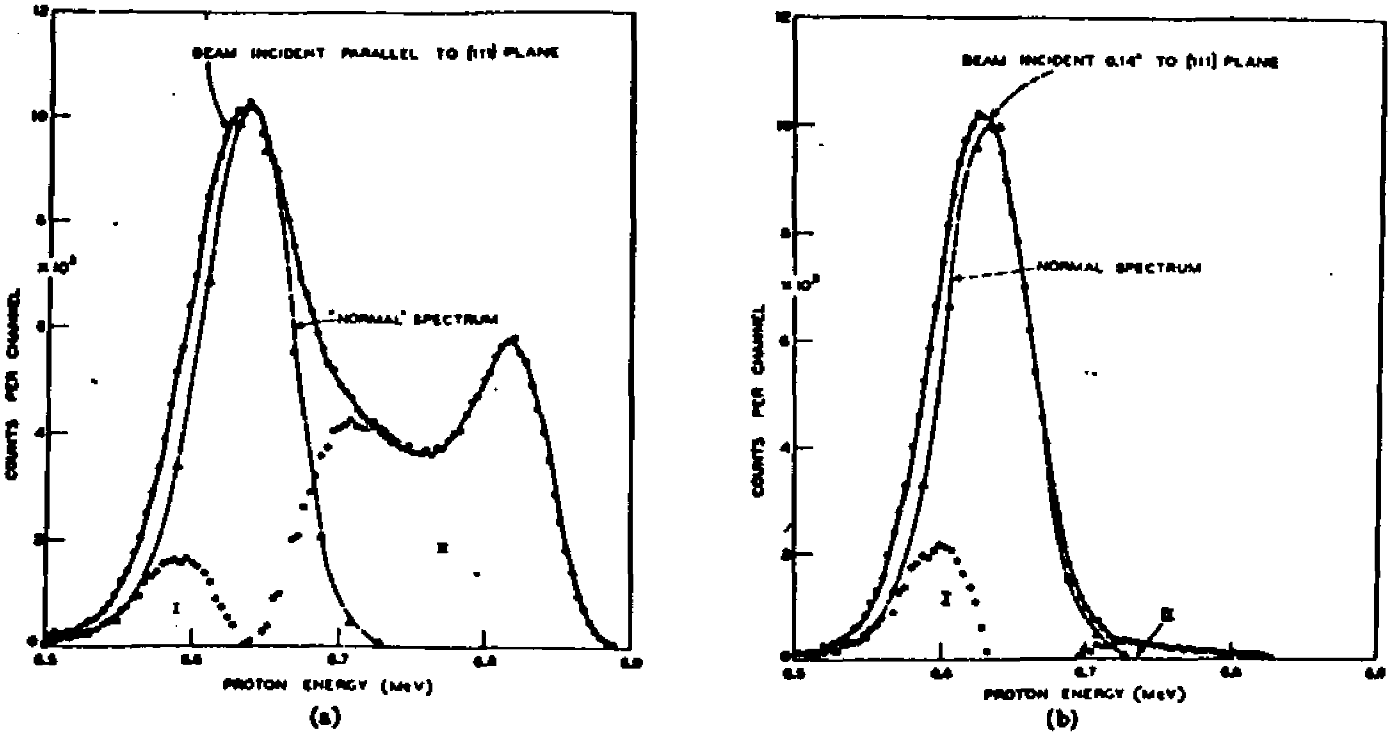


Fig. 3

Energy spectra for 7.0 MeV protons transmitted

(a) parallel to {111} planes and,

(b) 0.14° to the {111} planes of a 33μ thick

silicon crystal.[7]

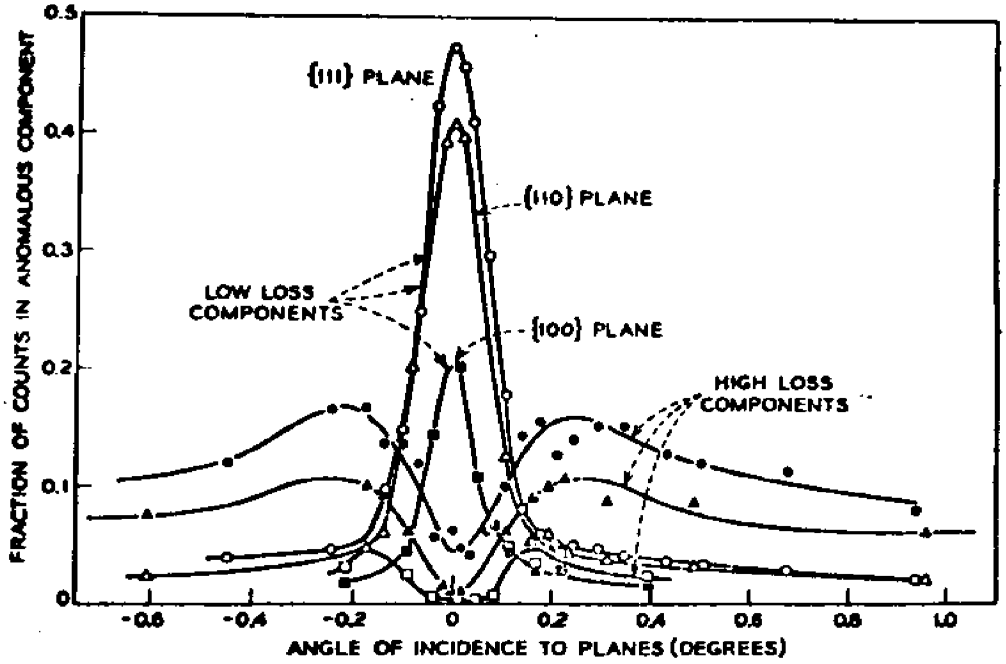


Fig. 4

Fraction of high loss and low loss particles in the transmitted energy distributions as a function of the incidence angle for 2.8 MeV protons relative to {111}, {110}, and {100} planes of a 33μ thick silicon crystal.[7]

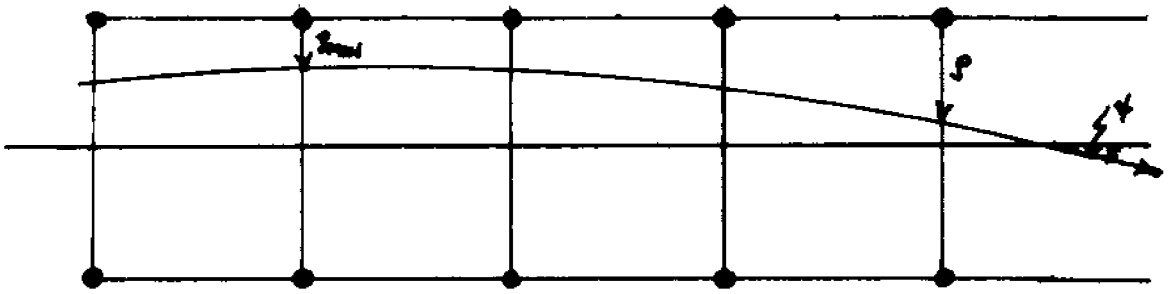


Fig. 5

Channeling in a Symmetry Plane

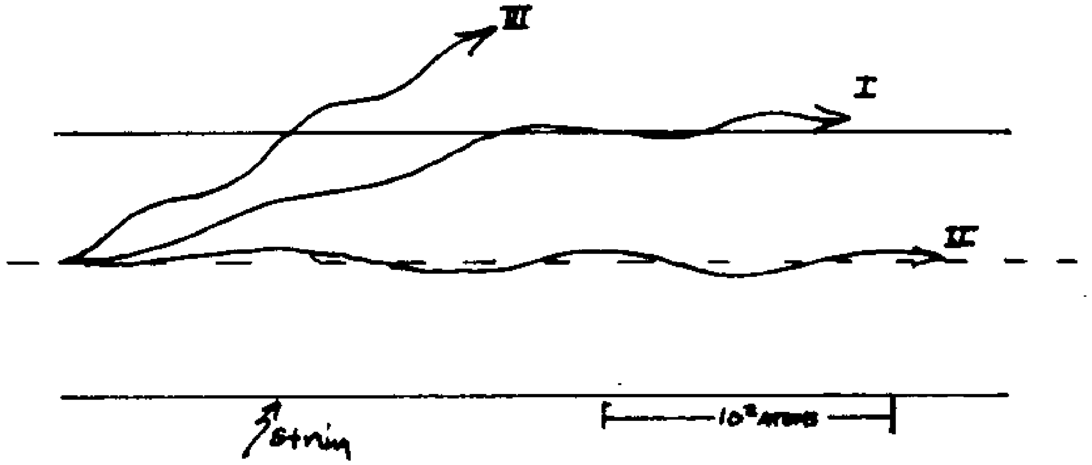
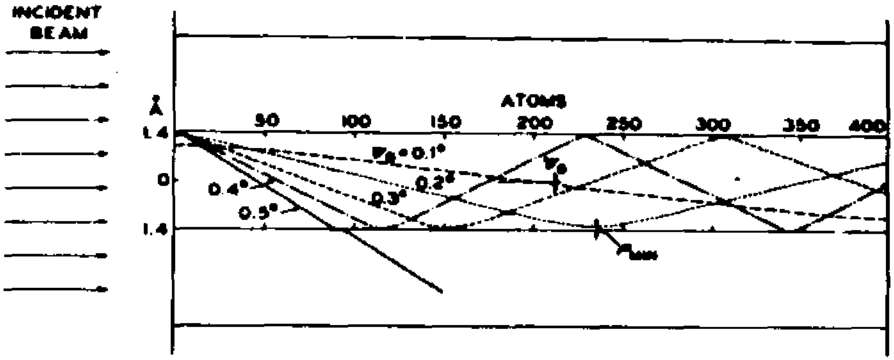


Fig. 6

Trajectories for Various Loss Compounds of Figs. 2 and 4



ψ_{INC} (DEGREES)	ρ_{MIN} (ANGSTROMS)	PERIOD (ATOMS)	$\langle\psi\rangle/\psi_0$ (PERCENT)
0.5	-	-	-
0.4	0.008	228	0.87
0.3	0.037	310	0.83
0.2	0.128	470	0.79
0.1	0.420	800	0.78

Fig. 7

Computer simulated trajectories of 5.0 MeV protons incident on static ⟨110⟩ rows of silicon.[8]

References

1. J. Stark, Phys. Z., 13, 973 (1912).
2. J. Stark and G. Wendt, Ann. Phys. 38, 921 (1912).
3. M. T. Robinson and O. S. Oen, "Computer Studies of the Slowing Down of Energetic Atoms in Crystals." Phys. Rev., 132, 2385 (1963).
4. J. Lindhard, "Influence of Crystal Lattice on Motion of Energetic Charged Particles." Mat. Fys. Medd. Dan. Vid. Selsk. 34, No. 14 (1965).
5. W. M. Gibson, "Particle Channeling Using Small Accelerators." Proceedings of the Conference on the Use of Small Accelerators for Teaching and Research, Oak Ridge (1968).
6. S. Datz, C. Erginsoy, G. Liebfried, and H. D. Lutz, "Motion of Energetic Particles in Crystals." Ann. Rev. of Nuclear Science 17, 129 (1967).
7. B. R. Appleton, C. Erginsoy, and W. M. Gibson, "Channeling Effects in the Energy Loss of 3-11 MeV Protons in Silicon and Germanium Crystals." Phys. Rev. 161, 330 (1967).
8. W. M. Gibson in "Interaction of Energetic Charged Particles with Solids." N.A.T.O. Advanced Study Institute Brookhaven Nat. Lab., 331 (1973).

Chapter 2

Equation of Motion for a Pair

2.1 Introduction

In the first chapter we showed that a proton in channeling through a single thin crystal maintained a correlated motion with consequently larger than normal impact parameters with the atoms of the solid. This in turn led to a sharp attenuation of processes dependent on string collisions. So a channeled proton will show an anonymously long range and low energy loss.† Therefore, we ask the following question. Will the motion of an electron relative to a proton in the channeling of a pair show any correlation as regards their relative positions? To put it more generally: will channeling atoms or ions reach charge equilibrium more slowly than random penetrating ones, and moreover might they not show smaller average charge states.

In this thesis, we intend to investigate this situation. We should point out here that although much of the formalism that follows is quite general we shall generally refer to the incident atom as an "electron-proton pair", or "pair", or atom. This choice of discussing the channeling of hydrogen is not only convenient for conceptual purposes but is also convenient for later computations. The emphasis on hydrogen clearly removes from consideration more difficult internal structure problems for the incident atom. Clearly, such problems would not elucidate the

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† Again, relative to random incidence.

basic aspects of atomic channeling. We should also look at this choice of hydrogen and the approximations discussed in the next sections as a first approximation. This point of view is similar to the one which considers the static string model as being a first approximation to the channeling of a proton, or the electron gas as being a first approximation for the motions of the electrons in a solid. We therefore shall try, in this exploratory investigation, to emphasize only those properties or attributes which we consider of primary importance to the phenomena under discussion. Further, we shall not hesitate at times to simplify or build models, so long as those models bring into sharp relief the basic qualities of pair channeling. At all times, the notion that this thesis is meant as an exploratory investigation of the nature of atomic channeling should be kept in mind.

In this chapter, we are primarily concerned with deriving an equation of motion for the channeling of an electron-proton pair. In section 2, we state the approximations we shall use subsequently. In section 3, we discuss the concept of a channeling subspace of Hilbert space. Concomitant with this, we discuss the use of appropriate projection operators and the superposition of quasi coherent quantum mechanical amplitudes. In section 4, we derive a general equation for the propagation of a pair. In section 5, we derive a specific equation for the problem at hand. What we ultimately obtain is a pseudo Schroedinger equation for the time development of the internal states of this pair. In section 6, we search for those states which have maximum lifetimes. A variational principal for maximum probability is stated whose solutions are shown to be, to an appropriate order in perturbation theory, nothing other than solutions to the pseudo Schroedinger equation previously derived. An appendix on biorthonormal sets is included for completeness.

2.2 Approximations

In the last chapter we observed that axial channeling has two components; one called simply the channeled ions and the second called the proper channeled ions. These are shown respectively in Figures 1b and 1a in Chapter 1. For the proper channeled group, 1a, we see again that the penetrating ion remains confined to one axis of the crystal. We shall concentrate on this group because of the simplicity even though they are a small portion of the total channeling population. We chose this group since here the motion in the transverse plane remains particularly ordered. For the non-proper channeled group the overlap between the channeling pairs charge distribution and that of the atoms of the solid would approach random behavior, insofar as transverse motion is concerned. We claim that for non-proper channeled pairs the correlation in their respective motions would approach that of a pair for random incidence. That is, we expect that the ionization rate would approach that for random penetrations.

Our second approximation entails replacing the protons dynamical motion with a prescribed one. In fact, we shall assume that the proton moves in a straight line down the center of a channel as a first step in the solution of the problem. We saw in the last chapter that a proton's motion is characterized by very gradual transverse motion, the longitudinal period being many hundreds of lattice spacings. It is clear that an adiabatic approximation is quite valid here since the transverse frequency of motion of the proton is of the order

$$\omega_T = \sqrt{\frac{2}{M} \cdot \frac{4 Z_1 Z_2 e^2}{d^2}} \qquad (1)$$

Here M is the proton mass, Z_1 the proton charge, Z_2 the core charge and d the lattice spacing. The electron's motion about the nucleus is of order

$$\omega = Z_1^2 \cdot \frac{e^2}{2 a_0 \hbar} \qquad (2)$$

where a_0 is the radius of the first Bohr orbit. For a proton-electron pair the ratio becomes

$$\frac{\omega_T}{\omega} \sim 4 \sqrt{Z_2 \left(\frac{a_0}{d}\right)^3} \cdot \sqrt{\frac{m}{M}} \qquad (3)$$

and so $\omega_T << \omega$. Therefore, we can prescribe the proton's motion, solve for the electronic motion given this nuclear position, choose another nuclear position, solve for the electronic motions and so forth. The different motions are then tied together adiabatically. Clearly, such an undertaking is rather formidable. Rather, we consider, except for a brief discussion later, only the straight line motion case. We are further assured that such a choice is reasonable by the fact that the proton can maintain in some cases, a distance of closest approach of one atomic radius. This was presented in the last chapter in Figure 7.

Our third approximation is that the lattice is rigid. This is really a minor problem and is mentioned more for completeness than any other reason. The motion of the lattice clearly will have an effect on the coupling of the pair. However, phonon energies are of the order of a fraction of a volt. Therefore, in single collisions we do not expect them to excite internal states. Phenomenologically, the motion of the lattice will be expressed by the size of the atomic cores, or better, by the range of the potential set up by them. Further, the mean square fluctuations (at STP) of the lattice would be a small fraction of the Thomas-Fermi screening radius of the atoms of the solid. Finally, this smearing out of the cores because of finite temperature effects can easily be incorporated into our work if desired. We shall not concern ourselves with this point any further.

In a later chapter, a fourth approximation will be made of averaging the potential, set up by the atoms of the solid, along the longitudinal direction. Such an average shall again be called a string potential. We showed earlier that the longitudinal frequency of lattice sites experienced by the incident pair is of the order,

$$\omega_L = \sqrt{\frac{2 \cdot E}{M d^2}} \qquad (4)$$

where E is the energy of the pair, while the electron's internal frequency of motion about the nucleus is given by equation 3. Their ratio is then

$$\frac{\omega_L}{\omega} \sim \left(\frac{a_0}{d}\right) \sqrt{\frac{m}{M}\left(E/\mathrm{Ryd.}\right)} \sim 10 \qquad (5)$$

for an MeV pair. This implies that we can make a string potential approximation. The reason for this is that on an atomic scale the potential has a high frequency component due to this longitudinal motion. Thus, the electron in a revolution samples only the average value. This is not the same approximation that was made in the last chapter. There, it was shown that the string potential is an acceptable approximation in describing the translational motion of an ion. Here it is shown that this approximation is valid for a description of the internal states of motion also.

In the derivations in the following sections we shall make approximations 2 and 4 at appropriate places. That is, we shall explicitly state when these are made so that the derivations can be expressed in their most general form until then.

2.2.1 Description of Channeling Space

We wish to solve the equation

$$\left\{ i \frac{\partial}{\partial t} - H(A,S) \right\} \Psi(A,S,t) = 0$$

looking for correlation of the electron and proton. Above, A and S refer to the incident electron and solid coordinates respectively. $H(A_1S)$ is the full Hamiltonian consisting of electron, solid and their interaction. In order to make such a search for correlation possible we look for a projection operator which projects the state $\psi(A,S,t)$ into such a subspace of Hilbert space. This subspace of correlated motion of the pair shall be referred to as "channeling space." This use of the words channeling space should cause no confusion if we remember that space here does not refer to Euclidian three space. Once we have found such an operator we can obtain an equation for the part of the wave function in this channeling space. To be more precise, we write

$$P + Q = 1 \tag{1}$$

where P is a projection operator which projects the full wave function onto that part of Hilbert space such that the pair is not decoupled. That is, there will be excitations of the solid for which the electron will remain in a quasi-stationary internal state as the pair channels through the solid. These states of the solid will be in P space. Furthermore, it is clear that P must be defined self-consistently. The choice of P will affect the lifetimes of the internal states and the lifetimes are used to select P. For example, excitations with momentum transfer less than the momentum of the electron in the first Bohr orbit will be contained in P space. So we expect that the projection operator and thus the potentials will depend upon such a parameter.

Exactly: P is defined as projecting onto that part of Hilbert space of the solid in which the pair remain in a quasi-stationary state of long lifetime. These states of long lifetime are amplitudes in P space.

2.3.2 Choice of Projection Operator

Although we shall not need an explicit form for P at the moment, it will lend some concreteness to the future discussions if we display P and give some of its properties now.

What we are, in fact, interested in is P ψ since this is the wave function in channeling space. This has the form

$$\underline{P}\Psi = \mathop{\sum\!\!\!\!\!\!\int}_{n\in C} \psi_n(A,t)\,U_n(s) \qquad (1)$$

where U_n is a solid state state satisfying the equation

$$H(S)\,U_n(S) = \nu_n\,U_n(S)$$

and H(S) is the non-interaction solid Hamiltonian and ν_n the energy of state n[†]. ψ_n are expansion coefficients and C is a dense set of excitations of the solid which comprises channeling space. The reason the set of excitations is dense is not hard to understand. Each atom of the crystal has a continuum of excitations to contribute to channeling space and they can be taken in all possible combinations. Physically, C contains small energy and momentum transfers between the pair and the solid. We must point out that a solid state of small energy and momentum transfer need not be in channeling space. The reason for this is that multiple collisions can lead to decoupling of the pair each collision comprising

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[†] We might consider the solid at absolute zero to start with. Then any excitation is then a result of a collision.

small exchanges. It is even possible for decoupling to occur in multiple collisions with the total exchanges small. On the other hand, we expect the primary ionization process to be hard single collisions. These collisions will definitely be contained in Q space. In fact, we shall see that the multiple soft collisions will affect the form of the internal states of the channeling pair. That is, they will be contained within a string potential experienced by the pair. Since our set of excitations is dense we make the following Ansatz:

$$P\Psi \simeq \Psi(A,t) \sum_{n\in C}{}' U_n(s)$$

We have assumed that the $\psi_n(A,t)$ are essentially independent of n and have taken them out of the sum. We are claiming that we need make no distinction between the many excitations in this space and can replace the various amplitudes by an average one. That $\psi(A,t)$ is an average state can be seen by equating 2 and 3 and projecting onto all of P space. We get

$$\Psi(A,t) = \frac{1}{N} \sum_{n\in C}{}' \psi_n(A,t)$$

where N is the number of excitations in P space.

Our projection operator now follows simply by inspection.

$$P = \frac{1}{N} \sum_{n\in C}{}' \sum_{m\in C}{}' |U_n\rangle\langle U_m|$$

Then we see that

$$\underline{P}\Psi = \frac{1}{N} \sum_{n\in C}{}' U_n \sum_{m \in C}{}' (U_m, \Psi)_A$$

whereby ($\quad$)$_A$ we mean the coordinate A is not integrated over. Identifying $(U_m, \psi)_A$ with $\psi_m(A,t)$ we see that 6 becomes identical with 3. Further, our operator P is a projection operator since

$$\underline{P}^{\dagger} = \frac{1}{N} \sum_{nm}{}' |U_m\rangle\langle U_n| = \underline{P}$$

$$\underline{P}^2 = \frac{1}{N^2} \sum_{nn'}{}' \sum_{mm'}{}' |U_n\rangle \langle U_{n'}, U_{m'}\rangle \langle U_m|$$

$$= \frac{1}{N^2} \left(\sum_{nm}{}' |U_n\rangle\langle U_m| \right) \sum_{n'}{}' 1$$

$$\underline{P}^2 = \frac{1}{N} \sum_{n\in C}{}' \sum_{m\in C}{}' |U_n\rangle \langle U_m| = \underline{P}$$

2.3.3 Addition of Amplitudes

In the last section we replaced the many amplitudes in channeling space by an average amplitude given explicitly by equation 2.3.2(4). What we are doing is neglecting fluctuations which we argue should be negligible here.

This approach is similar to the one used to describe nuclear resonance scattering[1]. There, instead of a dense set of excitations there exists a set of overlapping resonances. The prescription adopted is to replace the scattering amplitude by an average amplitude

$$\langle f \rangle = \frac{1}{\Delta E} \int f(E)\,dE \qquad (1)$$

where ΔE is a narrow energy range covering many resonances. The difference then between the average cross section and the one predicted by equation 1 is

$$\langle f^2 \rangle - [\langle f \rangle]^2 \qquad (2)$$

and this should be small if the fluctuations are small.

We argue that, in our case, such an addition in amplitudes is not entirely incorrect. We follow reference 2 in stating that quasi-elastic scattering of the pair is not necessarily incoherent with the incident wave, and then amplitudes may be added. Suppose that our incident electron suffers a collision with energy change $\Delta\epsilon$ and then suffers a second collision in time d/V, where again d is the lattice spacing and V is the incident pair's velocity. If the condition

$$\Delta\epsilon < \frac{\hbar V}{d}$$

is satisfied then the energy uncertainty of the scattered wave encompasses the range of incoherence $\Delta\epsilon$ and amplitudes for processes in this range can be added. Further, this inequality is exactly the one derived for the use of an average potential.

So our addition of amplitudes is consistent with our describing channeling in the standard way. What we are doing is smearing out the fluctuations in both the medium (as experienced by the pair) in the longitudinal direction and concurrently the fluctuations in the amplitudes of the atom. We might say that our electron is being scattered and rescattered but that if our pair is in channeling space we associate all these waves with the same state of the atom[†].

What we are ultimately interested in is the average charge at some point in the channel

$$\langle \rho \rangle = \frac{-e}{N} \sum_{n\in C}{}' \, |\psi_n(A,t)|^2 \qquad (4)$$

integrated over an appropriate portion of phase space. What we shall obtain from our average state is the distribution

$$\bar{\rho} = -e\,|\Psi(A,t)|^2 \qquad (5)$$

These differ by the amount

$$\bar{\rho} - \langle \rho \rangle = \frac{-e}{N} \sum_{n\neq m}{}' \, \psi_n^* \psi_m$$

where the sum is restricted to channeling space. For randomly varying phases and large N we claim that this term can be dropped. The closer the processes are to true coherence the smaller this term will be.

[†] Of course, this atom might have a further set of quantized internal states.

In order for the amplitudes we are adding to be incoherent we must, in principal, be able to measure (i.e. distinguish between) either the states of excitation of the solid or of the pair. New pair excitations of the order of $me^2/\hbar$ are not distinguishable. They are contained within uncertainties in the internal states of the pair. For the solid the consequent excitations will generally be local in nature with short lifetimes and therefore large energy uncertainties.

3.4 Equation of Motion

To find the motion of the pair we want to project the Schroedinger equation onto channeling space. To do this we begin with the full many body problem with Hamiltonian

$$H = H(A) + H(S) + V(A,S) \tag{1}$$

where again the free atom, free solid and atom solid interaction appear respectively.

We now let P be a projection onto channeling space and Q its orthogonal complement[†]. We look for an equation for $P\Psi(A,S,t)$ where $\Psi(A,S,t)$ satisfies

$$\left(i\frac{\partial}{\partial t} - H\right)\Psi(A,S,t) = 0 \tag{2}$$

[†] In this section we don't use the explicit representation of P.

We can rewrite this as

$$\left(i\frac{\partial}{\partial t}-H\right)(P+Q)\Psi=0 \qquad (3)$$

and project onto P to get

$$P\left(i\frac{\partial}{\partial t}-H\right)P\Psi = PHQ\Psi$$

We use the fact that P is time independent to write the above equation as

$$\left(i\frac{\partial}{\partial t}-H_{PP}\right)\Psi_P = H_{PQ}\,\Psi_Q \qquad (4)$$

with the obvious definitions

$$\Psi_p \equiv P\Psi$$

$$H_{pQ} \equiv PHQ$$

Similarly, if we project equation 3 onto Q space we get

$$\left(i\frac{\partial}{\partial t}-H_{QQ}\right)\Psi_Q = H_{QP}\,\Psi_P \qquad (5)$$

We want to solve the coupled equations 4 and 5 for the time development of Ψ_p under the initial conditions

$$\Psi_p = \Psi_Q = 0 \qquad t< 0$$

$$\Psi_p(0) = \Psi_0$$

$$\Psi_Q(0) = 0$$

We define the Laplace transform (one-sided Fourier transform)

$$\Psi(E) = \mathcal{L}(\Psi) = \frac{1}{2\pi}\int_0^\infty e^{iEt}\,\Psi(t)\,dt \qquad (6)$$

with the inversion

$$\Psi(t) = \int_\xi dE\; e^{-iEt}\,\mathcal{L}(\Psi)$$

where ξ is a contour above all the poles of $\mathcal{L}(\psi)$ in the complex E plane as is shown in Figure 8. Now we can Laplace transform equations 4 and 5 using the following result

$$\begin{aligned}\mathcal{L}\left(i\frac{\partial}{\partial t}\Psi\right) &\equiv \frac{1}{2\pi}\int_0^\infty e^{iEt}\, i\frac{\partial}{\partial t}\Psi(t)\,.\,dt \\ &= \frac{1}{2\pi}\int_0^\infty \left\{\frac{\partial}{\partial t}\left[e^{iEt}\,\Psi(t)\right] - i\frac{\partial}{\partial t}e^{iEt}\,.\,\Psi(t)\right\}dt \\ &= \frac{-i}{2\pi}\,\Psi(0) + \frac{1}{2\pi}\int_0^\infty E\, e^{iEt}\,\Psi(t)\,dt\end{aligned}$$

$$\mathcal{L}\left(i\frac{\partial}{\partial t}\Psi\right) = \frac{-i}{2\pi}\,\Psi(0) + E\,\mathcal{L}(\Psi)$$

where the condition that $e^{iEt}\,\psi(t) \to 0$ as $t \to \infty$ was used. So we obtain for the Laplace transforms of 4

$$[E - H_{pp}]\,\Psi_p(E) = H_{pQ}\,\Psi_Q(E) + \frac{i}{2\pi}\Psi_0$$

and 5

$$[E - H_{QQ}]\,\Psi_Q(E) = H_{Qp}\,\Psi_p(E)$$

where the initial conditions on ψ_p and ψ_Q have been used. We can now invert the latter equation

$$\psi_Q(E) = \frac{H_{Qp}}{E-H_{QQ}}\,\psi_p(E)$$

and substitute into the former to obtain

$$\{E - \mathcal{H}\}\,\Psi_p(E) = \frac{i}{2\pi}\Psi_0 \qquad (8)$$

where

$$\mathcal{H} \equiv H_{pp} + H_{pQ}\,\frac{1}{E-H_{QQ}}\,H_{Qp} \qquad (9)$$

If we solve 8 for ψ_p and substitute into 7 we have solved our problem formally. In 7 the contour ξ can be distorted so that it lies just above the real axis of E space. That is, the replacement,

$$E \rightarrow E + i\eta \quad (\lim \eta \rightarrow 0)$$

is valid with the new E being real. To prove this we shall show that if the imaginary part of E is greater than zero then the poles of $\psi_p(E)$ lie below the real E axis and if the imaginary part of E is greater than zero the poles of $\psi_p(E)$ lie above the real axis. But the poles of $\psi_p(E)$ must lie below the contour $\mathcal{C}$ and this will be satisfied for the contour distorted down onto the real E axis from above.

To prove the contention we must show that $I_m(E_m)$ has opposite sign to $I_m(E)$, where $I_m(E_m)$ means the imaginary part of E_m which is a pole of $\psi_p(E)$ and satisfies

$$\{E_m - \mathcal{H}(E)\}\,\varphi_m(E) = 0 \qquad (10)$$

In this equation $\mathcal{H}$ is the Hamiltonian of equation 9 and is non-hermitian. This statement shall be proved later. We want to point out that the solutions of 10 and

$$\{E_m^* - \mathcal{H}^+\}\,\hat{\varphi}_m = 0 \qquad (10a)$$

form a biorthonormal set of states. We review their properties in Appendix A of this chapter. We shall need the properties

$$\langle \hat{\varphi}_n, \varphi_m \rangle = \langle \varphi_n, \hat{\varphi}_m \rangle = \delta_{nm}$$

$$1 = \sum_m{}' \,|\hat{\varphi}_m\rangle\langle\varphi_m| = \sum_m{}' \,|\varphi_m\rangle\langle\hat{\varphi}_m|$$

Using the orthonormal set ω_S, a solution of

$$(\mathcal{E}_S - H_{QQ})\,\omega_S = 0$$

in equation 10 we get

$$\left(E_m - H_{PP} - \sum_{S}{}' \frac{H_{PQ}|\omega_s\rangle\langle\omega_s| H_{QP}}{E-\varepsilon_s} \right)\varphi_m(E) = 0$$

We then multiply by $\int d^3A\, d^3S\, \varphi_m^*(E)$ to get

$$E_m \langle\varphi_m,\varphi_m\rangle - \langle\varphi_m, H_{PP}\,\varphi_m\rangle - \sum_{S}{}' \frac{\langle\varphi_m H_{PQ}\,\omega_s\rangle\langle\omega_s, H_{QP}\varphi_m\rangle}{E-\varepsilon_s} = 0 \quad (11)$$

Since

$$\langle\varphi_m, H_{PQ}\,\omega_s\rangle = \langle P\varphi_m, H\, Q\omega_s\rangle$$
$$= \langle Q\omega_s, H\, P\varphi_m\rangle^*$$

$$\langle\varphi_m, H_{PQ}\,\omega_s\rangle = \langle\omega_s, H_{QP}\,\varphi_m\rangle \qquad (12a)$$

$$\langle\varphi_m,\varphi_m\rangle = \int d^3A\, d^3s\, |\varphi_m|^2 \geqslant 0 \qquad (12b)$$

We obtain on using 12a in 11 and then subtracting the complex conjugate equation

$$(E_m - E_m^*)\langle\varphi_m,\varphi_m\rangle = \sum_{S}{}' |\langle\varphi_m, H_{PQ}\,\omega_s\rangle|^2 \left\{ \frac{1}{E-\varepsilon_s} - \frac{1}{E^*-\varepsilon_s} \right\}$$

$$2i\, I_m(E_m)\langle\varphi_m,\varphi_m\rangle = \sum_{S}{}' |\langle\varphi_m, H_{PQ}\,\omega_s\rangle|^2 \left\{ \frac{-2i I_m(E)}{(Re(E)-\varepsilon_s)^2 + I_m^2(E)} \right\}$$

With equation 12b we conclude from the above that $I_m(E_m)$ has opposite sign of $I_m(E)$. Therefore 8 and 9 are written with E replaced by $E+i\eta$.

$$(E - \mathcal{H})\Psi_P(E+i\eta) = \frac{i}{2\pi}\Psi_0 \qquad (8')$$

$$\mathcal{H} = H_{PP} + H_{PQ}\frac{1}{E+i\eta-H_{QQ}}H_{QP} \qquad (9')$$

This Hamiltonian breaks naturally into P and Q space parts. The first term in 9' represents an average static Hamiltonian describing processes in P space only. The second term represents transitions from P space into Q space, propagation in Q space and then transition back into P space. This term is non-local in space and is also complex, its imaginary part describing loss of flux from P space. The loss of flux from P space is related to the fact that the imaginary part of the Hamiltonian is negative definite†. From the Dirac relation

$$\frac{1}{x\pm i\epsilon} = \frac{P}{x} \mp i\pi\delta(x)$$

we obtain from 9'

$$I_m\mathcal{H} = -\pi H_{PQ}\,\delta(E-H_{QQ})\,H_{QP}$$

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† This relationship is shown explicitly later.

If we take the expectation value in any state $\chi(A,S)$ we get

$$\langle \mathrm{Im}\,\mathcal{H} \rangle_{\chi} = -\pi \sum_{S}{}' \langle \chi, H_{PQ}\,\omega_S \rangle \langle \omega_S, H_{QP}\,\chi \rangle\, \delta(E-\mathcal{E}_S)$$

$$= -\pi \sum_{S}{}' \left| \langle \chi, H_{PQ}\,\omega_S \rangle \right|^2 \delta(E-\mathcal{E}_S) \leq 0$$

The loss of flux is interpreted as the decay of the internal state of the pair in going down a channel.

2.5 Equation of Motion for the Average Amplitude

It is clear that the equations derived in the last section are independent of the form of the projection operator. We now want to use these equations to obtain an equation of motion for the average amplitude and therefore remove the solid coordinates from the equation. Specifically,

$$\mathcal{P}\, \Phi(A,S,t) = \Phi(A,t) \cdot \sum_{n}{}' U_n(S)$$

and so it follows from 2.4(6) that the Laplace transform becomes

$$\mathcal{P}\, \Phi(A,S,E) = \Phi(A,E) \sum_{n}{}' U_n(S) \qquad (1)$$

We also need the result

$$\left\langle \frac{1}{N} \sum_{m\in C}{}' U_m(S),\ \sum_{n\in C}{}' U_n(S) \right\rangle = 1 \qquad (2)$$

First we rewrite 2.4(8') as

$$P\left(E-H-H\frac{Q}{E-H_{QQ}}H\right)P\Psi(E)=\frac{i}{2\pi}\Psi_0 \qquad (3)$$

Then we project onto P space, $\frac{1}{N}\sideset{}{'_1}\sum_{m\in c} U_m^+(S)$, in equation 3 using 1 and 2 to obtain

$$\left\{E-\frac{1}{N}\sideset{}{'_1}\sum_{n,m\in c}\langle U_n, HU_m\rangle-\frac{1}{N}\sideset{}{'_1}\sum_{nm\in c}\langle U_n\, H\frac{Q}{E-H_{QQ}}H\,U_m\rangle\right\}\Psi(A,E)=\frac{i}{2\pi}\Psi_0(A) \qquad (4)$$

where

$$\Psi(A,E)=\frac{1}{2\pi}\int_0^\infty dt\, e^{iEt}\,\Psi(A,t) \qquad (5a)$$

$$\Psi(A,t)=\int_\xi dE\, e^{-iEt}\,\Psi(A,E) \qquad (5b)$$

If we write as before

$$H = H(A) + H(S) + V(A_1S)$$

$$H(S)U_n(S) = \nu_n U_n(S)$$

equation 4 becomes

$$\left\{\left(E-\frac{1}{N}\sideset{}{'_1}\sum_{n\in c}\nu_n\right)-H(A)-\frac{1}{N}\sideset{}{'_1}\sum_{nm\in c}V_{nm}(A)\right\}\Psi(A,E)$$

$$-\frac{1}{N}\sideset{}{'_1}\sum_{nm\in c}\int d^3A'\left\langle U_n V\frac{Q}{E-H_{QQ}}V\,U_m\right\rangle_{AA'}\Psi(A',E)=\frac{i}{2\pi}\Psi_0(A) \qquad (6)$$

First note that this equation only contains the atomic coordinates the solids having been projected out. The first term on the left hand side of this equation is the energy of the pair in channeling space; the total energy less the average energy of excitations in channeling space. The second term is simply the free space Hamiltonian. The third term is the average static interaction in P space. This term in effect represents the solid frozen in one of its P state excitations and then averaged over all of P space. The atom interacts with the solid through this term as if the solid were incapable of dynamical response. If this were all there were many body problem would be simple. The rub is in the last term. It contains most of the dynamics of the problem by describing the coupling between channeling and non-channeling space. The coupling is accomplished through the interaction V(A,S) in the fourth term of equation 6. The operator is shown explicitly in its non-local form. It averages all transition, both real and virtual, out of channeling space, its imaginary part representing real transitions.

We shall generally write (6) in the form

$$[E - \mathcal{H}]\Psi = \frac{i}{2\pi}\Psi_0 \tag{7}$$

with

$$\mathcal{H} = H(A) - \frac{1}{N}\sum_{nm\epsilon C}{}' V_{nm}(A) - \frac{1}{N}\sum_{nm\epsilon C}{}' \int d^3A \left\langle U_n V \frac{Q}{E - H_{QQ}} V U_m \right\rangle_{A,A'} \tag{7a}$$

and we have made the replacement

$$E - \frac{1}{N}\sum_{n}{}' \nu_n \rightarrow E$$

2.6 States of Maximum Lifetime

In these sections we find an equation for the state ψ_0 that lives longest.

2.6.1 Variational Principle

First we look at the evolution of an arbitrary state ψ_0 by inverting equation 2.5(7a)

$$\Psi(A, E+i\eta) = \frac{\left(\frac{i}{2\pi}\right)\Psi_0}{E-\mathcal{H}}$$

and then use the biorthonormal set φ_m of

$$\{E_m - \mathcal{H}\}\varphi_m = 0$$

$$\{E_m^* - \mathcal{H}^+\}\hat{\varphi}_m = 0$$

to write

$$\Psi(E+i\eta) = \sum_{m}{}'(i/2\pi)\frac{\langle\hat{\varphi}_m, \Psi_0\rangle}{E-E_m+i\eta}\varphi_m$$

Substituting this into 2.5(5a) we find

$$\Psi(A,t) = \int_{-\infty}^{+\infty} dE\, e^{-iEt} \sum_m{}' (i/2\pi) \frac{\langle \hat{\varphi}_m, \Psi_0 \rangle}{E - E_m + i\eta} \varphi_m$$

$$\Psi(A,t) = \sum_m{}' e^{-iE_m t} a_m \varphi_m \qquad (1)$$

$$a_m \equiv \langle \hat{\varphi}_m, \Psi_0 \rangle \qquad (2)$$

In the second line we closed the contour in the lower half of the E plane. We assumed that the integrand fell off properly at infinity and has no singularities in the lower half plane. If it has singularities the argument that follows is not essentially changed.

We now ask the following question: Out of all states ψ_o that we could prepare at t = 0, which one would survive longest? We want to know what is the set of a_m which maximizes the probability at time t. These sets correspond to highly correlated pairs and possibly binding of the electron in the field of the proton. The time t here is considered a parameter, the transit time, and is fixed for a particular crystal being L/V the ratio of the channel length to atom velocity. We shall find that states of maximum lifetime will satisfy a Schroedinger equation which depends upon this parameter. The eigenstates of this equation therefore will also depend upon this parameter. However, except for very long times, our states of maximum lifetime are independent of this parameter. This is shown explicitly in the next section.

To maximize the probability we write

$$p = \mathrm{Prob}(t) = \int d^3A \; \Psi^*(A,t)\,\Psi(A,t) \Big/ \int d^3A \; \Psi^*(A,0)\,\Psi(A,0)$$

$$p = \sum_{mm'\in C}{}' \, e^{-i(E_m - E^*_{m'})t} \, a^*_{m'} \, a_m \, \alpha_{m'm} \,/N \qquad (2)$$

$$\alpha_{m'm} \equiv \int d^3A \; \varphi^*_{m'} \, \varphi_m$$

$$N \equiv \sum_{mm'\in C}{}' \, a^*_{m'} \, a_m \, \alpha_{m'm}$$

In going from the first to second line equation 1 was used. We now vary equation 2 with respect to a_m. Since the real and imaginary parts of a_m are independent we can vary them separately. As is usual we prefer to treat a_m and a^*_m as independent quantities and so we find

$$\frac{\partial p}{\partial a^*_{m'}} = \frac{1}{N^2}\left\{ N \sum_{m}{}' e^{-i(E_m - E^*_{m'})t} a_m \alpha_{m'm} - N p \sum_{m}{}' a_m \, \alpha_{m'm} \right\}$$

Setting this equal to zero which makes p stationary we obtain the equation

$$\sum_m{}' e^{-i(E_m - E_{m'}^*)t} a_m \alpha_{m'm} = p \sum_m{}' a_m \alpha_{m'm} \tag{4}$$

or in abstract vector space since $H \neq H^+$

$$e^{iH^+t} e^{-iHt} \Psi_0 = p \Psi_0 \tag{5}$$

States of maximum probability (lifetime) are eigenstates of the probability operator $e^{iH^+t} e^{-iHt}$ which is an hermitian operator with a complete set of states. The completeness follows from that fact that the eigenvalues of p are bounded. The spectrum is contained between zero and unity. We expect that the spectrum should look like Figure 9. The solution of equation 5 presents difficult mathematical problems. Since we consider this equation intractable in its present form we shall simplify this equation by showing that to an appropriate order in a pertubative expansion our solutions satisfy

$$e^{-iHt} \Psi = e^{-iEt} \Psi$$

2.6.2 Perturbation Theory

We shall attempt to solve the equation for the probability p in powers of the interactions and the interaction times the transit time. This equation in terms of the eigenstates of $\mathcal{H}$ was written in the last section as

$$\sum_m{}' e^{-i(E_m - E_m^*)t} a_m \alpha_{m'm} = p \sum_m{}' a_m \alpha_{m'm} \qquad 2.6.4$$

for the amplitude $a_{m'}$, with

$$\alpha_{m'm} = \langle \varphi_{m'}, \varphi_m \rangle \qquad 2.6.3$$

It might seem at first that such a perturbation expansion is incorrect here. It might be argued that the internal energies are of the order of the interaction at best (possibly much smaller) and so perturbation theory breaks down. This would be true for random penetrations. In the channel, however, the electron solid interaction can be a small fraction of its binding energy. We shall see this explicitly in the numerical results in chapters 5 and 6.

We write 2.6.1(7a) in the form

$$\mathcal{H} = H(A) + \mathcal{V}$$

$$\mathcal{V} = \mathcal{U} - i\vartheta$$

Then the eigenstates that diagnolize the operator $\mathcal{H}$ to first order are

$$\varphi_\ell = \chi_\ell + \sum_{m \neq \ell}{}' \frac{\mathcal{V}_{m\ell}}{W_\ell - W_m} \chi_m \qquad (1)$$

with eigenvalue

$$E_\ell = W_\ell + \mathcal{V}_{\ell\ell} + \sum_{m \neq \ell}{}' \frac{|\mathcal{V}_{\ell m}|^2}{W_\ell - W_m} \qquad (2)$$

The index l specifies the correspondence between φ and the unperturbed solution χ_ℓ which satisfies

$$H(A)\ \chi_\ell = W_\ell \chi_\ell$$

and represents freely moving hydrogen. In 1 $V_{m\ell}$ is the matrix element between free hydrogen states, and the sum in 2 is taken over all states not equal to the one of interest. In the event of degeneracy we need not rewrite equations 1 and 2 but we can merely interpret them more generally. In this case the index ℓ is interpreted not as specifying a state but rather a subspace of energy W_ℓ. Then χ_ℓ is the wave function in this subspace being the correct linear combination that diagnolizes V. The sum is over all subspaces with energy different than W_ℓ.

With this understanding we substitute 1 into 2.6.2(3) to get

$$\alpha_{mn} = \langle \varphi_m , \varphi_n \rangle = \delta_{mn} + \beta_{mn} + O(\gamma^2) \qquad (3)$$

$$\beta_{mn} = \left[\frac{V_{mn}}{W_n - W_m} + \frac{(V_{nm})^{+}}{W_m - W_n} \right] Q_{mn} \qquad (4)$$

$$Q_{mn} \equiv 1 - \delta_{mn}$$

Since $V = U - i\vartheta$ we get on substituting this into 4

$$\beta_{mn} = \frac{Q_{mn}}{W_n - W_m} \left(-2i\,\vartheta_{mn} \right) \qquad (5)$$

The operator β is hermitian since

$$\beta^*_{mn} = \frac{Q_{mn}}{W_n - W_m}\left(2i\,\vartheta^*_{mn}\right) = \frac{Q_{nm}}{W_m - W_n}\left(-2i\,\vartheta_{nm}\right) = \beta_{nm}$$

Using 3, 4 and 5 in 2.6.2(4) we obtain the equation for the amplitude m of maximum lifetime

$$\sum_n{}' i\,\delta_{nm}\, a_n \left(e^{-\Gamma_m t} - \mathfrak{p}\right) = \sum_n{}' i\, a_n\, \beta_{mn} \left(\mathfrak{p} - e^{-i\Omega_{mn} t}\right) + O(v^2) \qquad (6)$$

in which we defined (remembering that our eigenvalues E are complex)

$$E_n = \mathcal{E}_n - i\Gamma_n/2$$

$$\Omega_{nm} = E_n - E^*_m$$

We now make a perturbative expansion for the level ℓ in powers of v

$$a_n = a_n^{(0)} + a_n^{(1)} + \cdots = \delta_{n\ell} + a_n^{(1)} + \cdots$$

$$\mathfrak{p} = \mathfrak{p}_\ell^{(0)} + \mathfrak{p}_\ell^{(1)} + \cdots$$

and substitute these expressions in 6. We then equate equal powers of v to obtain the following:

<u>Zero Order solutions</u>

$$\delta_{m\ell}\left(e^{-\Gamma_m t} - \mathfrak{p}_\ell^{0}\right) = 0$$

so for m = ℓ

$$\mathfrak{p}_\ell^{0} = e^{-\Gamma_\ell t}$$

First Order Solutions

$$\delta_{m\ell}(-\mathcal{E}_\ell^{(1)}) + a_m^{(1)}(\mathcal{E}_m^{(0)} - \mathcal{E}_\ell^{(0)}) = \sum_n{}' \delta_{n\ell}\,\beta_{mn}\,(\mathcal{E}_\ell^{(0)} - e^{-i\Omega_{mn}t})$$

for m = ℓ we get

$$\mathcal{E}_\ell^{(1)} = 0 \qquad (8)$$

Using the fact that β is only off diagnal.

For m≠ ℓ we get

$$a_m^{(1)} = \beta_{m\ell} \quad \frac{(\mathcal{E}_\ell^{(0)} - e^{-i\Omega_{\ell m}t})}{(\mathcal{E}_m^{(0)} - \mathcal{E}_\ell^{(0)})} \qquad (9)$$

Second Order Solutions

$$a_m^{(2)}(\mathcal{E}_m^{(0)} - \mathcal{E}_\ell^{(0)}) - a_m^{(1)}\mathcal{E}_\ell^{(1)} - \delta_{m\ell}\,\mathcal{E}_\ell^{(2)} = \sum_n{}' a_n^{(1)}\beta_{mn}(\mathcal{E}_\ell^{(0)} - e^{-i\Omega_{nm}t})$$

$$+ \sum_n{}' \delta_{n\ell}\,\beta_{mn}\,\mathcal{E}_\ell^{(1)} + \sum_n{}' \delta_{n\ell}\,[\alpha(r^2)]_{mn}\,(\mathcal{E}_\ell^{(0)} - e^{-i\Omega_{nm}t})$$

For m = ℓ

$$-\mathcal{E}^{(2)} = \sum_n{}' a_n^{(1)}\beta_{\ell n}(\mathcal{E}_\ell^{(0)} - e^{-i\Omega_{n\ell}t}) - [\alpha(r^2)]_{\ell\ell}(\mathcal{E}_\ell^{(0)} - e^{-i\Omega_{\ell\ell}t})$$

We have on substituting 9 into this

$$\mathcal{E}_\ell^{(2)} = \sum_{n\neq\ell}{}' |\beta_{\ell n}|^2 \quad \frac{|(\mathcal{E}_\ell^{(0)} - e^{-i\Omega_{\ell n}t})|^2}{\mathcal{E}_\ell^{(0)} - \mathcal{E}_n^{(0)}} \qquad (10)$$

To write our results out in full we remember that the coefficients a_n

appeared in the expansion of Ψ_ℓ in

$$\Psi_\ell = \sum_n{}' a_n \varphi_n$$

$$\Psi_\ell = \varphi_\ell + a_\ell^{(1)} \varphi_\ell + \sum_{n \neq \ell}{}' a_n^{(1)} \varphi_n + \cdots$$

We choose $a_\ell^{(1)}$ so that Ψ_ℓ is normalized to unity to order V. This is satisfied by setting $a_\ell^{(1)} = 0$. Using 1 in the above with 9 we find

$$\Psi_\ell = \chi_\ell + \sum_{n \neq \ell}{}' \left(\frac{U_{n\ell} - i\mathcal{V}_{n\ell}}{W_\ell - W_n} \right) \chi_n + \sum_{n \neq \ell}{}' \frac{-2i\mathcal{V}_{n\ell}}{W_\ell - W_n} \frac{\left(\mathfrak{f}_\ell - e^{-i\Omega_{\ell n} t}\right)}{\mathfrak{f}_n^{(0)} - \mathfrak{f}_\ell^{(0)}} \chi_n + \cdots \qquad (10a)$$

And using 7, 8, and 9 we find

$$\mathfrak{f}_\ell = \mathfrak{f}_\ell^{(0)} + \sum_{n \neq \ell}{}' 4 \frac{|\mathcal{V}_{\ell n}|^2}{(W_\ell - W_n)^2} \left| \frac{\mathfrak{f}_\ell^{(0)} - e^{-i\Omega_{\ell n} t}}{\mathfrak{f}_\ell^{(0)} - \mathfrak{f}_n^{(0)}} \right|^2 + \cdots \qquad (11b)$$

$$\mathfrak{f}_\ell^{(0)} = e^{-\Gamma_\ell t} \qquad (11c)$$

These solutions have the following asymptotic property

$$\Psi_\ell \to \chi_\ell + \sum_{m \neq \ell}{}' \frac{V_{m\ell}}{W_\ell - W_m} \chi_m \qquad (\mathcal{V} \to 0)$$

$$\mathfrak{f}_\ell \to \mathfrak{f}_\ell^{(0)} \to 1 \qquad (\mathcal{V} \to 0)$$

The last result follows from $\Gamma_\ell \to 0$ as $\gamma \to 0$ and is proved below.

So the equation $e^{iH^+t} e^{-iHt} \psi = p\psi$ which makes the probability an extrenum yields wave functions and probabilities which have the property that if the imaginary part of the potential goes to zero the usual perturbed stationary states are obtained. These states have infinite lifetimes since $p_\ell = 1$. However, if the imaginary part of the perturbation does not vanish then the state decays at a rate given by the time derivative of 11b. If we prepare a state given by 11a it will live longer than other states but will ultimately decay if the transit time is made long enough. We notice that these states of maximum lifetime satisfy, to lowest order, the equation

$$\mathcal{H} \Phi_\ell = E_\ell \Phi_\ell \qquad (12)$$

$$\mathcal{H} = H(A) + V$$

So states of maximum lifetime satisfy a pseudo-Schroedinger equation with complex potential. Although this is not really a Schroedinger equation we shall solve it to obtain our states of maximum lifetime.

Our contention that the zero order decay rate goes to zero with the imaginary part of the potential follows directly from 12 by first projecting onto $\hat{\varphi}_m$ to get

$$< \hat{\varphi}_m , \mathcal{H} \varphi_n > = E_n \delta_{mn}$$

and then projecting the adjoint of 12 onto φ_m

$$< \varphi_m , \mathcal{H}^+ \hat{\varphi}_n > = E_n^* \delta_{nm}$$

and subtracting to get

$$\mathcal{H}_{mn} - (\mathcal{H}_{nm})^* = \delta_{nm}(E_n - E_m^*)$$

Using $H = H(A) + U - i\mathcal{V}$ and setting m=n we find

$$(-i\mathcal{V}_{nm}) - (-i\mathcal{V}_{nn}) = -i\Gamma_n$$

$$\Gamma_n = 2\mathcal{V}_{nn} = 2\langle\hat{\varphi}_n, \mathcal{V}\varphi_n\rangle$$

and so $\Gamma \to 0$ as $\mathcal{V} \to 0$.

At this point it would be worth our while to review what we have shown. First we have found that the pair propagates in the channel according to

$$\Psi = \sum_n{}' e^{-iE_n t} a_n \varphi_n$$

$$a_n = \langle\hat{\varphi}_n, \Psi_0\rangle$$

and Ψ_o is an initially prepared state in the channel. The φ_n satisfy

$$(E_n - \mathcal{H})\varphi_n = 0$$

where $\mathcal{H}$ is a complex non-local Hamiltonian. We now look for which Ψ_o will give maximum probability at the end of the transit. This is shown to be none other than φ_n if we only look at solutions to order V. Then

$$\Psi(t) = e^{-iEt}\,\Psi_0$$

or our states of maximum lifetime satisfy

$$\left(i\frac{\partial}{\partial t} - \mathcal{H} \right) \Psi = 0 \qquad (12)$$

$$\mathcal{H} = H(A) - \frac{1}{N} \sum_{\substack{1 \\ nm\in C}}' V_{nm} - \frac{1}{N} \sum_{\substack{1 \\ nm\in C}}' \int d^3A \left\langle U_n\, V \frac{Q}{E - H_{QQ}}\, V\, U_m \right\rangle_{A,A'} \qquad (12a)$$

We shall concentrate in the next few chapters on the explicit solution of this equation.

Appendix A

Biorthonormal Sets

Consider an eigenvalue problem for the non-hermitian operator $\mathcal{L}$ and its adjoint $\mathcal{L}^+$

$$\mathcal{L}\phi = \lambda\phi \qquad (1)$$

$$\mathcal{L}^+\hat{\phi} = \mu\hat{\phi} \qquad (2)$$

where $\mathcal{L}^+$ is defined by

$$<\mathcal{L}^+\psi, \phi> = <\psi, \mathcal{L}\phi>$$

We prove first that in 2 $\mu=\lambda^*$. Expand $\mathcal{L}, \mathcal{L}^+$ in a complete set of states γ of any hermitian operator

$$\mathcal{L} = \sum_{rs}{}' |\gamma_r> \mathcal{L}_{rs} <\gamma_s|$$

$$\mathcal{L}^+ = \sum_{rs}{}' |\gamma_r> \mathcal{L}^*_{sr} <\gamma_s|$$

$$<\gamma_r, \gamma_s> = \delta_{rs}$$

Then the adjoint of 1 and equation 2 become respectively

$$\sum_{s}{}' <\phi, \gamma_s>(\mathcal{L}^*_{sr} - \lambda^*\delta_{rs}) = 0$$

$$\sum_{s}{}' (\mu\delta_{rs} - \mathcal{L}^*_{sr}) <\gamma_s, \phi> = 0$$

Since the eigenvalues follow from

$$\det \left| \mathcal{L}_{sr}^{*} - \lambda^{*} \delta_{rs} \right| = 0$$

$$\det \left| \mu \delta_{rs} - \mathcal{L}_{sr}^{*} \right| = 0$$

we conclude $\lambda^{*} = \mu$. This does not necessarily imply that $\varphi = \varphi^{*}$.

Although the functions φ do not form an orthonormal set, φ and $\hat{\varphi}$ do form a biorthonormal set

$$\langle \hat{\varphi}_n , \varphi_m \rangle = \delta_{nm} \tag{3}$$

The proof follows from

$$(\lambda_n - \mathcal{L})\varphi_n = 0$$

$$(\lambda_m^{*} - \mathcal{L}^{+})\hat{\varphi}_m = 0$$

by projecting the first equation onto $\hat{\varphi}_m$, the complex conjugate of the second onto φ_n^{*} and subtracting

$$(\lambda_n - \lambda_m)\langle \hat{\varphi}_m , \varphi_n \rangle = 0$$

So by proper choice of the coefficients of φ_n and φ_n we can further set the normalization to one.

We assume without proof that our eigenstates are complete. This is expressed by

$$1 = \sum_r{}' \, |\hat{\varphi}_r\rangle \langle \varphi_r| = \sum_r{}' \, |\varphi_r\rangle \langle \hat{\varphi}_r|$$

These sets appear not only in the solution of non-hermitian eigenvalue problems but also in the solution of generalized eigenvalue problems

$$A\phi = \lambda B\phi$$

and appear in describing non-orthogonal coordinate systems. For example, the primitive vectors defining a crystal lattice and the reciprocal lattice of wave number space form a biorthonormal set of vectors. This might be more familiar to the reader under the heading contravariant and covariant components of a vector.

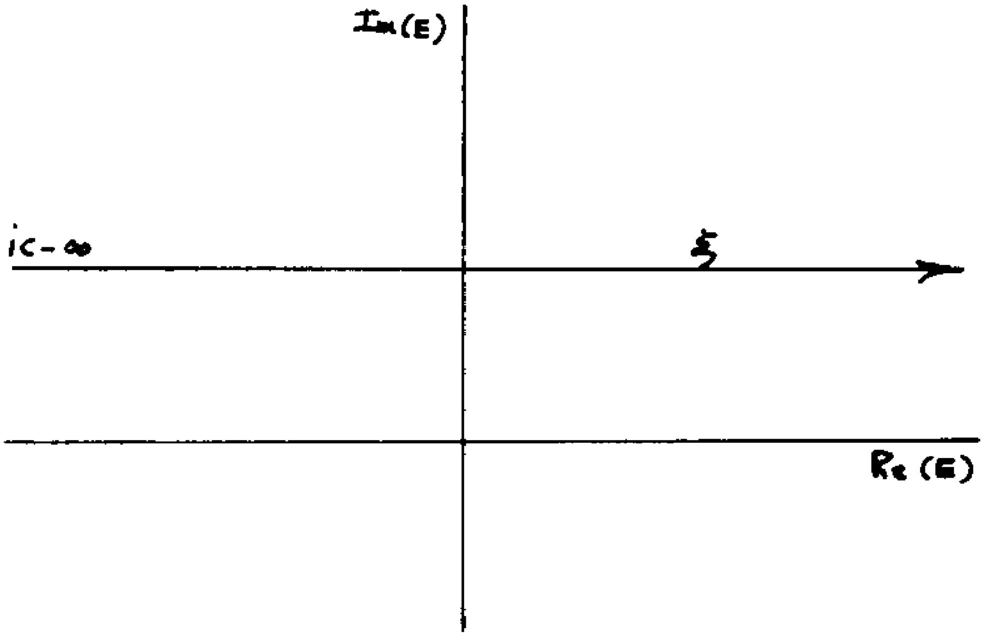

Fig. 8

Contour for Laplace Inversion

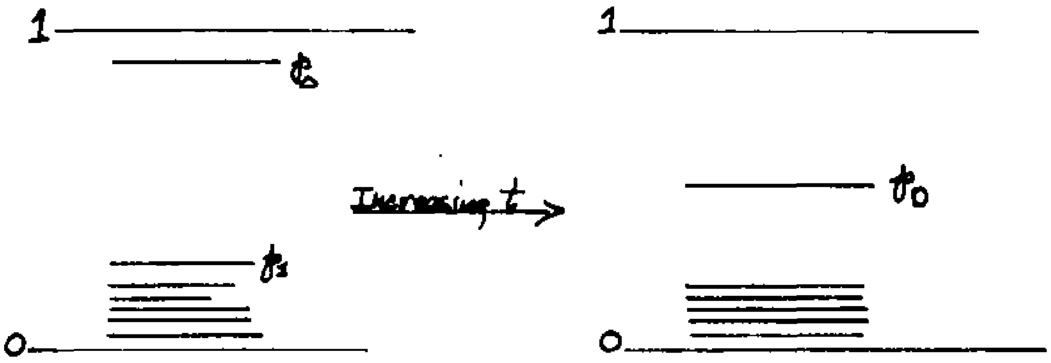

Fig. 9

Spectrum of Probability Operator

References

1. H. Feshbach, "A Unified Theory of Nuclear Reactions II", Annals of Phys. 19, 287 (1962).
2. K. M. Watson, "Quantum Mechanical Transport Theory I", Phys. Rev. 118, 886 (1960).

Chapter 3

Potentials

3.1 Introduction

In the last chapter, we derived our basic pseudo-Schroedinger equation 2.6.2(12) with Hamiltonian given by equation 2.6.2(12a). Since the proton's motion is fixed that Hamiltonian can be written

$$\mathcal{H} = H(\vec{r}, \vec{R}(t)) - \frac{1}{N} \sum_{n m \in C}{}' V_{nm}(\vec{r}) - \frac{1}{N} \sum_{n m \in C}{}' \int d^3r \left\langle U_n \, V \frac{Q}{E - H_{QQ}} V \, U_n \right\rangle_{\vec{r}, \vec{r}_1} \qquad (1)$$

where $\vec{R}(t)$ is the specified motion of the proton. The first term is the free space Hamiltonian

$$H(\vec{r}, \vec{R}(t)) = -\frac{1}{2m} \nabla_r^2 - \frac{Z_1 e^2}{|\vec{r} - \vec{R}(t)|} \qquad (2)$$

for an electron in the field of a moving proton. The second term in equation 1 is the interaction of the electron with the solid, averaged over the excitations of channeling space. This is the so-called state interaction and is clearly hermitian and local in configuration space. In section 3.2 we discuss this potential averaged over free single particle excitations of the solid. In section 3.3 we evaluate this potential for collective excitations. The last term in 1 is a non-local potential which is non-hermitian, and is interpreted as an ionization potential. In making this identification we approximate this potential by a local imaginary one. That is, we assume the real part has been absorbed into the static potential. The imaginary part representing real decoupling is calculated for a simple model in section 3.4. The set of potentials in 1 is sometimes referred to as the optical potential

3.2 Static Potential (Single Particle Excitations)

In the first part of this section we calculate the average static potential over states of free particle excitations. We show that both the diagnol and off-diagnol terms are zero. In the second part we show that the potential exists for a non-uniform distribution of charge in the channel, and a phenomenological model for it is proposed.

3.2.1 Free Electron Approximation

We want to evaluate

$$V_S = \frac{1}{N_C} \sum_{mm' \in C}' V_{m'm}(\vec{r}) \qquad (1)$$

where V_S stands for the static potential and $V_{m'm}$ is the incident electron solid interaction taken between states of excitation of the solid which are contained in P space. N_C is the number of excitations in P space. In the free electron approximation

$$V = \sum_{j=1}^{N}{}' \frac{e^2}{|\vec{r} - \vec{r}_j|} - \int \frac{(Ne^2/\Omega)}{|\vec{r} - \vec{r}\,'|} \, d^3r'$$

represents the interaction between the incident electron at $\vec{r}$ and the electrons of the solid located at $\vec{r}_j$. The last term represents the interaction between the incident electron and a uniform background of charge. N represents the number of electrons and Ω the volume of the solid. We shall evaluate 1 by expressing V in second quantized form[10].

As is standard wave operators are introduced and they are conveniently expended in a complete set of states φ_i,

$$\Psi(x) = \sum_i{}' \varphi_i(x)\, C_i$$

$$\Psi^+(x) = \sum_i{}' \varphi_i^*(x)\, C_i^+$$

where the wave operators satisfy the anti-commutation relations for form fermions

$$\Psi(x)\, \Psi^+(x) + \Psi^+(x)\Psi(x) = \delta(x - x')$$

The amplitudes C_i, C_i^+ are operators which annihilate and create particles in the state φ_i respectively. Further, we define the states φ_i so that they form a complete orthonormal set. Then the above anti-commutation rule yields for the annihilation and creation operators,

$$C_i C_j^+ + C_j^+ C_i = \delta_{ij} \qquad (2)$$

all other pairs anti-commuting. Finally, the following prescription is used for going from a discrete sum over N particles to a continuous integral

$$\sum_{\text{particles}}{}' f(\text{particle}) \longrightarrow \int dx\ \Psi^+(x) f(x) \Psi(x)$$

In our free particle case it is clearly advantageous to take the states φ_i as free particle one and so

$$\Psi(\vec{x}) = \sum_{\vec{p},\sigma}' \frac{e^{i\vec{p}\cdot\vec{x}}}{\sqrt{\Omega}} \delta_\sigma(s)\, C_{\vec{p},\sigma}$$

where σ and S take on the "values" up and down for the spin quantum number and coordinate respectively. Then

$$\sum_{j=1}^{N}{}' \frac{e^2}{|\vec{r}-\vec{r}_j|} = \sum_{\vec{K},\vec{k},\sigma}' e^{-i\vec{K}\cdot\vec{r}}\, \tilde{V}(\vec{K})\, C^{+}_{\vec{K}+\vec{k},\sigma} C_{\vec{k}\sigma}$$

where

$$\tilde{V}(\vec{K}) = \frac{e^2}{\Omega}\int d^3x\, \frac{e^{-i\vec{K}\cdot\vec{x}}}{x} = \frac{4\pi e^2}{K^2\Omega}$$

Then we can write the potential as

$$V = \sum_{\vec{K},\vec{k},\sigma}' e^{-i\vec{K}\cdot\vec{r}}\, \tilde{V}(\vec{K})\, C^{+}_{\vec{K}+\vec{k},\sigma} C_{\vec{k},\sigma} - N\,\tilde{V}(0) \qquad (4)$$

We recognize that this expression contains the wave density operator,

$$\rho^{+}_{\vec{K}} = \sum_{\vec{k},\sigma}' C^{+}_{\vec{K}+\vec{k},\sigma} C_{\vec{k},\sigma}$$

that is, this operator creates density fluctuations with momentum $\vec{K}$. To see this we note that this operator is the Fourier transform of the space density

$$\rho(\vec{x}) = \Psi^+(\vec{x})\,\Psi(\vec{x})$$

For on taking the transform of

$$\rho(\vec{x}) = \sum'_{\vec{k},\vec{k}',\sigma} c^+_{\vec{k}',\sigma}\, c_{\vec{k},\sigma}\, \frac{e^{+i(\vec{k}-\vec{k}')\cdot\vec{x}}}{\Omega}$$

we get

$$\rho_{\vec{K}} = \int d^3x\; e^{-i\vec{K}\cdot\vec{x}}\, \rho(\vec{x}) = \sum'_{\vec{k},\vec{k}',\sigma} c^+_{\vec{k}',\sigma}\, c_{\vec{k},\sigma}\, \delta_{\vec{K},\,\vec{k}-\vec{k}'}$$

$$\rho_{\vec{K}} = \sum'_{\vec{k},\vec{K},\sigma} c^+_{\vec{k}-\vec{K},\sigma}\, c_{\vec{k},\sigma}$$

therefore

$$\rho_{-\vec{K}} = \rho^+_{\vec{K}} = \sum'_{\vec{k},\sigma} c^+_{\vec{k}+\vec{K},\sigma}\, c_{k,\sigma}$$

We then write 4 in terms of this density fluctuation operator

$$V = \sum'_{\vec{K}} e^{-i\vec{K}\cdot\vec{r}}\; \tilde{V}(\vec{K})\, \rho^+_{\vec{K}} - N\, V(0) \qquad (5)$$

Further, we divide the average potential into diagnol and non-diagnol parts

$$V_S = \frac{1}{N_B} \sum_{m \in C}' V_{mm} + 2 \frac{1}{N_C} \sum_{m' > m}' V_{m'm}$$

We now proceed to calculate these separate parts in 6 using 5.

Diagnol Element: We now use the representation 5 in the first part of equation 6 to obtain

$$V_S^{DIAG} = \frac{1}{N_C} \left\{ \sum_{\vec{K}}' e^{-i\vec{K}\cdot\vec{r}} \tilde{V}(\vec{K}) \sum_{m \in C}' \langle m | \rho_K^+ | m \rangle - N_C \tilde{V}(0) \sum_{m \in C}' \langle m | m \rangle \right\}$$

The only term in the $\vec{K}$ sum to survive is K=0. This is so since momentum must be conserved between the electron gas and the incident electron. Therefore,

$$V_S^{DIAG} = \frac{1}{N_C} \left\{ \tilde{V}(0) \sum_{m \in C}' \langle m | \rho_0^+ | m \rangle - N \tilde{V}(0) \sum_{m \in C}' \cdot 1 \right\}$$

Now

$$\langle m | \rho_0^+ | m \rangle = \sum_{\vec{k},\sigma}' \langle m | C_{\vec{k}\sigma}^+ C_{\vec{k},\sigma} | m \rangle$$

$$= N$$

which follows from

$$\langle m | C^{+}_{\vec{k}\sigma} C_{\vec{k}\sigma} | m \rangle = 1 \qquad \text{if } \vec{k},\sigma \text{ occupied}$$
$$= 0 \qquad \text{if } \vec{k},\sigma \text{ not occupied}$$

there being N such occupied single particle states for each state of excitation m. Therefore,

$$V_S^{DIAG} = \frac{1}{N_c}\left\{ \tilde{V}(0)\, N N_c - \tilde{V}(0)\, N N_c \right\} = 0$$

<u>Non-diagnol Element</u>: Here we shall evaluate the coupling between the ground state $|0\rangle$ and excitations of the form $\rho_{\vec{p}}|0\rangle$. The ground state is, of course, two filled fermi spheres of radii k_F. The excited states are coherent superpositions of electron hole pairs with definite momentum. The state $\rho_{\vec{p}}|0\rangle$ represents a momentum transfer of $\vec{P}$ to the electron gas by the incident electron. Channeling space consists only of transfers of momentum less than some maximum momentum, otherwise the electron is ionized. This maximum momentum is of the order of the inverse first Bohr radius. Our choice of the above coherent superposition is consistent with our addition of amplitudes in channeling space.

Using the representation 5 in the non-diagnol part of 6 and applying the above remarks we find

$$V_S^{ND} = \frac{2}{N_c} \sum_{P<P_M}{}' \left\{ \sum_{\vec{K}}{}' e^{-i\vec{K}\cdot\vec{r}}\, \tilde{V}(K) \langle 0 | \rho_{\vec{K}}\, \rho^{+}_{\vec{K}} | 0 \rangle - N\, \tilde{V}(0) \langle 0 | 0 \rangle \right\} \qquad (1)$$

For K=0 the matrix element in 1 becomes

$$M_{\vec{K}=0} = \langle 0 | \rho_0 (\rho_0^+ - N) | 0 \rangle$$

But

$$\rho_0^+ |0\rangle = \sum_{\vec{K},\sigma}{}' C^+_{\vec{K},\sigma} C_{\vec{K},\sigma} |0\rangle = \sum_{\vec{K},\sigma}{}' n_{\vec{K}\sigma} |0\rangle = N|0\rangle$$

where $n_{k\sigma}$ represents the distribution of momenta and spins in the ground state. So we see

$$M_{\vec{K}=0} = \langle 0 | \rho_0 (N-N) | 0 \rangle = 0$$

In fact, $\rho_0 + |0\rangle$ is the ground state again and this is not part of the sum in 1. We can now write 1 in the following form

$$V_S^{ND} = \frac{2}{N_c} \sum_{p<p_M}{}' \sum_{\vec{K}}{}' e^{-i\vec{K}\cdot\vec{r}}\, \tilde{V}(\vec{K}) \langle 0 | \rho^+_{-\vec{P}}\, \rho^+_{\vec{K}} | 0 \rangle \qquad (2)$$

By conservation of momentum $\vec{K} = \vec{P}$ in equation 2 and so

$$V_S^{ND} = \frac{2}{N_c} \sum_{p<p_M}{}' e^{-i\vec{P}\cdot\vec{r}}\, \tilde{V}(p) \langle 0 | \rho^+_{-p}\, \rho^+_{p} | 0 \rangle \qquad (3)$$

But

$$\langle 0 | \rho^{+}_{-p} \, \rho^{+}_{p} | 0 \rangle = \sum_{\vec{k}\sigma}{}' \sum_{\vec{k}',\sigma}{}' \langle 0 | c^{+}_{\vec{k}\sigma} \, c_{\vec{k}+\vec{p},\sigma} \, c^{+}_{\vec{k}'+\vec{p},\sigma} \, c_{\vec{k}'\sigma'} | 0 \rangle \qquad (4)$$

Clearly we see in 4 that k=k' and σ=σ' so

$$\langle 0 | \rho^{+}_{-p} \, \rho^{+}_{p} | 0 \rangle = \sum_{\vec{k},\sigma}{}' n_{\vec{k}\sigma} \left(1 - n_{\vec{k}+\vec{p},\sigma}\right) \qquad (5)$$

where at zero temperature

$$n_{\vec{k}\sigma} = a(k_F^2 - k^2)$$

$$(1 - n_{\vec{k},\sigma}) = a(k^2 - k_F^2)$$

where

$$a(x) = 1 \qquad x > 0 \qquad (6)$$

$$= 0 \qquad x < 0$$

We show in Appendix 3A that the sum in equation 5 becomes

$$F(p) = \sum_{\vec{k}\sigma}{}' n_{\vec{k},\sigma} \left(1 - n_{\vec{k}+\vec{p},\sigma}\right) = N\left(\frac{3}{4}\frac{p}{k_F} - \frac{1}{16}\frac{p^3}{k_F^3}\right) \qquad p < 2k_F \qquad (7a)$$

$$= N \qquad p > 2k_F \qquad (7b)$$

Then 5 becomes

$$V_S^{ND}(\vec{r}) = \frac{2}{N_c} \sum_{p<P_M}{}' e^{-i\vec{p}\cdot\vec{r}} V(p) F(p)$$

$$= \frac{2}{N_c} \frac{4\pi e^2}{(2\pi)^3} 4\pi \int_0^{P_M} dp\, F(p) \frac{\sin pr}{pr} \qquad (8)$$

If $P_M > 2k_F$ then use of 7a in 8 yields

$$V_S^{ND}(\vec{r}) = \frac{2}{N_c} \frac{4e^2 N}{\pi} \left\{ \int_0^{2k_F} \frac{dp}{p} \left(\frac{3}{4} \frac{p}{k_F} - \frac{1}{16} \frac{p^3}{k_F^3} \right) \sin pr + \int_{2k_F}^{P_M} \frac{dp}{p} \frac{\sin pr}{r} \right\} \qquad (9a)$$

if $P_M < 2k_F$ use of 7b in 8 yields

$$V_S^{ND}(\vec{r}) = \frac{1}{N_c} \frac{4e^2}{\pi} N \int_0^{P_M} \frac{dp}{p} \left(\frac{3}{4} \frac{p}{k_F} - \frac{1}{16} \frac{p^3}{k_F^3} \right) \frac{\sin pr}{r} \qquad (9b)$$

Since the integrals in equations 9a and 9b are finite we find that

$$V_{ND}^{S} \to \frac{1}{\Omega} \to 0 \quad \text{as} \quad \Omega \to \infty \qquad (10)$$

This follows from the fact that $N \sim \Lambda$ but $N_C \sim \Lambda^2$. Notice also that the integrals in 9a and 9b are finite for $r \to 0$ and $r \to \infty$. Therefore 10 holds for all values of r.

3.2.2 Screened Field

An important point to notice is that the vanishing of the non-diagnol part of the potential is independent of the approximations made in the last section. So we need only consider the diagnol term. This should not be too surprising since the non-diagnol term in the static potential represents fluctuations about the average.

In a solid the electrons and background deviate from the uniform average distribution of a free electron gas. In such a case our one electron wave functions will take the form

$$\varphi_{\vec{k},\sigma}(\vec{x}) = \gamma_{\vec{k}}(\vec{x})\, \delta_\sigma(s)$$

where $\gamma_{\vec{k}}(\vec{x})$ is a so-called Bloch function and is an eigenstate of a one electron Hamiltonian, and represents the motion of this electron in a fixed lattice. With this choice

$$\sum_{j=1}^{N}{}' \frac{e^2}{|\vec{r}-\vec{r}_j|} = \sum_{\vec{p},\vec{k}\sigma}{}' \tilde{V}(\vec{p},\vec{p}+\vec{k})\, C^{+}_{\vec{p}+\vec{k},\sigma} C_{\vec{p}\sigma} \qquad (2a)$$

$$\tilde{V}(\vec{p},\vec{p}+\vec{k}) = \frac{e^2}{\Omega} \int d^3x\, \frac{e^{-i\vec{k}\cdot\vec{x}}}{|\vec{r}-\vec{x}|} \gamma^{*}_{\vec{p}+\vec{k}}(\vec{x})\, \gamma_{\vec{p}}(\vec{x}) \qquad (2b)$$

then

$$V_S^{DIAG} = \frac{1}{N_c} \sum_{\vec{p}\vec{k}\sigma}{}' \tilde{V}(\vec{p},\vec{p}+\vec{k}) \sum_{m\in C}{}' \langle m| C^{+}_{\vec{p}+\vec{k},\sigma} C_{\vec{p},\sigma} |m\rangle + \sum_{\vec{R}_\ell}{}' \frac{Z_2 e^2}{|\vec{r}-\vec{R}_\ell|}$$

where $\vec{R}_\ell$ represents the position of the lattice sites with charge $Z_2 e$. If we neglect the small differences in the sum over excitations, i.e.

$$\sum_{m\in C}{}' \langle m| C^{+}_{\vec{p}+\vec{k},\sigma} C_{\vec{p},\sigma} |m\rangle \simeq N_c \langle 0| C^{+}_{\vec{p}+\vec{k},\sigma} C_{\vec{p},\sigma} |0\rangle$$

$$= N_c\, n_{\vec{k}\sigma} \quad \text{if } \vec{k} = 0 \qquad (4a)$$

$$= 0 \quad \text{if } \vec{k} \neq 0 \qquad (4b)$$

Using 4 and 2 in equation 3 we get

$$V_S^{DIAG} \simeq \int d^3x \frac{n_p(\vec{x})}{|\vec{r}-\vec{x}|} + \sum_{\vec{\ell}}{}' \frac{Z_2 e^2}{|\vec{r}-\vec{R}_\ell|} \qquad (5a)$$

$$n_p(\vec{x}) = \frac{e^2}{\Omega} \sum_{\vec{p}<p_M}{}' |\gamma_{\vec{p}}(\vec{x})|^2 \qquad (5b)$$

Here n_p represents the local density distribution of electric charge. The derivation of 5 is meant in a purely heuristic way. That is, we only mean to point out that the static potential is basically the field set up by a charge density of the solid, that density being an average one. At this point, we are not interested in continuing the calculation of the potential.

In fact, its further development from first principles is intractable. Also the range of accuracy aimed at in this work does not necessitate a first principles calculation. In fact, since our potential 5a looks rather harmless and shows no unusual characteristics, we shall replace it by one of the standard interatomic potentials.

$$V_S = \sum_{\ell}{}' \frac{Z_2 e^2}{|\vec{r}-\vec{R}_\ell|} e^{-\lambda|\vec{r}-\vec{R}_\ell|}$$

This then represents the average static interaction between the electron and solid.

This looks very much like a Bohr potential(1). However, we are leaving the screening length λ as a free parameter. For a Bohr potential λ would be chosen to be $\sqrt{1+(Z_2)^{2/3}}$ in atomic units. There are many phenomenological potentials to choose from and they are discussed at length in reference 1. We have chosen this particular one for both conceptual reasons and computational convenience.

This choice of potential might be claimed to be poor in two respects. First one might argue rightly that a Bohr potential falls off too rapidly(1). We have chosen λ as a variable parameter because of this difficulty. Secondly, one might also argue that pseudo potential calculations imply that the field at the origin is much weaker than equation 6 predicts. This would be true if we were looking at the interaction between a valence electron and a core of the solid. In that case the pseudo potential is attenuated at the origin due to the neglect of exchange forces. That is, the Pauli principle keeps the valence electron in question away from the electrons surrounding the nucleus. If exchange is neglected in the construction of a potential experienced by that electron one should then weaken the strength of that potential at the nucleus to accomodate this effect. In our case, the incident electron has much higher energy than the valence electrons. Therefore, exchange effects are negligible and one need not attenuate the potential at the origin.

We should also point out that the screening of the Yukawa form in equation 6 follows from the screening of the cores by the valence electrons. That is, the gas of valence electrons in attempting to neutralize local charge imbalances will screen out the fields of the cores on an atomic scale of length.

We have only attempted to make the transition from 5 to 6 plausible. It is by no means necessary that 6 be used but rather it is consistent with our picture of the interactions in channeling.

3.3.1 Electron Gas

In the last section we found the average potential energy experienced by the incident electron for single particle excitations of the solid. However, there is also a collective response which is manifested in plasma oscillations of the electron gas of the solid. We are interested in these sections in calculating this effect on the potential energy.

At first, we might argue the electron gas completely screens out the field of the proton and so the incident electron cannot in any real sense be bound to the proton. This argument is based upon the fact that if a proton is placed at rest at some point in the solid the potential field, φ, around it is not coulombic but rather,

$$\varphi(r) = \frac{Z_1 e^2}{r} e^{-k_{TF} r} \qquad (1)$$

where k_{TF} is a constant of order unity in atomic units and Z_1 the charge of the "proton." This result was mentioned in the last section in reference to the screening of the cores by the valence electrons and will be derived later in this section. Suffice it to say, that 1 implies that the field is screened out at a distance of the order of a Bohr radius.

However, in deriving equation 1, the proton is considered at rest. While this is true for the cores of the solid it is not true for our incident proton. In fact, the velocity of the proton becomes important when considering the effect of the screening by the electron gas. On intuitive grounds we expect that if

$$\frac{V}{\omega_p} >> \lambda_D$$

then screening is not important. Here V is the velocity of the proton, ω_p the so-called plasma frequency is a number that characterizes the relaxation rate (of order one) and λ_D, the Debye length, a number characterizing the wavelength of an oscillation (of order one). Equation 2 expresses the fact that during the time of one oscillation the proton covers many wavelengths in its motion. That is, the plasma oscillations are slow on the scale of linear motion and so the oscillations are essentially frozen. But it is these oscillations which lead to polarization phenomena and screening. In fact, we shall show that the potential field due to these oscillations goes inversely with V. Finally, we remark that equation 2 implies $V >> v_F$ where v_F is the Fermi velocity.

In our case

$$10 \lesssim V \lesssim 10^2 \qquad (3)$$

while

$$v_F \sim 1 \qquad (4)$$

and so 1 is satisfied for MeV channeling.

3.3.2 Maxwell Lorentz Equations

We consider the solid in the following limit. It consists of fixed cores at their equilibrium positions plus essentially free valence electrons. Further, we smear the positive charged background so it is removed from the problem except insofar as providing electrical neutrality. This approximation is based upon two notions; first, that the distribution of valence charge in a metal, say, is essentially uniform and second, that the nuclear motion is slow on the scale of electronic motion. This model is called an electron gas and we now wish to describe this system subject to a small disturbance. We must point out the discussions in the rest of this section are not new. They are rather included for completeness. References 3 through 7 inclusive should be consulted for more details.

We begin our study by taking the Lorentz point of view in that we write down separately Maxwell's equations in vacuum and the equations of motion of the charges present. Maxwell's equations are

$$\nabla\cdot\vec{E} = 4\pi(\rho_0 + \rho) \qquad (1a)$$

$$\nabla\times\vec{E} = -\frac{1}{c}\frac{\partial\vec{B}}{\partial t} \qquad (1b)$$

$$\nabla\cdot\vec{B} = 0 \qquad (1c)$$

$$\nabla\times\vec{B} = \frac{4\pi}{c}(\vec{J}_0 + \vec{J}) + \frac{1}{c}\frac{\partial\vec{E}}{\partial t} \qquad (1d)$$

Here $\vec{E}$ and $\vec{B}$ are the electric and magnetic fields and ρ_0 and j_0 are the external charge and current densities. The charges and currents of matter ρ and $\vec{j}$ are taken to satisfy the Vlasov equation

$$\frac{\partial f}{\partial t} + \vec{v}\cdot\nabla_r f + \vec{a}\cdot\nabla_v f = -\nu f \qquad (2)$$

where $f(\vec{r}, \vec{v}, t)\, d^3r\, d^3v$ is the probability that an electron of the gas is between spatial positions $\vec{r}$ and $\vec{r}+d\vec{r}$ and velocity positions $\vec{v}$ and $\vec{v}+d\vec{v}$ at time t. Further, ν is the collision operator and the charges and currents are related to f through

$$\rho(\vec{r},t) = ne - ne\int f(\vec{r},\vec{v},t)\, d^3v$$

$$\vec{J}(\vec{r},t) = -ne\int f(\vec{r},\vec{v},t)\,\vec{v}\, d^3v$$

where n is the average number of electrons per unit volume and the smeared positive background is contained in the term ne in $\rho(\vec{r}, t)$. Lastly, the coupling between the charges of matter and their fields E and B are contained in the acceleration term of equation 2 by the relation

$$\vec{a} = -\frac{e}{m}\left(\vec{E} + \frac{\vec{v}}{c}\times\vec{B}\right)$$

We have chosed to describe the motion of the electron gas in a semi-classical way by using equation 2 to describe the electronic motion[4]. We say semi-classical since we shall take the equilibrium distribution as being a Fermi-Dirac one. For our purposes this is sufficient since we will be concerned with the plasma oscillations. They contribute undamped motion for wavelength larger than the Debye wavelength. However, quantum mechanical considerations become important at small wavelengths.

3.3.3 Dielectric Formulation (Linear Theory)

To obtain the equations of fields for matter we define the dielectric tensor ϵ_{ij} from

$$D_i(\vec{r},t) = \int_{-\infty}^{t} dt' \int d^3r'\, \epsilon_{ij}(\vec{r},\vec{r}\,',t-t')\, E_j(\vec{r}\,',t')$$

where $D(\vec{r}, t)$ is defined by

$$\vec{D}(\vec{r},t) = \vec{E}(\vec{r},t) + 4\pi \int_{-\infty}^{t} \vec{J}(\vec{r},t')\,dt'$$

We see that the auxiliary field D_i is related to the electric field E_j by the non-local (space and time) linear operator ϵ_{ij}. To understand this relationship imagine an electric field incident on an atom. If inertial effects are important in the response of the atom then D does not follow E but lags and ϵ_{ij} becomes non-local in time (time dispersion). Also suppose that in calculating the response of the atom the dipole approximation does not hold then ϵ_{ij} becomes non-local in space (spatial dispersion). Using the relations between D and j the Maxwell equations become

$$\nabla\cdot\vec{D} - 4\pi\int_{-\infty}^{t}\nabla\cdot\vec{J}(\vec{r},t')\,dt' = 4\pi(\rho+\rho_0)$$

$$\nabla\times\vec{B} = \frac{4\pi}{c}(J+\vec{J}_0) + \frac{1}{c}\frac{\partial\vec{D}}{\partial t} - \frac{4\pi}{c}\vec{J}$$

$$\nabla\cdot\vec{B} = 0$$

$$\nabla\times\vec{E} = -\frac{1}{c}\frac{\partial\vec{B}}{\partial t}$$

By charge conservation the first equation above becomes

$$\nabla\cdot\vec{D} - 4\pi\int_{-\infty}^{t}\frac{\partial\rho(\vec{r},t')}{\partial t'}\,dt' = 4\pi(\rho+\rho_0)$$

We assume the condition

$$\rho(\vec{r},\, t=-\infty) = 0$$

which states that there is no net charge before the action of disturbances.

This can also be seen by assuming

$$f(\vec{r},\vec{v},\, t=-\infty) = f_0(v)$$

This condition then allows us to write the Maxwell equations in the form

$$\nabla\cdot\vec{D} = 4\pi\rho_0 \qquad (1a)$$

$$\nabla\times\vec{B} = \frac{4\pi}{c}\vec{J}_0 + \frac{1}{c}\frac{\partial\vec{D}}{\partial t} \qquad (1b)$$

$$\nabla\cdot\vec{B} = 0 \qquad (1c)$$

$$\nabla\times\vec{E} = -\frac{1}{c}\frac{\partial\vec{B}}{\partial t} \qquad (1d)$$

In these equations all the polarization effects are contained in the vector D (magnetic polarization also). We now assume homogeniety of space. This is actually true for our electron gas but clearly an approximation if the crystal lattice background is restored. Thus ϵ is defined by

$$D_i(\vec{r},t) = \int_{-\infty}^{t} dt' \int d^3r' \, \epsilon_{ij}(\vec{r}-\vec{r}', t-t') \, E_j(\vec{r}', t') dt'$$

with the relationship between D and E given by

$$\frac{\partial D_i}{\partial t} = \frac{\partial E_i}{\partial t} + 4\pi j_i$$

These relationships are now Fourier analyzed by expanding all functions as

$$h(\vec{r},t) = \int h(\vec{k},\omega) \, e^{i(\vec{k}\cdot\vec{r}-\omega t)} \, d^3k \, d\omega$$

$$h(\vec{k},\omega) = \frac{1}{(2\pi)^4} \int d^3r \, dt \, e^{-i(\vec{k}\cdot\vec{r}-\omega t)} \, h(r,t)$$

Then the above relations become

$$D_i(\vec{k},\omega) = \epsilon_{ij}(\vec{k},\omega) \, E_j(\vec{k},\omega)$$

$$-i\omega D_i(\vec{k},\omega) = -i\omega E_i(\vec{k},\omega) + 4\pi j_i(\vec{k},\omega)$$

Eliminating the auxiliary function D we get

$$j_i(\vec{k},\omega) = -\frac{i\omega}{4\pi} \left(\epsilon_{ij}(\vec{k},\omega) - \delta_{ij} \right) E_j(\vec{k},\omega) = \sigma_{ij} E_j$$

where σ_{ij} is the conductivity tensor.

Now for an isotropic system, which we assume, we may write

$$\epsilon_{ij}(\vec{k},\omega) = \left(\delta_{ij} - \frac{k_i k_j}{k^2}\right)\epsilon^{tr}(\vec{k},\omega) + \frac{k_i k_j}{k^2}\epsilon^{l}(\vec{k},\omega)$$

That is, only two constants are needed to specify the tensor at $\vec{k}, \omega$. If we had used the conventional formulation of Maxwell's equations, then the dielectric tensor would have been a scalar called for example, $\epsilon(\vec{k}, \omega)$. But there would also be another scalar called, say, $\mu(\vec{k}, \omega)$ relating B and a new vector H. For a further discussion of this point see reference 5 and for the use of the latter formulation see reference 6. In either case, if one gives two functions of k and ω relating the appropriate fields and one also gives the external sources then the motion of the system can be solved. In our case, the information on ϵ_{ij} will be provided by the Vlasov equation.

3.3.4 Solution of the Vlasov Equation

In order to obtain a closed expression for the dielectric tensor, we need the induced current. If we turn to the Vlasov equation to supply the answer we find that we need the electric and magnetic fields. But to find these we need to solve the Maxwell equations and so need the induced currents. So we are faced with a self-consistent problem. If we linearize the Vlasov equation and solve it self-consistently with the Maxwell equations, we shall find the dielectric tensor in terms of the system properties only. That is, it will be independent of the external sources. What follows will be valid only in this linear response limit.

Our discussion here follows Lindhard[4].

We write

$$f(\vec{r},\vec{v},t) = f_0(v) + g(\vec{r},\vec{v},t)$$

and assume g is small relative to the equilibrium distribution f_0. We also assume a relaxation time approximation, that is ν is a small constant collision frequency. We finally linearize the Vlasov equation and find for g

$$\frac{\partial g}{\partial t} + \vec{v}\cdot\nabla_r g - \frac{e}{m}\left(\vec{E}+\frac{\vec{v}}{c}\times\vec{B}\right)\cdot\nabla_v f_0 = -\nu g \qquad (1)$$

We have retained ν to provide the proper boundary conditions, that is that we obtain retarded solutions. In fact, the constant ν provides the following properties for the system: Ultimate return to equilibrium (entropy increase), causality and energy dissipation.

We Fourier analyze equation 1 to obtain

$$-i\omega g(\vec{k},\omega) + i\vec{k}\cdot\vec{v} g - \frac{e}{m}\vec{E}\cdot\nabla_v f_0 = -\nu g$$

where the term proportional to B in equation 1 has been dropped since it vanishes for an initial distribution that is isotropic in the velocity. The above equation becomes on solving for g

$$g(\vec{k},\vec{\omega},\vec{v}) = -\frac{ie}{m}\,\frac{\vec{E}(\vec{k},\omega)\cdot\nabla_v f_0(v)}{\vec{k}\cdot\vec{v}-\omega-i\nu}$$

Now

$$\rho(\vec{r},t) = Ne - Ne\int f_0(v)\, d^3v - Ne\int g\, d^3v = -Ne\int g(\vec{r},\vec{v},t)\, d^3v$$

$$\vec{J}(\vec{r},t) = -Ne\int g(\vec{r},\vec{v},t)\, \vec{v}\, d^3\vec{v}$$

since

$$\int f_0(v)\, d^3v = 1$$

$$\int f_0(v)\, \vec{v}\, d^3v = 0$$

So on Fourier analysis ρ and j become

$$\rho(\vec{k},\omega) = -Ne\int g(\vec{k},\omega,\vec{v})\, d^3v$$

$$\vec{J}(\vec{k},\omega) = -Ne\int g(\vec{k},\omega,\vec{v})\, \vec{v}\, d^3v$$

Using 2 in the above we find

$$\vec{J}(\vec{k},\omega) = \frac{ie^2N}{m}\int \frac{\vec{E}\cdot\nabla_v f_0}{\vec{k}\cdot\vec{v}-\omega-i\nu}\, \vec{v}\, d^3v$$

or

$$j_i(\vec{k},\omega) = \frac{ie^2N}{m}\int \frac{\frac{1}{v}\left(\frac{\partial f_0}{\partial v}\right)}{\vec{k}\cdot\vec{v}-\omega-i\nu}\, v_i v_j\, d^3v \cdot E_j \qquad (3)$$

Using 3.3.3(1) in equation 3 we get

$$\epsilon_{ij}(\vec{k},\omega) = \delta_{ij} - \frac{4\pi}{i\omega}\left(\frac{ie^2}{m}\right) N \int \frac{\left(\frac{1}{v}\frac{\partial f_0}{\partial v}\right)}{\vec{k}\cdot\vec{v}-\omega-i\nu} v_i v_j \qquad (4)$$

This result is true for a linear theory with space and time homogeneity.

If further we substitute 3.3.2(2) into equation 4 and left multiply the resultant equation by $\frac{k_i k_j}{k^2}$ we obtain

$$\epsilon^{l}(\vec{k},\omega) = \frac{k_i k_j \delta_{ij}}{k^2} - \frac{4\pi e^2 N}{m\omega} \int \frac{\left(\frac{1}{v}\frac{\partial f_0}{\partial v}\right)}{\vec{k}\cdot\vec{v}-\omega-i\nu} \frac{k_i k_j}{k^2} v_i v_j \, d^3v \qquad (5a)$$

and by $(\delta_{ij} - \frac{k_i k_j}{k^2})$ we obtain

$$2\epsilon^{tr}(\vec{k},\omega) = \left(\delta_{ij} - \frac{k_i k_j}{k^2}\right)\delta_{ij} - \frac{4\pi e^2 N}{m\omega} \int \frac{\left(\frac{1}{v}\frac{\partial f_0}{\partial v}\right)}{\vec{k}\cdot\vec{v}-\omega-i\nu} \left(\delta_{ij} - \frac{k_i k_j}{k^2}\right) v_i v_j \qquad (5b)$$

where we have used

$$\frac{k_i k_j}{k^2}\epsilon_{ij} = \epsilon^{l}$$

$$\left(\delta_{ij} - \frac{k_i k_j}{k^2}\right)\epsilon_{ij} = 2\epsilon^{tr}$$

Finally, we write using 4 and 5a and 5b

$$\epsilon^{\ell}(\vec{k},\omega) = 1 - \frac{\omega_p^2}{\omega}\int \frac{\left(\frac{1}{v}\frac{\partial f_0}{\partial v}\right)}{\vec{k}\cdot\vec{v}-\omega-i\nu}\frac{(\vec{k}\cdot\vec{v})^2}{k^2}\,d^3v \qquad (6a)$$

$$\epsilon^{tr}(\vec{k},\omega) = 1 - \frac{\omega_p^2}{2\omega}\int \frac{\left(\frac{1}{v}\frac{\partial f_0}{\partial v}\right)}{\vec{k}\cdot\vec{v}-\omega-i\nu}\left[\vec{v}\cdot\vec{v}-\frac{(k\cdot v)^2}{k^2}\right]d^3v \qquad (6b)$$

with the plasma frequency defined by

$$\omega_p^2 = \frac{4\pi N e^2}{m}$$

3.3.5 Evaluation of the Dielectric Constants (semi-classically)

To evaluate the dielectric constants we need the equilibrium distribution which we assume is a Fermi-Dirac distribution in the zero temperature limit. That is

$$f_0(v) = \frac{3}{4\pi v_F^3}\,a(v_F - v)$$

where v_F is the Fermi velocity a constant which depends upon the mass density of the gas and is equal to the velocity of the most energetic electron. Again, a is a step function which vanishes for negative arguments and is unity for positive ones. The constant multiplying a is chosen so that the distribution is normalized to one. Since

$$\frac{\partial f_0}{\partial v} = \frac{-3}{4\pi v_F^3}\,\delta(v-v_F)$$

the longitudinal constant becomes

$$\epsilon^{\ell}(\vec{k},\omega) = 1 - \frac{\omega_p^2}{\omega} 2\pi \int_0^\infty dv\, v^2 \int_{-1}^{+1} d\xi \left(\frac{-3}{4\pi v_F^3}\right) \frac{\delta(v-v_F)}{kv\xi-\omega-i\nu}\, v\xi^2$$

where $\xi = \cos(k \cdot v)$ and k is the z axis of ξ space. Simplifying we get

$$\epsilon^{\ell}(\vec{k},\omega) = 1 + \frac{3\omega_p^2}{2\omega} I(k, v_F, \omega) \qquad (2a)$$

$$I(k, v_F, \omega) = \int_{-1}^{+1} d\xi \frac{\xi^2}{kv_F\xi-\omega-i\nu} \qquad (2b)$$

Similarly

$$\epsilon^{tr}(\vec{k},\omega) = 1 + \frac{3\omega_p^2}{4\omega} J(k, v_F, \omega) \qquad (3a)$$

$$J(k, v_F, \omega) = \int_{-1}^{+1} \frac{d\xi}{kv_F\xi-\omega-i\nu} - I(k, v_F, \omega) \qquad (3b)$$

3.3.6 Electron Proton Pair in Medium

In this section we want to obtain a general expression for the potential energy of an electron in the field of a proton embedded in a medium. We begin with the Maxwell equations

$$\nabla \cdot \vec{D} = 4\pi \rho_0$$

$$\nabla \times \vec{B} = \frac{4\pi}{c} \vec{J}_0 + \frac{1}{c} \frac{\partial \vec{D}}{\partial t}$$

$$\nabla \cdot \vec{B} = 0$$

$$\nabla \times \vec{E} = -\frac{1}{c} \frac{\partial \vec{B}}{\partial t}$$

The homogeneous equations allow the introduction of the potentials A and φ by

$$\vec{B} = \nabla \times \vec{A}$$

$$\vec{E} = -\nabla \varphi - \frac{1}{c} \frac{\partial \vec{A}}{\partial t}$$

The fields B and E are invariant under the gauge transformation

$$\vec{A} \rightarrow \vec{A}' + \nabla \Lambda$$

$$\phi \rightarrow \varphi' = \varphi - \frac{1}{c} \frac{\partial \Lambda}{\partial t}$$

where Λ is arbitrary. This invariance allows us to choose the gauge

$$\nabla \cdot \vec{A} = 0$$

We now Fourier analyze the non-homogeneous Maxwell equations and potentials to get in $\vec{k}, \omega$ coordinates

$$i \vec{k} \cdot \overleftrightarrow{\epsilon} \cdot \vec{E} = 4\pi \rho_0$$

$$i \vec{k} \times \vec{B} = \frac{4\pi}{c} \vec{J}_0 - \frac{i\omega}{c} \overleftrightarrow{\epsilon} \cdot \vec{E}$$

with

$$\vec{B} = i\,\vec{k}\times\vec{A}$$

$$\vec{E} = -i\vec{k}\varphi + \frac{i\omega}{c}\vec{A}$$

and the Coulomb gauge condition

$$\vec{k}\cdot\vec{A} = 0$$

Using the fact that

$$\vec{\epsilon}\cdot\vec{E} = \epsilon^{tr}\vec{E}^{tr} + \epsilon^{L}\vec{E}^{L}$$

the non-homogeneous equations become

$$ik\,\epsilon^{\ell}E^{\ell} = 4\pi\rho_0(\vec{k},\omega)$$

$$i\vec{k}\times\vec{B} = \frac{4\pi}{c}\vec{J}_0 - \frac{i\omega}{c}\left(\epsilon^{\ell}\vec{E}^{\ell} + \epsilon^{tr}\vec{E}^{tr}\right)$$

Introducing the potentials A and φ introduced before we get

$$i\,k\,\epsilon^{\ell}(-ik\varphi) = 4\pi\rho_0 \qquad (1)$$

$$i\vec{k}\times(i\vec{k}\times\vec{A}) = \frac{4\pi}{c}\vec{J}_0^{tr} - \frac{i\omega}{c}\left(\frac{i\omega}{c}\vec{A}\right) + \frac{4\pi}{c}J_0^{L} - \frac{i\omega}{c}\epsilon^{\ell}(-ik\varphi) \qquad (2)$$

where we used

$$\vec{J}_0 = \vec{J}_0^{tr} + \vec{J}_0^{\ell}$$

with longitudinal and transverse signifying parallel and perpendicular to $\vec{k}$ respectively. Since charge conservation in $\vec{k}, \omega$ space is

$$i\vec{k}\cdot\vec{J}_0 - i\omega\rho_0 = 0$$

we find

$$\vec{k}\cdot\vec{J}_0^{\ell} = \omega\rho_0$$

which forces the last two terms in equation 2 to vanish. Then equations 1 and 2 become with the introduction of the Coulomb gauge condition

$$\epsilon^{\ell}(\vec{k},\omega)\,k^2\,\varphi(\vec{k},\omega) = 4\pi\rho_0(\vec{k},\omega) \qquad (3a)$$

$$\left(k^2 - \frac{\omega^2}{c^2}\epsilon^{tr}(\vec{k},\omega)\right)\vec{A}(\vec{k},\omega) = \frac{4\pi}{c}\vec{J}_0^{tr}(\vec{k},\omega) \qquad (3b)$$

We now want to solve the set 3 for an electron proton pair penetrating the electron gas whose properties are now contained in the two constants ϵ^{L} and ϵ^{tr}. Since the electron's internal motion is slow relative to its linear motion for an MeV pair we consider the case of a fixed dipole moving with velocity V with coordinates shown in Figure 10. For this case the densities

$$\rho(\vec{r},t) = e[z_1\delta(\vec{r}-\vec{V}t) - \delta(\vec{r}-\vec{V}t-\vec{a})]$$

$$\vec{J}_0(\vec{r},t) = e\vec{V}[z_1\delta(\vec{r}-\vec{V}t) - \delta(\vec{r}-\vec{V}t-\vec{a})]$$

yield Fourier amplitudes

$$\rho_0(\vec{k},\omega) = \frac{e}{(2\pi)^3}\left[z_1\delta(\omega-\vec{k}\cdot\vec{v}) - e^{-i\vec{k}\cdot\vec{a}}\delta(\omega-\vec{k}\cdot\vec{v})\right]$$

$$\vec{J}_0(\vec{k},\omega) = \vec{v}\,\rho_0(\vec{k},\omega)$$

To obtain the potentials we invert equations 3.3.5(3) to get

$$\varphi(\vec{k},\omega) = \frac{4\pi e}{8\pi^3}\frac{\delta(\omega-\vec{k}\cdot\vec{v})}{\epsilon^l k^2}\left(z_1 - e^{-i\vec{k}\cdot\vec{a}}\right) = \varphi_p(\vec{k},\omega)+\varphi_e(\vec{k},\omega)$$

$$\vec{A}(\vec{k},\omega) = \frac{4\pi}{c}\frac{e}{8\pi^3}\frac{\vec{v}^{tr}\delta(\omega-\vec{k}\cdot\vec{v})}{k^2-\frac{\omega^2}{c^2}\epsilon^{tr}}\left(z_1-e^{-i\vec{k}\cdot\vec{a}}\right) = \vec{A}_p(\vec{k},\omega)+\vec{A}_e(\vec{k},\omega)$$

where

$$\vec{v}^{tr} = \vec{v} - \frac{\vec{k}\cdot\vec{v}}{k^2}\vec{k}$$

By Fourier's theorem we obtain for the spatial potentials

$$\varphi(\vec{r},t) = \frac{e}{2\pi^2}\int d^3k\, \frac{\left(z_1-e^{-i\vec{k}\cdot\vec{a}}\right)}{k^2\epsilon^l(k,\vec{k}\cdot\vec{v})}\, e^{i\vec{k}\cdot(\vec{r}-\vec{v}t)}$$

$$\vec{A}(\vec{r},t) = \frac{e}{c2\pi^2}\int d^3k\, \frac{\vec{v}^{tr}\left(z_1-e^{-i\vec{k}\cdot\vec{a}}\right)}{k^2-\frac{\omega^2}{c^2}\epsilon^{tr}(\vec{k},\vec{k}\cdot\vec{v})}\cdot e^{i\vec{k}\cdot(\vec{r}-\vec{v}t)}$$

We now evaluate the fields at the position of the electron. We also subtract away the self field. A check on our procedure is that the potentials should reduce to the well-known results for the free space limits

$\epsilon^{\ell} \rightarrow 1$, $\epsilon^{tr} \rightarrow 1$. Since A is of order V/C relative to φ we shall only consider the potential polarization field in the following sections. The potential at the electrons is

$$\varphi(\vec{r} = \vec{V}t + \vec{a}) = \frac{e}{2\pi^2} \int d^3k \, \frac{Z_1 e^{i\vec{k}\cdot\vec{a}}}{k^2 \epsilon^{\ell}} - \frac{e}{2\pi^2} \int \frac{d^3k}{k^2} \left(\frac{1}{\epsilon^{\ell}} - 1 \right) \qquad (3)$$

Adding and subtracting the first term with $\epsilon^{\ell} = 1$ unit yields from equation 3

$$\varphi \text{ (at electron)} = \frac{e}{2\pi^2} \int d^3k \, \frac{Z_1 e^{i\vec{k}\cdot\vec{a}}}{k^2} + \frac{e}{2\pi^2} \int \frac{d^3k}{k^2} \left(Z_1 e^{ika} - 1 \right) \left(\frac{1}{\epsilon^{\ell}} - 1 \right) \qquad (4)$$

where the first term integrates to $Z_1 e/a$ and the last term represents corrections due to the presence of matter. This term vanishes in the limit $\epsilon^{\ell} \rightarrow 1$ and so equation 4 reduces to the correct value for vacuum. In the next sections we find approximate values for the proton field in matter in the limit of high and low velocity of translation.

In the next chapter we shall evaluate the potential due to matter, that is the second term in equation 4, for the plasma oscillation contribution. This is certainly a P space contribution, since it can act to distort the internal state of the electron proton pair. To amplify this point we first note that the dielectric constant contains contributions for $k > k_D$ and $k < k_D$, where $k_D = 2\pi/\lambda_D$. For excitations with $k > k_D$ the system will not support plasma oscillations since they will decay into single particle excitations. These single particle excitations are Q space contributions to the potential and represent ionizations. They are taken up at the end of this chapter. However, since they are single particle effects they are treated as such rather than in the dielectric formulation. For $k < k_D$ there are both single particle excitations and plasma oscillations. These are the P space contributions since they distort the internal state of the pair rather than decouple it. The single particle aspect of this has already been treated and so we are interested only in the plasma contribution to the second term in equation 4.

3.3.7 Screening

Since we are no longer interested in the transverse response of the system due to its V/C dependence we drop the superscript ℓ on the dielectric constant. Using 3.3.6(2a) and (2b) we find on integrating

$$\epsilon(k,\omega) = 1+\frac{3\omega_p^2}{(kv_F)^2}\left\{1+\frac{1}{2}\frac{\omega}{kv_F}\ln\left(\frac{kv_F-\omega}{kv_F+\omega}\right)+i\pi\left(\frac{\omega}{kv_F}\right)\right\} \quad |\omega|<kv_F \qquad (1)$$

$$= 1+\frac{3\omega_p^2}{(kv_F)^2}\left\{1+\frac{1}{2}\frac{\omega}{kv_F}\ln\left(\frac{kv_F-\omega}{kv_F+\omega}\right)\right\} \quad |\omega|>kv_F \qquad (2)$$

If we left

$$x \equiv \frac{\omega}{kv_F}$$

$$k_{TF}^2 \equiv \frac{3\omega_p^2}{v_F^{\,2}}$$

and

$$\epsilon = \epsilon_1 + i\,\epsilon_2$$

we get

$$\epsilon_1(k,x) = 1 + \frac{k_{TF}^2}{k^2} \begin{cases} 1 + \frac{x}{2} \ln\left(\frac{1-x}{1+x}\right) & |x|<1 \\ 1 + \frac{x}{2} \ln\left(\frac{x-1}{x+1}\right) & |x|>1 \end{cases} \qquad (3a)$$

$$\epsilon_2(k,x) = \frac{k_{TF}^2}{k^2} \begin{cases} \pi x & |x|<1 \\ 0 & |x|>1 \end{cases}$$

First we consider the case of a stationary proton in an electron gas. By 3.3.6(3) the potential field is given by

$$\varphi(\vec{r}) = \frac{e}{2\pi^2} \int d^3k \, \frac{e^{i k \cdot r}}{k^2 \epsilon(\vec{k}, \vec{k}\cdot\vec{v})}$$

Since the charge is stationary we need to substitute in the above expression for φ

$$\epsilon(k,0) = 1 + \frac{k_{TF}^2}{k^2}$$

This yields

$$\varphi(\vec{r}) = \frac{e}{2\pi^2} \int d^3k \, \frac{e^{i\vec{k}\cdot\vec{r}}}{k^2 + k_{TF}^2} = e \, \frac{e^{-k_{TF} r}}{r}$$

which is a result referred to earlier.

We now want to show that the field about a fast moving proton ($V > v_F$) is not shielded as above. To consider the effect of the plasma mode on the incident proton we note that the electron gas can support free oscillations (plasma oscillations) when

$$\epsilon(\vec{k}, \omega_{\vec{k}}) = 0 \qquad (4)$$

This follows from the Maxwell equation for the potential φ with no external sources

$$k^2 \epsilon(\vec{k}, \omega)\, \varphi(\vec{k}, \omega) = 0$$

This admits the two solutions

$$\varphi = 0 \qquad \epsilon \neq 0$$

$$\varphi \neq 0 \qquad \epsilon(\vec{k}, \vec{\omega}_k) = 0$$

the second solution being the source of density oscillations. We also remark that if $k < k_D = \omega_p / V_F$ then these oscillations are undamped as can be seen from 3b with the knowledge that $\omega \sim \omega_p$. Since the modes given by 4 can be excited by the incident proton, these modes will be the plasma contribution to the potential field. Using 3 in 4 we obtain an approximate expression for the plasma contribution to the dielectric constant

$$\epsilon_{\text{plasmon}} = 1 - \frac{\omega_k^2}{\omega^2} + i\eta \qquad (5a)$$

$$\omega_k^2 = \omega_p^2 + k^2 \langle v^2 \rangle \qquad (5b)$$

$$\langle v^2 \rangle = \frac{3}{5} v_F^2$$

If we substitute 5a into

$$\varphi(\vec{a}) = \frac{e}{2\pi^2} \int \frac{d^3k}{k^2} e^{i \vec{k}\cdot\vec{a}} \left(\frac{1}{\epsilon^l(k, \vec{k}\cdot\vec{v})}^{-1} \right) \quad ; \vec{a} = \vec{r} - \vec{v}t$$

for the proton's field and use

$$d^3k = d\phi \, dk_z \, k_\perp dk_\perp$$

$$\omega = k_z V$$

$$\vec{k}\cdot\vec{a} = \vec{k}_\perp \cdot \vec{a}_\perp + k_z a_z \hat{v}$$

with $\vec{V}$ as the Z axis we get

$$\varphi(\vec{a}) = \frac{eV}{\pi} \int_0^\infty dk\, k\, J_0(k a_\perp) \int_{-\infty}^{+\infty} \frac{d\omega}{\omega^2 + k^2 V^2} \frac{e^{i \frac{\omega}{V} a_z}}{\epsilon\left(\sqrt{k^2 + \left(\frac{\omega}{V}\right)^2}, \omega\right)} \qquad (6)$$

For both $a_Z > 0$ and $a_Z < 0$ there is a contribution from the poles to the integral in 6. These give for $a_z > 0$

$$\varphi(\vec{a}) = \frac{ev}{\pi}\int_0^\infty dk\, \frac{k\, J_0(ka_\perp)}{2ikv\,\epsilon(0,ikv)}\, e^{-ka_z} \simeq \frac{e}{a} \qquad ; \; a < \lambda_D$$

and for $a_z < 0$

$$\varphi(\vec{a}) = \frac{ev}{\pi}\int_0^\infty dk\, k\, \frac{J_0(ka_\perp)}{-2ikv\,\epsilon(0,-ikv)}\, e^{ka_z} \simeq \frac{e}{a} \qquad ; \; a < \lambda_D$$

The plasma mode contributes to 6 using 5

$$\varphi(\vec{a}) = 0 \qquad a_z > 0$$

$$\varphi(\vec{a}) \cong \frac{ev}{\pi}\int_0^\infty dk\, k\, J_0(ka_\perp)\int_{-\infty}^{+\infty} \frac{d\omega}{\omega^2 + k^2 v^2}\, e^{i\frac{\omega a_z}{v}}\, \frac{\omega^2}{(\omega - \omega_p + i\eta)(\omega + \omega_p + i\eta)} \qquad a_z < 0$$

and closing the contour in the lower half ω plane

$$\varphi(\vec{a}) = \frac{2e\omega_p}{v}\int_0^\infty dk\, \frac{k\, J_0(ka_\perp)}{\left(\frac{\omega_p}{v}\right)^2 + k^2}\, \sin\left(\frac{\omega_p}{v} a_z\right) e^{-\eta a_z} \qquad a_z < 0$$

$$\varphi(\vec{a}) = \frac{2e\omega_p}{v}\, K_0\left(\frac{\omega_p}{v} a_\perp\right) \sin\left(\frac{\omega_p}{v} a_z\right) e^{-\eta a_z} \qquad a_z < 0$$

This result was first obtained by Ritchie[7]. The fact that the potential blows up at $a_1 = 0$ is the result of including oscillations with k greater than k_D in the last integral. Also the damping η has been retained since all real systems have some damping. We derived this to show the approximate nature of the potential and its dependence on V. It is clear that for sufficiently large V as this contribution vanishes we are left with a Coulomb field. We note that if we had calculated the induced charge density by a similar technique we would have found that this charge is confined to a cone behind the moving particle of half angle $\sqrt{v_{F}/V}$. See reference 7 for details. Again as V increases the cone narrows as the proton outraces the induced plasma oscillations.

3.4 Ionization Potential

In this last section we derive an expression for the rate of ionization of the incident atom. This rate is then related to the imaginary part of the optical potential.

The ionization arises from a strong collision between the incident electron and an electron of the solid. This collision is treated here in an impulse approximation. By this we mean that both the incident and core electrons wave functions are expanded in a Fourier series. Thus a free electron free electron collision is considered for each of the respective Fourier components. A differential cross section is then obtained and then averaged over the respective momentum distributions given by the previous Fourier expansions. For a complete discussion see for example reference 8. The ionization cross section is taken as the sum of all cross sections for momentum transfers greater than some minimum necessary for ionization to occur (see below).

First we consider the scattering of two free particles of masses, m_1, m_2 and velocities $\vec{v}_1$ and $\vec{v}_2$. The subscript one refers to the electron of the incident pair and the subscript two refers to the electron of the solid. Conservation of momentum states

$$m_1\vec{v}_1 + m_2\vec{v}_2 = M\vec{V}_g = m_1\vec{v}_1{}' + m_2\vec{v}_2{}' \tag{1}$$

with

$$M = m_1 + m_2 \tag{2}$$

The primes refer to after the collision and $\vec{V}g$ is the velocity of the center of mass. We let

$$\vec{V} \equiv \vec{v}_1 - \vec{v}_2 \tag{3}$$

$$\vec{V}' \equiv \vec{v}_1{}' - \vec{v}_2{}' \tag{4}$$

then the momentum transferred to the incident electron is

$$\vec{P} = m_1(\vec{v}_1{}' - \vec{v}_1)$$

Using 3 and 1 and then 4 and 1 we get

$$\vec{v}_1 = \vec{V}_g + \frac{m_2}{M}\vec{V}$$

$$\vec{v}_1{}' = \vec{V}_g + \frac{m_2}{M}\vec{V}'$$

so

$$\vec{P} = \mu(\vec{V}' - \vec{V}) \tag{5a}$$

$$\mu \equiv \frac{m_1 m_2}{M} \tag{5b}$$

Since the scattering is elastic, both particles being free, the vector $\vec{V}$ is simply rotated to $\vec{V}'$ through an angle Θ with no change in length.

We argue that if

$$P \geqslant P_I$$

then the incident electron is ionized. The constant P_I is given by

$$\frac{P_I^2}{2m_1} = I_0$$

with I_0 the energy necessary to ionize the incident atom (ionization potential).

We need the cross section for a particular momentum transfer. The differential cross section for a scattering through the angle Θ in the center of mass frame for a particle of mass μ and velocity V is given by[8]

$$\sigma(\Theta) = \left(\frac{e^2}{2\mu V^2}\right)^2 \frac{1}{\sin^4\left(\frac{\Theta}{2}\right)} \tag{7}$$

This can be related to P since on using equation 5 we get

$$P^2 = \mu^2 V^2 + \mu^2 (V')^2 - 2\mu V V' \cos\Theta$$

$$P^2 = 2\mu^2 V^2 (1 - \cos\Theta)$$

$$P\,dP = \frac{\sin\Theta}{\mu^2 V^2}\,d\Theta \tag{8}$$

with

$$0 \leq P \leq 2\mu V$$

In using 8 in 7 we get

$$\sigma(\theta) = (2\mu e^2)^2 \frac{1}{p^4} \equiv \sigma(P)$$

Then

$$\sigma_{ION} = \int d\phi \int_{\substack{\text{IONIZ.}\\ \text{RANGE}}} \sin\theta \, \sigma(\theta) d\theta$$

$$\sigma_{ION} = 2\pi \frac{(2\mu e^2)^2}{(\mu V)^2} \int_{P_I}^{2\mu V} dp \frac{P}{P^4}$$

$$\sigma_{ION} = 2\pi \left(\frac{2e^2}{V}\right)^2 \frac{1}{2} \left\{ \frac{1}{P_I^2} - \frac{1}{(2\mu V)^2} \right\}$$

so

$$\sigma_{ION} = \frac{2\pi e^4}{m_1 V^2} \left\{ \frac{1}{I_0} - \frac{1}{E_0} \right\} \tag{9a}$$

$$E_0 \equiv \frac{2 m_1 m_2^2 V^2}{M^2} \tag{9b}$$

This procedure might seem crude but it is well known[11] to give results as good or better than much more elaborate calculations. At this point we should integrate 9a over the velocity distributions v_1 and v_2 contained in σ_{ION} through the relative velocity V. This would be in keeping with the impulse approximation. However we assume that the translational energy far exceeds the binding energies involved. Then the two electrons can be treated as truly free. The incident electrons velocity is taken as $\vec{v}_1$ = V i.e. only its translational part. The solid electron is taken at rest $\vec{v}_2$ = 0. This result is rigorous except for the inner electron in the core of the solid. The result 9 is the Thompson cross section.[9] Since the ionization dI/dt is related to the ionization cross section by

$$\frac{dI}{dt} = n_e V \sigma_{ION}$$

where ne is the electronic density of the scatterers, we find

$$\frac{dI}{dt} = n_e V \frac{2\pi e^4}{m_1 V^2} \left\{ \frac{1}{I_0} - \frac{1}{E_0} \right\} \tag{10}$$

This ionization rate can be related to the imaginary part of the optical potential u_I. The Schroedinger equation we derived for the motion of the incident electron in P space is

$$\left\{ i \frac{\partial}{\partial t} - H_A - V_S - i V_I \right\} \psi(\vec{r}, t) = 0 \tag{11}$$

where V_I the imaginary part of the optical potential is now interpreted as the ionization potential. If we multiply 11 by Ψ^* and subtract the complex conjugate equation after multiplying it by Ψ we get

$$\frac{\partial}{\partial t} |\psi|^2 = -2i \, \psi^* V_I \psi$$

If we then integrate this overall space we get

$$\frac{d}{dt} \int |\psi(\vec{r}, t)|^2 d^3r = -2i \int \psi^* V_I(r) \psi \, d^3r \tag{12}$$

The left hand side is the rate of change of probability which is related to the ionization rate by

$$\frac{d}{dt}\int |\psi|^2 d^3r = -\frac{dI}{dt} \tag{13}$$

Then

$$\frac{dI}{dt} = 2i\int \psi^*(\vec{r},t)\, V_I(r)\, \psi(\vec{r},t) \tag{14}$$

We shall return to these formulas after we have evaluated the ionization potential I_o for channeling pairs.

Appendix 3A

In this appendix we want to calculate

$$F(p) = {\sum_{\vec{k}\sigma}}' n_{\vec{k}\sigma}(1-n_{\vec{k}+\vec{p}\sigma}) = \frac{2\Omega}{(2\pi)^3}\int d^3k \; a(k_F^2-k^2)\, a((\vec{p}+\vec{k})^2-k_F^2)$$

with a(x) defined by 3.2.1 (8).

The integral above is the shaded area in Figure A1

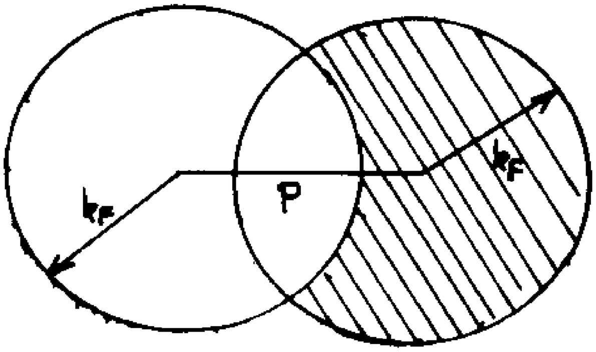

FIGURE A1

Suppose $p \leq 2k_F$ then the spheres in A1 overlap. The second step function $a((p+k)^2-k_F^2)$ demands that a lower limit on

$$\cos\theta = \nu = \hat{k}\cdot\hat{p}$$

be given by

$$k_F^2 = k^2+p^2+2pk\nu_L$$

or

$$\nu_L = \frac{k_F^2-k^2-p^2}{2kp}$$

This can be understood with the aid of Figure A2. For given k the variable θ must be such that the tip of the vector k lies only in the shaded portion. Therefore it can only sweep through the angle θ_L in Figure A2(b)

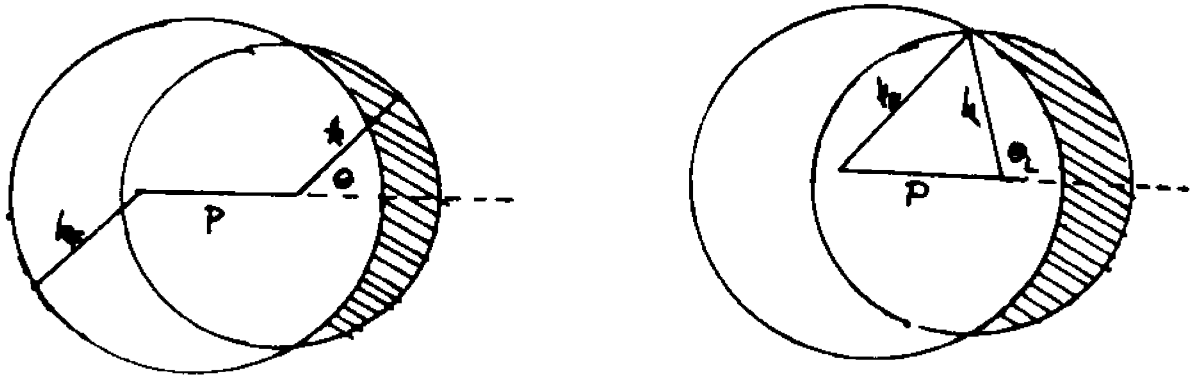

FIGURE A2

(a) (b)

so we get

$$F(p) = 2\,\frac{\Omega}{(2\pi)^3}\,2\pi \int dk\, k^2\, a(k_F^2-k^2) \int_{\nu_L}^{1} d\nu$$

$$= \frac{2\Omega}{(2\pi)^2} \int dk\, k^2 \left(1 - \frac{k_F^2-k^2-p^2}{2pk}\right) a(k_F^2-k^2)$$

If $p \le k_F$ then the integration over k has the limits k_F-p to k_F. If $2k_F \ge p \ge k_F$ then the integral over k has the limits $p-k_F$ to k_F. We can now easily integrate the above equation and after some straight forward algebra

$$F(p) = \frac{\Omega}{(2\pi)^2}\, p\left(k_F^2 - \frac{1}{12}p^2\right) \tag{1}$$

For $p \ge 2k_F$ the two spheres separate in Figure A1 and so

$$F(p) = \frac{2\Omega}{(2\pi)^3}\left(\frac{4}{3}\pi k_F^3\right) \tag{2}$$

Since N/2 electrons, with spin up say, satisfy

$$\frac{N}{2} = \sum_{k<k_F}{}' 1 = \frac{\Omega}{(2\pi)^3}\int_{k<k_F} d^3k = \frac{\Omega}{(2\pi)^3}\left(\frac{4}{3}\pi k_F^3\right) \tag{3}$$

Using 3 in 1 and 2 we find

$$F(p) = N\left(\frac{3}{4}\frac{p}{k_F} - \frac{1}{16}\frac{p^3}{k_F^3}\right) \qquad p \leq 2k_F$$

$$= N \qquad p \geq 2k_F$$

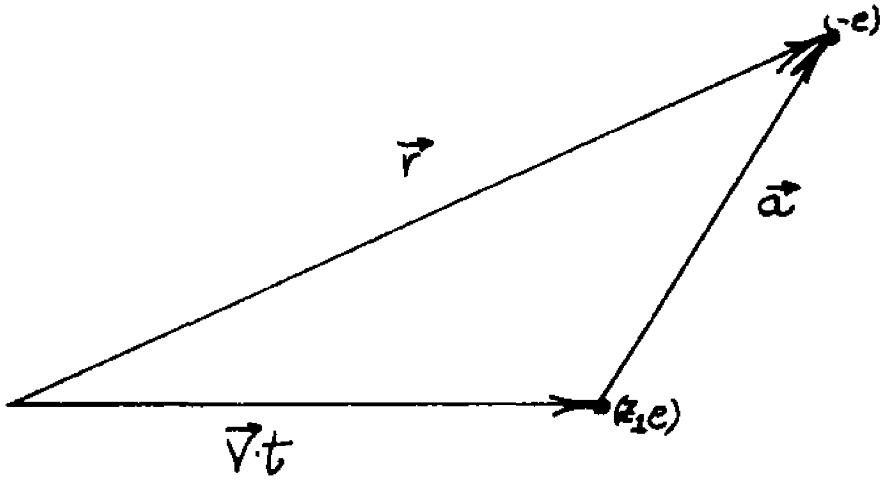

Fig. 10

Coordinates of Electron and Proton

References Chapter 3

1. I.M. Torrens, "Interatomic Potentials", Academic Press, New York (1972).
2. W.A. Harrison, "Pseudopotentials in the Theory of Metals", Benjamin, New York (1966).
3. D. Pines, "Elementary Excitations in Solids", Benjamin, New York (1964).
4. J. Lindhard, Dan. Mat. Fys. Medd. 28, No. 8 (1954).
5. A.A. Rukhadze and V.P. Silin, Soviet Phys. Usp. 4, 459 (1961).
6. L.D. Landau and E.M. Lifshitz, "Electrodynamics of Continuous Media", Addison-Wesley, Massachusetts (1960).
7. J. Neufeld and R.H. Ritchie, Phys. Rev. 98, 1632 (1955).
8. M.L. Goldberger and K.M. Watson, "Collision Theory", John Wiley and Sons, (1964).
9. J.J. Thompson, Phil. Mag. 23, 449 (1912).
10. L.I. Schiff, "Quantum Mechanics", McGraw Hill Book Co., New York (1968).
11. M. Gruyzinski, Phys. Rev. 115, 374 (1959).

Chapter 4

Solutions of the Equations of Motion

4.1 Introduction

In this chapter we are concerned with the explicit solution of the equation of motion for the electron. Our approach will be to diagnolize the Hamiltonian of this equation with respect to a basis of states of a hydrogenic atom in free space.

First in section 2 we transform the equation of motion to a frame of reference at rest with respect to the translating proton. Then we discuss in some detail our method of solution. Section 3 contains an evaluation of the matrix elements of the static potential. Finally section 4 consider the matrix elements of the polarization potential.

We shall see that numerical techniques are necessary for the diagnolization and in obtaining the matrix elements of the static potential. A discussion of the details of the particular numerical techniques used and the solutions themselves are deferred until Chapter 6 where the results of Chapters 2 through 5 are brought together.

4.2 Equation of Motion in the Protons Frame of Reference

Our basic equation of motion for the electron has been derived previously in a frame at rest with respect to the solid. In that frame we found that the electron satisfied

$$\left(i\frac{\partial}{\partial t} - H_{LOCAL} \right)\psi(\vec{r},t) = 0 \qquad (1a)$$

with

$$H_{LOCAL} = -\frac{1}{2m}\nabla^2 - \frac{Z_1 e^2}{|\vec{r}-\vec{R}(t)|} - \sum_{\vec{\ell}}{}' \frac{Z_2 e^2}{|\vec{r}-\vec{R}_\ell|} e^{-\lambda |\vec{r}-\vec{R}_\ell|} + V_{POL}(\vec{r}-\vec{R}(t)) - i \sum_{\vec{\ell}}{}' V_I(\vec{r}-\vec{R}_\ell) \qquad (1b)$$

The Bohr representation for the electron core interaction has been written down explicitly in the third term of equation 1b. The fourth term is the ionization potential and the fifth the polarization potential. The vector $\vec{R}_{\vec{\ell}}$ labels the positions of the cores and again $\vec{R}$ (t) is the specified motion of the proton.

We showed in Chapter 2 that the concept of average string potential should be used to describe the interaction between the electron and lattice. We say should rather than might in the last sentence since this concept seems very deeply intertwined with channeling itself. Perhaps this r emark is somewhat extreme, whatever the case might be we shall use the string potential. Then the sum over lattice points in 1b is replaced by

$$\sum_{\vec{\ell}}{}' \rightarrow \sum_{\text{strings}}{}' \int \frac{dZ}{D}$$

where Z is the coordinate of $\vec{R}_\ell$ in the direction of $\vec{V}$ and D is the lattice spacing in that direction. Whenever an $\vec{\ell}$ sum appears here it shall mean the averaging and sum over strings indicated above.

With this in mind we perform a Gallilean transformation to a reference system moving with the proton. We define the electrons coordinates in that frame by $\vec{r}'$; t' which are related to the coordinates $\vec{r}, t$ in the rest frame by

$$\vec{r}\,' = \vec{r} - \vec{R}(t) \qquad (2a)$$

$$t' = t \qquad (2b)$$

Further we write equation 1 in a more compact form by combining potentials of similar arguments, thus

$$i\frac{\partial\psi}{\partial t} = \left\{ -\nabla^2 + V_1(\vec{r} - \vec{R}(t)) + \sum_{\ell}{}' V_2(\vec{r} - \vec{R}_\ell) \right\} \psi(\vec{r}, t) \qquad (3)$$

To transform equation 3 we first note that by using equations 2a and 2b we can write

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t'} - \dot{\vec{R}} \cdot \nabla' \qquad (4a)$$

$$\nabla = \nabla' \qquad (4b)$$

Further if $\Psi'(\vec{r}\,', t')$ is the wave function in the moving system then since probability and volume are conserved in a Gallilean transformation we have

$$|\psi'(\vec{r}\,', t')|^2 = |\psi(\vec{r}, t)|^2$$

which implies $\Psi(\vec{r}, t) = \Psi'(r', t')\, e^{i(\text{phase})}$. It is clear that this can be written

$$\psi(\vec{r}, t) = \psi'(\vec{r}\,', t')\, e^{i[a\,\vec{r}\,' \cdot \dot{\vec{R}} - \epsilon(t')]}$$

where and and ϵ are arbitrary.

Then using 4a, 4b and 5 in 3 we find

$$\left[\frac{(-\nabla')^2}{2m} - \frac{ia}{m}\mathring{\vec{R}}\cdot\nabla + \frac{a^2\mathring{R}^2}{2m} + V_1(\vec{r}') + \sum_{\ell}{}' V_2(\vec{r}'+\vec{R}(t)-\vec{R}_\ell)\right]\psi'$$

$$= i\frac{\partial\psi'}{\partial t} + \left(-a\vec{r}'\cdot\ddot{\vec{R}} + \mathring{\epsilon} + a\mathring{R}^2 - i\mathring{\vec{R}}\cdot\nabla'\right)\psi' \qquad (6)$$

If we make the choices

$$a = m \qquad (7a)$$

$$\epsilon(t) = -\frac{m}{2}\int^{t}\mathring{R}^2(t')dt' \qquad (7b)$$

then equation 6 becomes

$$\left\{-\frac{1}{2m}\nabla'^2 + V_1(\vec{r}') + \sum_{\ell}{}' V_2(\vec{r}'+\vec{R}(t)-\vec{R}_\ell)\right\}\psi' = i\frac{\partial\psi'}{\partial t'} - m\vec{r}'\cdot\ddot{\vec{R}}\psi'$$

which becomes on dropping primes

$$\left\{-\frac{1}{2m}\nabla^2 + V_1(\vec{r}) + m\vec{r}\cdot\ddot{\vec{R}} + \sum_{\ell}{}' V_2(\vec{r}+\vec{R}(t)-\vec{R}_\ell)\right\}\psi(\vec{r},t) = \frac{i\partial\psi(\vec{r},t)}{\partial t}$$

The third term on the left hand side of the above equation is called the shakeoff potential and is due exclusively to the acceleration of the proton. According to our approximation $\vec{R} = \vec{V}t$ so for the protons motion this term vanishes. Further the last term in the above equation can be written

$$\sum_{\ell}{}' V_2(|\vec{r}+Vt\hat{z}-\vec{R}_\ell|) = \sum_{\text{strings}}{}' \int_{-\infty}^{\infty}\frac{dz}{D} V_2(|\vec{r}_\perp - \vec{R}_\ell^\perp, Vt-z|)$$

$$= \sum_{\text{strings}}{}' \int_{-\infty}^{\infty}\frac{dz}{D} V_2(|\vec{r}-\vec{R}_\ell^\perp - z\hat{V}|)$$

$$= \sum_{\ell}{}' V_2(\vec{r}-\vec{R}_\ell)$$

which says simply that a string is invariant under linear transformation along its length. So we obtain in a system at rest with respect to the proton the following equation

$$\left\{-\frac{1}{2m}\nabla^2 + V_1(\vec{r}) + \sum_{\vec{\ell}}{}' V_2(\vec{r}-\vec{R}_\ell)\right\}\psi(\vec{r},t) = i\frac{\partial\psi(\vec{r},t)}{\partial t}$$

which becomes under the substitution

$$\psi(\vec{r},t) = \psi(\vec{r})\,e^{-iEt}$$

$$\left\{-\nabla^2 + V_1(r) + \sum_{\vec{\ell}}{}' V_2(\vec{r}-\vec{R}_\ell)\right\}\psi(\vec{r}) = E\psi(\vec{r}) \qquad (8)$$

where E is complex and atomic (Rydberg) units are used

A direct solution of the partial differential equation 8 seems untenable because of the symmetry of the problem. Rather we shall attempt to solve this in a hydrogenic basis. This in fact seems to be a logical procedure since for large Z_1 and high incident velocity V our solution would approach that of a hydrogenic atom. That this is a reasonable choice is not difficult to understand since for high Z_1 there will be negligible overlap between the electronic density of the incident atom and the cores of the solid which act to distort and ionize the atom. Further we have already pointed out that the polarization potential itself decreases as V increases as does the ionization potential. In section 4 we shall see this even more clearly for the polarization effect. So in this limit of high translational velocity and high Z_1 we have a tightly bound hydrogenic atom in the ground state. Since this is the case we should expect that as we relax the severity of the conditions some mixing of higher states will ensue. Specifically we write

$$\psi(r) = \sum_{\mu}{}' a_{\mu} \phi_{\mu}(r) \qquad (9a)$$

expecting that only a few terms make large contributions where the states ϕ satisfy

$$\left(-\nabla^2 - \frac{2Z_1}{r}\right) \phi_{nlm}(\vec{r}) = \frac{-Z_1 e^2}{n^2} \phi_{nlm}(\vec{r}) = W_n(Z_1) \phi_{nlm}(\vec{r})$$

$$\mu = (n, l, m)$$

On substituting 9 in 8 we get

$$\sum_{\nu}{}' \left[\left(E - W_n(Z_1)\right) \delta_{\mu\nu} - V_{\mu\nu} \right] a_{\nu} = 0. \qquad (10a)$$

where $V_{\mu\nu}$ is the matrix element

$$V_{\mu\nu} = \langle \phi_{\mu} V_{pa} \phi_{\nu} \rangle + \sum_{\text{strings}}{}' \int_{-\infty}^{\infty} \frac{dZ}{D} \langle \phi_{\mu} \left[\frac{e^{-\lambda|\vec{r} - \vec{R}|}}{|\vec{r}' - \vec{R}|} \quad - i\, V_I(\vec{r} - \vec{R}) \right] \phi_{\nu} \rangle \qquad 10b$$

Now diagnolization of 10a leads to our solution. However there are some points to be cleared up. First the matrix elements of the static potential (the second term in 10b) are by no means trivial to evaluate and in fact entail numerical integration. Secondly the diagnolization itself must be done numerically if any reasonably sized basis is chosen in 9a. We should also point out again that the Hameltonian in 10a is non hermitian due to the ionization potential. However this complicates our solution only in detail[1]. The last point is that we do not know the ionization potential since it is itself related to the wave function we are seeking. This was shown explicitly in section 3.4 where we found that it was related to the ionization rate $^{dI}/dt$ through

$$\frac{1}{q}\frac{dI}{dt} = \int \psi^*(iV_I)\psi(\vec{r},t))d^3r$$

We could then attempt a self consistant solution. This would comprise a guess of the wave function and then inversion of the above relationship to obtain V_I. This would then be substituted in 10a which would then be diagnolized.

The consistancy of the solution to equation 10a with the initial guess is then the criterion for termination of the process. However, we would rather treat the ionization potential as a perturbation. As a first solution this seems the most direct approach since it is consistant with our assumption that the atom is long lived. For example suppose V = 50 then this would lead to a decay rate using 3.4 (13) of order .1 (Rydberg units). This would correspond to a lifetime of order 10. But for thin crystals, in such a time the atom can already have traversed the solid.

This implies that the ionization potential has a small effect on the eigenvalues. In our perturbation treatment we will in fact be neglecting the affect of the ionization potential on the states themselves. We shall only look at the ionization potentials perturbation of the eigenvalue.

So our solution takes the following form. We solve the eigenvalue 10a with the ionization potential absent. This solution yields a set of states and their eigenvalues. These eigenvalues represent the binding energy of the states relative to the proton and strings. We then find among this set the state of tightest binding relative to the proton. This state Ψ_0 called the ground state has its binding to the proton given by

$$\mathcal{E}^B = \langle \psi_0 | -\nabla^2 - \frac{2Z_1}{r} | \psi_0 \rangle \qquad (11)$$

Then from the relation derived in Chapter 3

$$\frac{dI}{dt}(E_i, I_0) = \frac{d}{dt}\int |\psi(\vec{r},t)|^2 \, d^3r$$

where E_i the incident energy and I_0 the ionization potential, we obtain on writing

$$E = \mathcal{E} - i\,\Gamma/2$$

and using 11 a value for Γ at $t = 0$.

$$\frac{dI}{dt}(E_{i}) - \mathcal{E}^{B}) = \Gamma \qquad (12)$$

We now turn to the evaluation of the potentials.

4.3 Static Potential

We want to evaluate the matrix elements of the potential

$$V_S = \sum_{\vec{\ell}}{}' \frac{-2Z_1}{|\vec{r}-\vec{R}_\ell|} e^{-\lambda|\vec{r}-\vec{R}_\ell|} \qquad (1)$$

in a hydrogenic basis. In this potential λ is left at our disposal. This potential must of course be averaged over the direction of motion of the proton. Suppose for simplicity that we were considering channeling in a simple cubic crystal. Then the situation would appear as in figure 11, where only the four nearest neighbors are shown. The direction of motion of the proton is out of the paper. The string numbered 1 would appear as in figure 12 where the coordinates of the vector $\vec{R}$ are shown. The electrons coordinates are (r, θ, ϕ). Before doing the necessary integrals to evaluate the matrix elements we can take advantage of some symmetry properties.

First we expand $V_S(r)$ in spherical harmonics

$$V_S(\vec{r}) = \sum_{LM}{}' Y_{LM}(\theta,\phi)\, V_{LM}(\vec{R}, r)$$

We see from figure 11 that V must satisfy

$$V(r,\theta,\phi) = V(r,\theta,\phi + \frac{n\pi}{2})$$

with η an integer. This implies on using 2 that

$$e^{iM\frac{\eta\pi}{2}} = 1$$

or

$$\eta \cdot M = 4\,(\text{integer})$$

From this we conclude that

$$V_S = 0 \quad \text{unless} \quad M = 0,\ \pm 4,\ \pm 8, \ldots$$

We also see that a matrix element of equation 2 in a hydrogenic basis reads

$$\langle n'\ell'm'|V(\vec{r})|n\ell m\rangle = \sum_{LM}{}' \int_0^\infty dr\, r^2 R^*_{n'\ell'}(r) R_{n\ell}(r) V_{LM} \cdot \int d\phi\, d\theta \sin\theta\, Y^*_{\ell'm'}(\theta\phi)\, Y_{LM}(\theta\phi)\, Y_{\ell m}(\theta,\phi)$$

where we have written

$$|n\ell m\rangle \equiv \phi_{n\ell m}(\vec{r}) = R_{n\ell}(r)\, Y_{\ell m}(\theta,\phi) \qquad (4)$$

The angular integral is invariant under the transformation

$$(\theta,\phi) \to (\pi-\theta,\ \phi+\pi) \qquad (5a)$$

but

$$Y_\ell^m(\pi-\theta,\ \phi+\pi) = (-1)^\ell\, Y_\ell^m(\theta,\phi) \qquad (5b)$$

Therefore we conclude that the only terms to survive in the sum over L above are those for which

$$(-1)^{\ell+\ell'+L} = 1$$

or

$$\ell+\ell'+L = \text{even}$$

Finally we write our matrix element in the form

$$V_{\mu'\mu} = \sum_{\text{Strings}} (-2Z_L) \int_{-\infty}^{+\infty} \frac{dZ}{D} \int d^3r \, \phi^*_{\mu'}(\vec{r}) \frac{e^{-\lambda|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} \phi_\mu(\vec{r}) \qquad (7a)$$

where the sum is over the strings numbered one through four which are shown in figure 11. The transformation $\vec{R} \rightarrow -\vec{R}$ takes us from string number one to string three and from string number two to string four. Therefore the sum over strings in 7a above is invariant under this transformation and we get

$$V_{\mu'\mu} = \sum_{\text{Strings}}{}' (-2Z_L) \int_{-\infty}^{+\infty} \frac{dZ}{D} \int d^3r \, \phi^*_{\mu'}(\vec{r}) \frac{e^{-\lambda|\vec{r}+\vec{R}|}}{|\vec{r}+\vec{R}|} \phi_\mu(\vec{r}) \qquad (7b)$$

Then we can make the transformation $\vec{r} \rightarrow -\vec{r}$ in the integral in 7b above. Using 5a and 5b we then find

$$V_{\mu'\mu} = (-1)^{\ell+\ell'} \sum_{\text{Strings}}{}' \int_{-\infty}^{+\infty} \frac{dZ}{D} \int d^3r \, \phi^*_{\mu'}(\vec{r}) \frac{e^{-\lambda|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} \phi_\mu(\vec{r})$$

from which we conclude that the matrix element vanishes unless $\ell + \ell'$ is even. Combining this result with (6) we have

$$V_{\mu'\mu} = 0 \quad \text{unless} \quad \ell + \ell' = \text{even}$$

and in the L sum in equ unless $\ell + \ell' = \text{even}$

$$L = \text{even}$$

are non zero.

We have proved the conditions 3 and 7 for a set of four lattice strings. But in reality for a cubic lattice we have a set of lattice points in the transferse plane given by

$$\vec{\rho} = D \left\{ (n_x - \tfrac{1}{2}) \hat{i} + (n_y - \tfrac{1}{2}) \hat{j} \right\}$$

where $\vec{\rho}$ is a two dimensional vector from the incident proton to a lattice point in the transverse plane. These lattice points are shown in Figure 13 where they are grouped in sets of four. For example the first set has the lattice numbers $n_x = \pm 1$, $n_y = \pm 1$. Further, for this set we see that

$$\rho = D/\sqrt{2}$$

We note that all these sets are squares and so our relations 3 and 7 still hold. We merely add strings in groups of four. Using the numbering of the figure we obtain the important parameters given in table I. The angle ϕ is taken with respect to a convenient axis say χ.

In our numerical calculation we shall use sodium for the crystal. This is a simple metal with a body centered cubic lattice rather than being simple cubic. However if we consider channeling along ⟨0, 0, 1⟩ then the lattice would appear in the transverse plane as in Figure 14. Therefore we would have the same symmetry in the transverse plane. However the lattice parameter in table I would be given by $D = a/\sqrt{2}$ while the lattice spacing along the direction of motion would be $D = a$. For sodium the lattice parameter is(2) $a = 4.225$ angstroms.

We finally point out that for other crystals and different directions of incidence would in general no longer have a square lattice in the transverse plane. However this would affect the calculations that follow in computational details only.

It can be shown that$^{(3)}$

$$\frac{e^{-\lambda|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} = \sum_{LM}{}' \, 8\lambda \, i_L(\lambda S_<) \, k_L(\lambda S_>) \, Y^*_{LM}(\hat{R}) \, Y_{LM}(\hat{r})$$

where $S_<(S_>)$ is the lesser (greater) of r and R. The functions i_L and k_L are spherical Bessel functions of an imaginary argument. They are simple transcendental functions, for example

$$i_0(x) = \frac{\sinh x}{x}$$

and

$$k_0(x) = \frac{\pi}{2x} e^{-x}$$

Their properties can be found in reference 3 if we write them in the form

$$\begin{Bmatrix} i_L \\ k_L \end{Bmatrix} = \sqrt{\frac{\pi}{2x}} \begin{Bmatrix} I_{L+\frac{1}{2}}(x) \\ K_{L+\frac{1}{2}}(x) \end{Bmatrix}$$

Using the above expansions of the Bohr potential we get for the matrix element of the static potential

$$(V_S)_{n'\ell'm'|n\ell m} = \sum_{\text{strings}}{}' -2Z_1 \frac{8\lambda}{D} \int_{-\infty}^{+\infty} dz \, Y^*_{LM}(\hat{R}) \int d^3r \, \phi^*_{n'\ell'm'}(r) \, \phi_{n\ell m}(r) \times i_L(S_<) \, k_L(S_>) \, Y_{LM}(\hat{r}) \qquad (8)$$

If we write the hydrogenic wave functions explicitly as

$$\phi_{n\ell m}(\vec{r}) = R_{n\ell}(r) \, P_{\ell m}(\theta) \, \frac{e^{im\phi}}{\sqrt{2\pi}}$$

where $R_{n\ell}(r)$ is a radial hydrogenic function and $P_{\ell m}(\theta)$ is proportional to an associated Legendre polynomial. In substituting this we find that equation 8 becomes

$$(Y_3)_{\mu'\mu} = -2Z_0 \frac{8\lambda}{D} \sum_{LM}{}' C(L\ell'm'\ell m) \sum_{g}{}' J_L(g)$$

where

$$C(L\ell'm'\ell m) = \int d\Omega \, Y^*_{\ell'm'}(\Omega) \, Y_{LM}(\Omega) \, Y_{\ell m}(\Omega) \quad ; \Omega = (\theta,\phi)$$

The sum over strings is written as a sum over sets of strings. That is g represents a set which contains four strings as in Figure 13 and Table I. If we use figure 12 and the representation

$$Y^*_{LM}(\hat{R}_g) = \mathcal{P}_{\ell m}(\cos\theta_g) \frac{e^{-iM\phi_g}}{\sqrt{2\pi}}$$

$$= \mathcal{P}_{\ell m}\left(\frac{z}{\sqrt{\rho_g^2+z^2}}\right) \frac{e^{-iM\phi_g}}{\sqrt{2\pi}}$$

we find that $J_L(g)$ in 9 can be written

$$J_L(g) = \left\{ \frac{e^{-iM\phi_g}}{\sqrt{2\pi}} + \frac{e^{-iM(\phi_g+\pi/2)}}{\sqrt{2\pi}} + \frac{e^{-iM(\phi_g+\pi)}}{\sqrt{2\pi}} + \frac{e^{-iM(\phi_g+\frac{3\pi}{2})}}{\sqrt{2\pi}} \right\} S_L(g) \qquad (11a)$$

$$S_L(g) = \int_{-\infty}^{\infty} dz \, P_{LM}\left(\frac{z}{\sqrt{\rho_g^2+z^2}}\right) k_L\left(\lambda\sqrt{\rho_g^2+z^2}\right) \int_0^{\sqrt{\rho_g^2+z^2}} dr \, r^2 \mathcal{R}_{n'\ell'}(r) \mathcal{R}_{n\ell}(r) \, i_L(\lambda r)$$

$$+ \int_{-\infty}^{\infty} dz \, P_{LM}\left(\frac{z}{\sqrt{\rho_g^2+z^2}}\right) i_L\left(\lambda\sqrt{\rho_g^2+z^2}\right) \int_{\sqrt{\rho_g^2+z^2}}^{\infty} dr \, r^2 \mathcal{R}_{n'\ell'} \mathcal{R}_{n\ell}(r) \, k_L(\lambda r) \qquad (11b)$$

The bracket in 11 a contains the sum over the four strings in the set g. Using 3 we find that 11 a becomes

$$J_L(g) = 4\,\frac{e^{-iM\phi_g}}{\sqrt{2\pi}}\,\mathcal{S}_L(g) \qquad (12)$$

Now we can rewrite 11 (b) on using the fact that the integrands are even in z. This follows from equation 5 b and the explicit dependence shown in 11 b. So we get

$$\begin{aligned}\mathcal{S}_L(g) = {} & 2\int_0^\infty dz\, P_{LM}\left(\frac{z}{\sqrt{\rho_g^2+z^2}}\right) k_L\left(\lambda\sqrt{\rho_g^2+z^2}\right)\int_0^{\sqrt{\rho_g^2+z^2}} dr\, Q_{n'l'}\, Q_{nl}\, i_L(\lambda r)\, r^2 \\ & + 2\int_0^\infty dz\, P_{LM}\left(\frac{z}{\sqrt{\rho_g^2+z^2}}\right) i_L\left(\lambda\sqrt{\rho_g^2+z^2}\right)\int_{\sqrt{\rho_g^2+z^2}}^\infty dr\, Q_{n'l'}\, Q_{nl}\, k_L(\lambda r) \qquad (13)\end{aligned}$$

The second term in 13 is integrated in the r, z plane as shown in Figure 15 a. That is z is held fixed, r is integrated inside the parabola and then z is integrated over the half plane. If we reverse the procedure the second term in 13 can be written, where the order of integration

$$\int_{\rho_g}^\infty dr\, r^2 Q_{n'l'}\, Q_{nl}(r)\, k_L(\lambda r)\int_0^{\sqrt{r^2-\rho_g^2}} dz\, P_{LM}\left(\frac{z}{\sqrt{\rho_g^2+z^2}}\right) i_L\left(\lambda\sqrt{\rho_g^2+z^2}\right)$$

is shown in Figure 15 b. Substituting this in equation 13 and then into 12 we get after some obvious change of variables

$$J_L(g) = 8\,\frac{e^{-iM\phi_g}}{\sqrt{2\pi}}\,\rho_g^4\,(J_1+J_2) \qquad (14a)$$

$$J_1 = \int_0^\infty dz\, P_{LM}\left(\frac{z}{\sqrt{1+z^2}}\right) k_L(\lambda\rho_g\sqrt{1+z^2}) \int_0^{\sqrt{1+z^2}} dr\, r^2 R_{n'l'}(\rho_g r) R_{nl}(\rho_g r)\, i_L(\lambda\rho_g r) \qquad (14b)$$

$$J_2 = \int_1^\infty dr\, r^2 R_{n'l'}(\rho_g r) R_{nl}(\rho_g r)\, k_L(\lambda\rho_g r) \int_0^{\sqrt{r^2-1}} dz\, P_{LM}\left(\frac{z}{\sqrt{1+z^2}}\right) i_L(\lambda\rho_g\sqrt{1+z^2}) \qquad (14c)$$

This must then be combined in equation 9 to give

$$(V_s)_{\mu'\mu} = -2Z_0 \frac{8\lambda}{D} \sum_{LM}{}' C(L,l'm'/lm) \sum_g{}' \frac{e\, e^{-iM\phi_g}}{\sqrt{2\pi}} \rho_g^4 (J_1+J_2)$$

The evaluation of the integral over the three spherical harmonies C(L, l'm', lm) is standard. Therefore a brief description is relegated to appendix A.

We should point out that the result 14 d entails extensive numerical work. We defer until Chapter 6 a discussion of the numerical techniques used in the evaluation of the set of equations 14 and equation A 8.

4.4 Polarization Potential

In Chapter 3 we derived the result

$$V_{Pol} = \frac{e}{2\pi^2} \int \frac{d^3k}{k^2} \left(Z_1 e^{+i\vec{k}\cdot\vec{r}} - 1\right)\left(\frac{1}{\epsilon(\vec{k},\vec{P},\vec{v})} - 1\right) \qquad (1)$$

for the potential in matter at the position of the electron in a frame at rest with respect to the proton. This potential is due entirely to the presence of matter vanishing in free space where $\epsilon = 1$. We now want to evaluate this in a hydrogen basis taking into account the plasma contribution to 1.

Since $\vec{r}$ will be of order unity when evaluated between low lying states of a hydrogenic atom and further, since the plasma contributions occur only for $k < k_D$ we make the dipole expansion for the exponential in equation 1. This expansion should not be taken too seriously for coupling to higher states. The contributions to the k integral (see equation 3) come from the region $k \sim \omega_p/V$. Since we shall be interested in $Z_1 = 1$ (see Chapter 6) we obtain

$$(V_{POL})_{\mu'\mu} = \frac{i\, r_{\mu'\mu}}{2\pi^2}\, e \int \frac{d^3k}{k^2}\, \vec{k} \left(\frac{1}{\epsilon(k, \vec{k}\cdot\vec{v})} - 1 \right)$$

Since

$$\epsilon(k, \vec{k}\cdot\vec{v}) = \epsilon\left(\sqrt{k_x^2+k_y^2+k_z^2},\ k_z v \right)$$

is even in k_x and k_y we get

$$(V_{POL})_{\mu'\mu} = \frac{i(z)_{\mu'\mu}}{2\pi^2}\, e \int \frac{d^3k}{k^2}\, k_z \left(\frac{1}{\epsilon(k, k_z v)} - 1 \right) \qquad (2)$$

If we make the substitutions

$$k_z v = k\cdot v = k v \mu$$

$$\omega = k_z v$$

$$d\omega = k v\, d\mu$$

into equation 2 we obtain

$$(V_{POL})_{\mu'\mu} = \frac{i(\zeta)_{\mu'\mu}}{2\pi 2}\, e\, \frac{2\pi}{V^2} \int_0^{k_D} \frac{dk}{k} \int_{-kV}^{kV} d\omega\, \omega \left(\frac{1}{\epsilon(k,\omega)} - 1 \right) \tag{3}$$

where the fact that plasma oscillations exist only for $k < k_D$ is shown explicitly in the upper limit on the k integral. It should be clear that higher powers in the expansion of the exponential in 1 would bring higher powers of V into the denominator of equation 3. To continue, we note from section 3.37 that

$$Re \left(\frac{1}{\epsilon(k,\omega)} - 1 \right) = \text{even in } \omega$$

$$Im \left(\frac{1}{\epsilon(k,\omega)} \right) = \text{odd in } \omega$$

where Re, Im mean real part of and imaginary part of respectively. In fact this result is more general than our derivation in that section. The reader is referred to Pines, 4 for the details. With these properties we get for 3

$$(V_{POL})_{\mu'\mu} = \frac{-(\zeta)_{\mu'\mu}}{\pi}\, \frac{e}{V^2}\, Im \int_0^{k_D} \frac{dk}{k} \int_{-kV}^{kV} d\omega\, \omega\, \frac{1}{\epsilon_{PLASMA}(\vec{k},\omega)} \tag{4}$$

If we use the representation for the plasma contribution to the dielectric constant given by equation 3.37 (5a) we have

$$\frac{1}{\epsilon_p(k,\omega)} = \frac{\omega^2}{(\omega-\omega_k-i\eta)(\omega+\omega_k+i\eta)} \qquad (5)$$

where ω_k is the frequency of oscillation of the plasma mode. Equation 5 yields

$$\mathrm{Im}\left(\frac{1}{\epsilon_p(k,\omega)}\right) = -\frac{\pi\omega_{\vec{k}}}{2}\left[\delta(\omega-\omega_{\vec{k}}) - \delta(\omega+\omega_{\vec{k}})\right]$$

and in fact is odd in ω as stated. If we make the approximation $\omega_k \simeq \omega_p$[+] and substitute equation 6 into equation 4 we get

$$V_{\mu'\mu} = (3)_{\mu'\mu}\, e \left(\frac{\omega_p}{V}\right)^2 \ln\left(V/v_F\right) \qquad (7)$$

where we used the relationship

$$\omega_p = k_D v_F$$

It is interesting to note that equation 4 (or 7) is proportional to the stopping power of an electron gas. For a proton transversing a solid the energy lost per unit path length (stopping power) is

$$\frac{dW}{dz} = \frac{dW}{dt}\cdot\frac{1}{V} = \frac{e}{V}\vec{E}\cdot\vec{V}\Big|_{\substack{\text{Position}\\ \text{of Proton}}} \qquad (8)$$

That is the field set up in media by the proton acts to slow it down. In fact the potential at the field point $\vec{r}$ at time t set up by the moving

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[+] This causes negligible error in the limit $V >> {}_F$. See Pines in reference 5 for the details of this point proton was shown in Chapter 3 to be

$$\phi(\vec{r},t) = \int \frac{d^3k}{k^2} \frac{e^{ik\cdot(\vec{r}-\vec{v}t)}}{\epsilon(k,\vec{k}\cdot\vec{v})}$$

$$-\vec{E} = \nabla\phi = \int \frac{d^3k}{k^2}\, i\vec{k}\, \frac{e^{ik\cdot(\vec{r}-\vec{v}t)}}{\epsilon(k,k\cdot v)} \qquad (9)$$

Then making the substitutions following equation 2 into 8 and using 9 we get

$$\frac{dW}{dz} = e\frac{2\pi}{v^2}\int_0^{k_D}\frac{dk}{k}\int_{-kv}^{kv} d\omega\, \omega\, \mathrm{Im}\left(\frac{1}{\epsilon(k,k\cdot v)}\right)$$

Therefore according to equation 4

$$(V_{POL})_{\mu'\mu} = \frac{-(z)_{\mu'\mu}}{2\pi^2}\left(\frac{dW}{dz}\right)$$

Therefore knowledge of the energy loss gives no information about the polarization potential. This should not be surprising since in making a dipole approximation earlier we were evaluating the fields at the proton as in equation 8.

We also note that that factor multiplying $z_{\mu',\mu}$ in equation 7 is of order .01 in our case. The factor $z_{\mu'\mu}$, is obtained by a standard calculation. Briefly, with z = r cos θ

$$(z)_{\mu'\mu} = \int_0^\infty dr\, r^2 R_{n'l'}(r)\, R_{nl}(r)\int d\Omega\, Y_{l'm'}(\Omega)\cos\theta\, Y_{lm}(\Omega) \qquad (10)$$

Using appendix A or more simply [6]

$$Y_{\ell m} = \mathcal{P}_{\ell m} \frac{e^{im\phi}}{\sqrt{2\pi}}$$

$$\mathcal{P}_{\ell m}\cos\theta = \sqrt{\frac{(\ell+1)^2-m^2}{(2\ell+3)(2\ell+1)}}\,\mathcal{P}_{\ell+1,m} + \sqrt{\frac{\ell^2-m^2}{(2\ell+1)(2\ell-1)}}\,\mathcal{P}_{\ell-1,m} \qquad (11)$$

we find that $z_{\mu'\mu}$ vanishes unless

$$\ell-\ell' = \pm 1$$

$$m'-m = 0$$

Specifically 10 becomes on using 11

$$\langle n', \ell+1, m | z | n \ell m \rangle = \sqrt{\frac{(\ell+1)^2-m^2}{(2\ell+3)(2\ell+1)}}\,\mathcal{R}_{n\ell}^{n'\ell+1} \qquad (12a)$$

$$\langle n', \ell-1, m | z | n \ell m \rangle = \sqrt{\frac{\ell^2-m^2}{(2\ell+1)(2\ell-1)}}\,\mathcal{R}_{n\ell}^{n'\ell-1} \qquad (2b)$$

where $R_{n\ell}^{n'\ell'}$ represents the radial integral in equation 10. The squares of the elements $R_{n\ell}^{n'\ell'}$ are tabulated in reference 6. The signs given below have been obtained by inspection. We list those non-vanishing matrix elements of interest to us. (in atomic units)

$$\langle 1s | z | 2p(0) \rangle = +.75$$

$$\langle 1s | z | 3p(0) \rangle = +.32$$

$$\langle 2s | z | 2p(0) \rangle = -3.20$$

$$\langle 2s | z | 3p0 \rangle = +1.83$$

$$\langle 2p(-1) | z | 3d(-1) \rangle = 2.14$$

$$\langle 2p(0) | z | 3s(0) \rangle = .50$$

$$\langle 2p(0) | z | 3d(0) \rangle = 2.48$$

$$\langle 2p(1) | z | 3d(1) \rangle = 2.14$$

$$\langle 3s | z | 3p(0) \rangle = -23.4$$

$$\langle 3p(-1) | z | 3d(-1) \rangle = -4.67$$

$$\langle 3p(0) | z | 3d(0) \rangle = -5.42$$

$$\langle 3p(1) | z | 3d(1) \rangle = -4.67$$

So we see that the low lying states of hydrogen contribute according to 7 an order of magnitude value of •1 Rydbergs for the polarization potential. This is in keeping with our remarks about the smallness of this potential for high incident velocities.

At this point we have all that is necessary to find the ground state and its lifetime for a pair channeling in a sodium crystal. Since capture is possible if the atom ionizes, we shall first consider some capture problems in Chapter 5 before returning to the numerical solution of 4.2 (10 a).

Appendix A

We follow Messiah[7] in writing a solution for the integral

$$C(L\ell_2 m_2\, \ell_1 m_1) \equiv \int d\Omega\, Y^*_{\ell_2 m_2}(\Omega)\, Y_{LM}(\Omega)\, Y_{\ell_1 m_1}(\Omega) \qquad (1)$$

in the form

$$C(L\ell_2 m_2\, \ell_1 m_1) = (-1)^{m_2}\left[\frac{(2\ell_1+1)(2\ell_2+1)(2L+1)}{4\pi}\right]^{1/2}\begin{pmatrix} \ell_1 & \ell_2 & L \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \ell_1 & \ell_2 & L \\ m_1 & -m_2 & M \end{pmatrix} \qquad (2)$$

The terms on the right of the square root in 2 are 3j symbols which are proportional to Clebsch-Gordon coefficients. Their appearance in 2 is quite natural since we can reduce 1 to the addition of angular momentum. The first term appears due to the fact that the coordinates are the same for the angular momentum states and specifically has the properties and values

$$\begin{pmatrix} \ell_1 & \ell_2 & L \\ 0 & 0 & 0 \end{pmatrix} = 0 \quad \text{if } \ell_1+\ell_2+L = \text{odd} \qquad (3)$$

$$\begin{pmatrix} \ell_1 & \ell_2 & L \\ 0 & 0 & 0 \end{pmatrix} = (-1)^p \sqrt{\Delta(\ell_1 \ell_2 L)}\; \frac{p!}{(p-\ell_1)!(p-\ell_2)!(p-L)!} \qquad (4)$$

$$2p \equiv \ell_1+\ell_2+L$$

$$\Delta(\ell_1 \ell_2 L) = \frac{(\ell_1+\ell_2-L)!\,(\ell_2+L-\ell_1)!\,(L+\ell_1-\ell_2)!}{(\ell_1+\ell_2+L+1)!} \qquad (7)$$

And

$$\begin{pmatrix} \ell_1 & \ell_2 & L \\ m_1 & -m_2 & M \end{pmatrix} = (-1)^{\ell_1-\ell_2-M} \Delta(\ell_1 \ell_2 L) \sqrt{(\ell_1+m_1)!\,(\ell_1-m_1)!\,(\ell_2-m_2)!\,(L-M)!\,(L+M)!}$$

$$\times \sum_t{}' (-1)^t \left[t!\,(L-\ell_2+t+m_1)!\,(L-\ell_1+t+m_2)!\,(\ell_1+\ell_2-L-t)!\,(\ell_1-t-m_1)!\,(\ell_2-t-m_2)! \right]^{-1} \quad ($$

where

$$\begin{pmatrix} \ell_1 & \ell_2 & L \\ m_1 & -m_2 & M \end{pmatrix} = 0 \qquad \text{if} \quad M \neq m_2 - m_1 \qquad (9a)$$

and the sum in 8 is only over those terms for which angular momentum is conserved

$$|\ell_1-\ell_2| \leq L \leq (\ell_1+\ell_2) \qquad 9b)$$

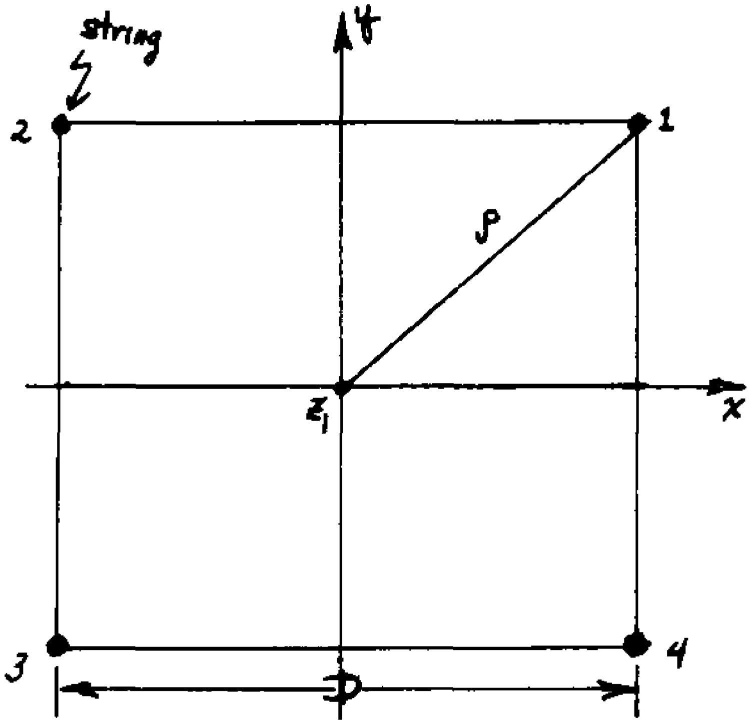


Fig. 11

Configuration of Strings in Transverse Plane

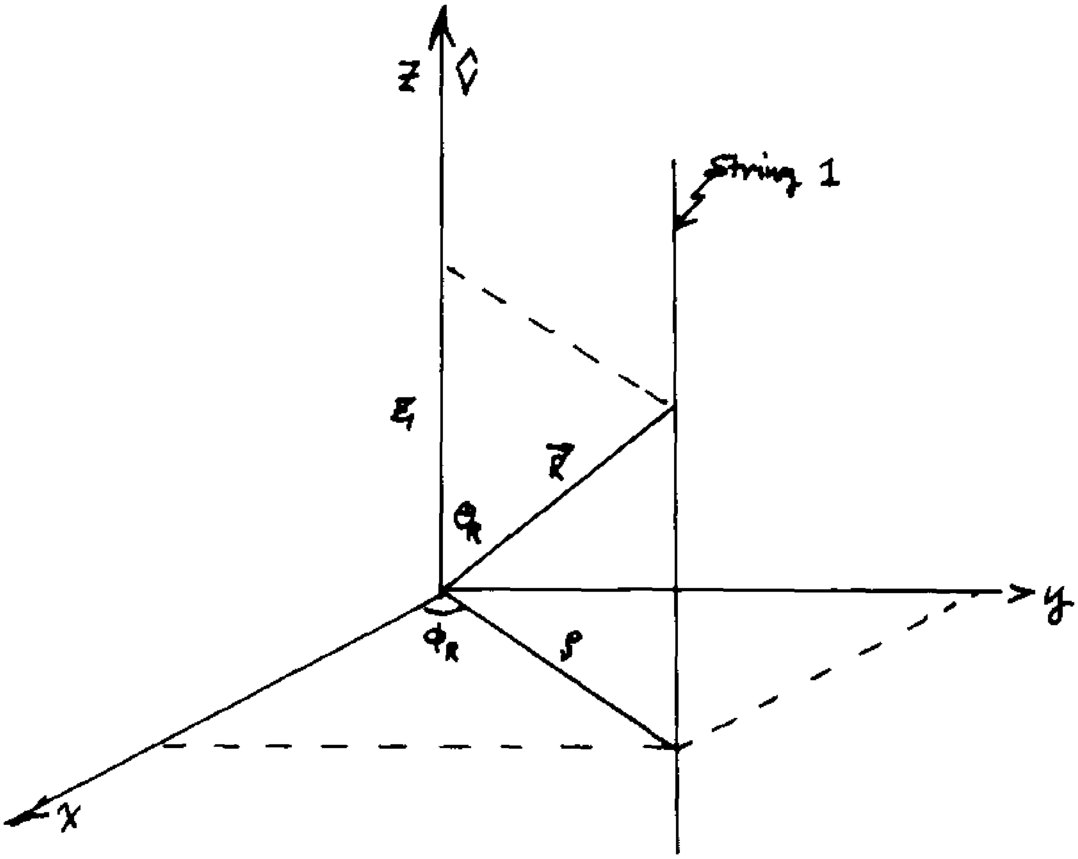


Fig. 12

Coordinates of a String

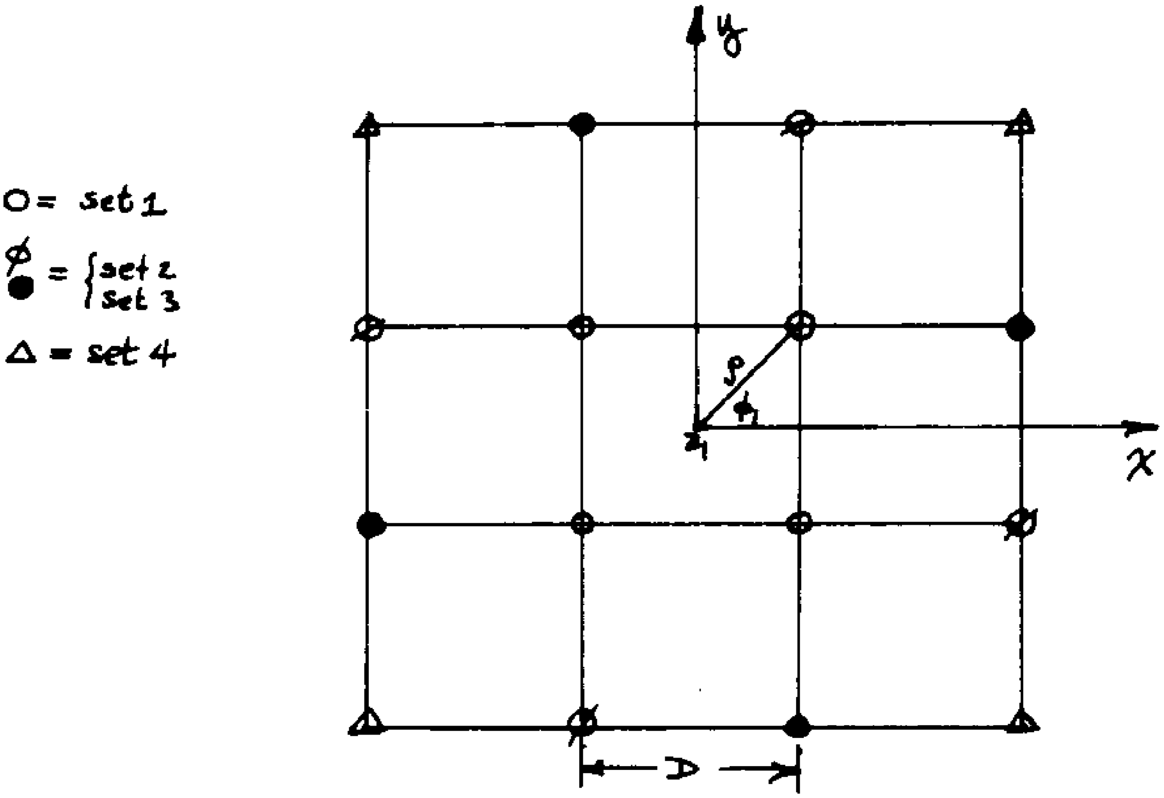


Fig. 13

Configuration of FIRST FOUR Sets of Strings

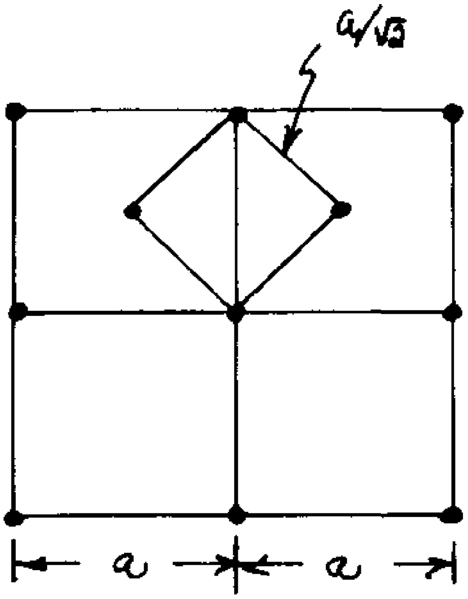


Fig. 14

B.C.C. Lattice Along ⟨0,0,1⟩

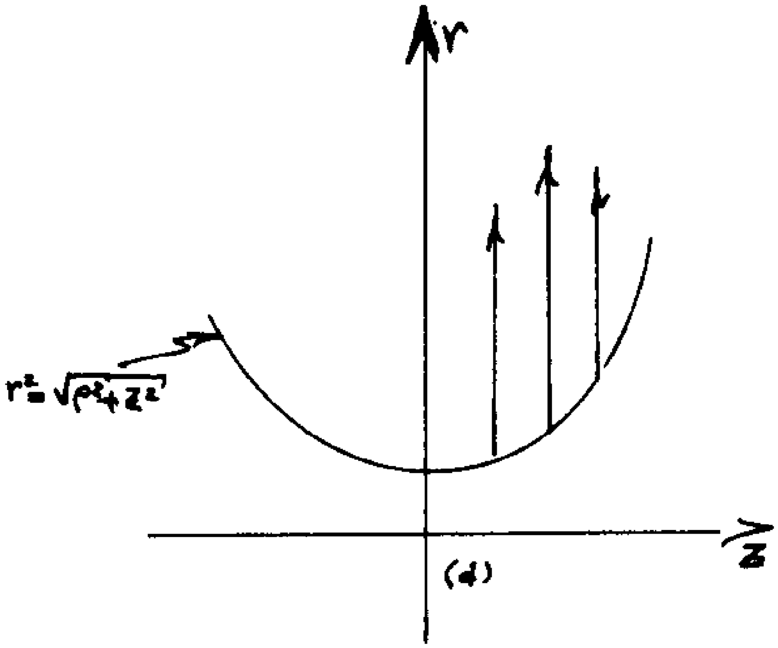
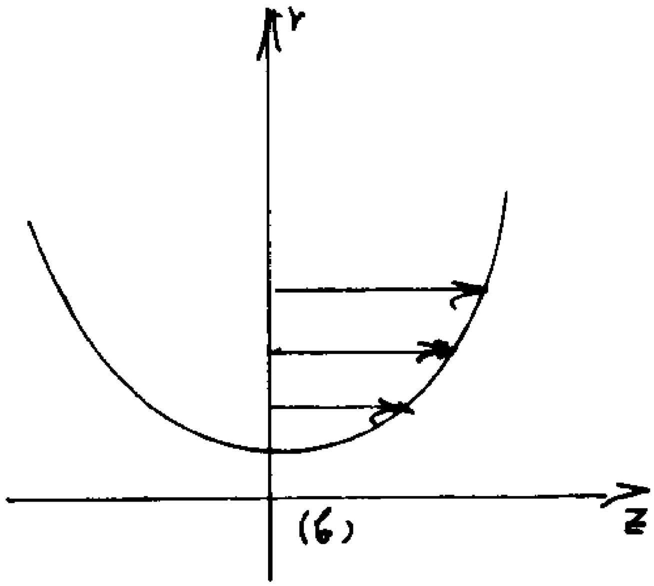


Fig. 15

Order of Double Integration



GROUP g	ρ_g (BOHR RADII)	ϕ_g (RADIANS)
1	$D/\sqrt{2}$	$\pi/4$
2	$D \cdot \sqrt{5/2}$	$\pi/10$
3	$D \cdot \sqrt{5/2}$	$2\pi/5$
4	$D \cdot \sqrt{3}/2$	$\pi/4$

Table I

Table of Sodium Parameters Taken From Figure 13

References Chapter 4

1. J.G.F. Francis, Comput. J. **4**, 265 (1961).

2. C. Kittel, "Introduction to Solid State Physics," 3rd Edition, John Wiley and Sons, New York (1968).

3. M. Abramowitz and I. Stegun, "Handbook of Mathematical Functions", Dover (1965).

4. D. Pines, "Elementary Excitations in Solids", Benjamin (1963).

5. D. Pines, Phys. Rev. **92**, 626 (1953).

6. H.A. Bethe and E.E. Salpeter, "Quantum Mechanics of One and Two Electron Atoms", Academic Press, New York (1957).

7. A. Messiah, "Quantum Mechanics", John Wiley and Sons, New York, (1961).

Chapter 5

Charge Capture

5.1 Introduction

In order to obtain the number of channeling pairs we need to consider capture rates by the stripped proton. That is, if an ionization occurs the beam can replenish its supply of hydrogen by having the protons capture electrons. Although for MeV energies of translation the capture rate is neglibible relative to the ionization rate, the capture process can become important as the energy is lowered. Therefore we shall consider in this chapter the formal theory of capture and some of its consequences for capture in a solid. In particular we shall consider capture from a sea of electrons in a Born approximation wave treatment and also capture from the cores in a Born approximation impact parameter treatment.

The reader might wonder why the capture process has not been included previously in the imaginary part of the optical potential. That is, if ionization implies a loss of electron flux and a negative definite imaginary potential, does not capture imply an increase of flux and so a positive definite imaginary potential? This is not correct since capture is not a coherent or quasi-coherent process. For an MeV proton an exchange of energy of the order of a few Kev is necessary to raise a valence electron into a bound state of the moving proton. Further for the capture from localized cores the energy necessary is even higher. Such processes are truely incoherent and so cannot be contained in channeling space. This implies further that a capture potential could not exist otherwise we would be adding amplitudes for capture processes. The absence of a capture potential is reflected in equation 2.4 (13).

5.2 Formal Theory

We wish to calculate the rate of capture of an electron by a proton passing through a solid. The solid consists of N electrons which of course obey the Pauli principle. In describing this process of capture we shall explicitly take into account antisymmetrization. Although the results we obtain could be termed intuitively obvious their derivation requires enough complexity to warrant a full trdatment here.

We describe the reaction in the center of mass frame for a proton of charge Z_1e, mass M and velocity $\vec{V}$ incident on a solid which is at rest. This initial state is

$$\chi_{\xi(i)} = \frac{e^{i\vec{P}_i\cdot\vec{R}}}{\sqrt{\Omega}}\, g_{\xi(i)}(1,2,\cdots,N)$$

where P_1 is the relative momentum of the two systems with separation $\vec{R}$ from the center of mass of the solid to the proton. The numbers 1, 2, ··N signify the space and spin coordinates of electrons 1, 2 through N the subscript notation ξ(i) means the projection of a state i onto the subspace totally antisymmetric in electronic coordinates. We are following reference 1 in the notation for identical particle. Ω is the quantization volume. Finally we point out that we are neglecting the Pauli principle for the heavier protons, which is valid for these energies. Our initial state satisfies

$$(E_i - H_i)\,\chi_{\zeta(i)} = 0 \qquad (1a)$$

where

$$H_i = -\frac{1}{2M}\nabla_R^2 + H_S(1,2,\cdots N) \qquad (1b)$$

$$H_S(1,2,\cdots N)\, g_{\zeta(i)} = \nu_i\, g_{\zeta(i)}$$

$$E_i = \frac{P_i^2}{2M} + \nu_i$$

A_i represents the Hamiltonian before interaction between the proton and solid. The interaction in this initial channel[+] of the reaction is defined by $V_i = H - H_i$ with H the full Hamiltonian. H_S above is the solid Hamiltonian.

In orbital form we can write

$$g_{\zeta(i)} = \frac{1}{\sqrt{N!}} \sum_P{}' (-1)^p P\, \gamma_1(1)\gamma_2(2)\cdots\gamma_N(N) \qquad (2)$$

where P is one of the N!. permitations of the coordinates and the states γ_i are eigenstates of a one-electron Hamiltonian used to describe the motion of an electron in the solid. The subscript in the state γ_1

[+] The use of the term refers to the assymptotic configurations in a reaction. It has nothing to do with channeling!

represents quantum numbers, say spin and wave number. The state given by equation 2 is normalized to unity as can easily be shown.

For the final channel we suppose an electron is captured from the state γ_1 and attaches itself to the proton in a bound state ϕ_b moving with momentum P_f. So

$$\chi_{\zeta(f)} = \frac{c}{N!} \sum_{Q}{}' (-1)^{Q} Q \left\{ \frac{e^{i P_f \cdot R_1'}}{\sqrt{\Omega}} \phi_b(1') \gamma_\zeta(2) \cdots \gamma_N(N) \right\}$$

The term in brackets represents the final state with electron number one captured. Then all permutations Q of the N electronic coordinates are taken. The coordinates are shown in figure 16.

Since

$$\vec{r}_1{}' = \vec{r}_1 - \vec{R}$$
$$\vec{R}_1{}' = \frac{M}{m+M}\vec{R} + \frac{m}{M+m}\vec{r}_1$$

we can write

$$\chi_{\zeta(f)} = \frac{e^{i P_f \cdot \frac{M}{m+M} \vec{R}}}{\sqrt{\Omega}} \frac{c}{N!} \sum_{Q}{}' (-1)^{Q} Q \left\{ e^{\frac{im}{m+M} \vec{r}_1 \cdot \vec{P}_f} \phi_b(1') \gamma_\zeta(2) \cdots \gamma_N(N) \right\} \quad (4a)$$

Further note that

$$\phi_b(1') \equiv \varphi_b(\vec{r}_1 - \vec{R})\,(\text{Spin})$$

and that the rest of the states are assumed to be unperturbed by the change in the assymptotic Hamiltonian of the solid due to the capture. Since N is large $(\sim 10^{22}\,\text{cm}^{-3})$ this is a good approximation. Our state $\chi_{\zeta(f)}$ does not satisfy a reaction channel equation as $\chi_{\zeta(1)}$ did (equation 1a), but each of its separate permutations satisfy

$$\left\{ E_f - Q H_f Q^{-1} \right\} \chi_{Q(f)} = 0 \qquad (5a)$$

$$\chi_{Q(f)} = Q \left\{ e^{i \vec{P}_f \cdot \frac{M}{m+M} \vec{R}} \, e^{i \frac{m}{m+M} \vec{r}_1} \phi_1(1') \gamma_2(2) \cdots \gamma_N(N) \right\} \qquad (5b)$$

$$H_f = -\frac{1}{2(m+M)} \nabla^2_{R_1'} - \frac{1}{2\mu} \nabla^2_{r_1'} - \frac{Z_1 e^2}{r_1'} + H_s(2,3,\cdots,N) \qquad (5c)$$

$$E_f = \frac{P_f^2}{2(m+M)} - W_b + \nu_f \qquad (5d)$$

$$\left(-\frac{1}{2\mu} \nabla^2_{r_1'} - Z_1 e^2 / r_1' \right) \phi_b(1') = -W_b \, \phi_b(1') \qquad (5e)$$

and

$$\mu = \frac{mM}{m+M}$$

H_f is the Hamiltonian for the final channel in which the proton-electron system is not in interaction with the solid. If we consider final states in which the proton is in the solid then the coulomb potential in 5c and 5e is supplemented by our optical potential. In either case the interaction in the final channel is obtained by

$$V_f = H - H_f$$

If we write

$$\chi_{s(f)} = \frac{e^{i \vec{P}_f \cdot \frac{M}{m+M} \cdot \vec{R}}}{\sqrt{\Omega}} \, g_{s(f)} \qquad (6a)$$

$$g_{s(f)} = \frac{c}{N!} \sum_Q{}' (-1)^Q \left\{ \tilde{\varphi}_b(1') \gamma_2(2) \cdots \gamma_N(N) \right\} \qquad (6b)$$

$$\tilde{\varphi}_b(1') = e^{i \frac{m}{m+M} \vec{P}_f \cdot \vec{r}} \, \phi_b(1') \qquad (6c)$$

then the normalization of χ_f to unity implies that the constant C in 6b be chosen so that

$$\langle g_{\zeta(f)}, g_{\zeta(f)} \rangle = 1$$

on

$$1 = \frac{C^2}{N!} \int d\tau_1 \cdots d\tau_N \left[\left(1 - \sum_{j=2}^{N}{}' X_{1j}\right) \left[\tilde{\phi}_b^*(1') \gamma_2^*(2) \cdots \gamma_N^*(N) \right] \hat{\phi}_b(1') \gamma_2(2) \cdots \gamma_N(N) \right] \quad (7)$$

where $d\tau_1$ etc. are generalized spin-space volume elements and X_{1j} is an operator which exchanges coordinates 1 and j. For example X_{12} would place electron 2 in the outgoing proton and electron 1 in the state γ_2. Using the orthonormality of the set γ_i we find that equation 7 becomes

$$1 = \frac{C^2}{N!} \left(1 - \sum_{j=2}^{N}{}' \left| \int d\tau \, \phi_b^* \gamma_j \right|^2 \right) \simeq \frac{C^2}{N!}$$

The approximately equal sign above follows from the fact that the overlap between the outgoing electron bound to the proton and a solid state is vanishingly small for large separation although not strictly so. The fact that these states are not strictly orthogonal follows from the fact that they are eigenstates of different Hamiltonians. So our final state in this approximation can be written

$$\chi_{\zeta(f)} = \frac{1}{\sqrt{N!}} \sum_{Q} (-1)^Q Q \left\{ \frac{e^{i P_f \cdot R_1'}}{\sqrt{\Omega}} \phi_b(1') \gamma_2(2) \cdots \gamma_N(N) \right\} \quad (8)$$

The scattering which grows out of the State $\chi_{\xi(i)}$ is denoted by $\Psi^+_{\zeta(i)}$ and satisfies the Lippman Schwinger equation$^{(1)}$

where the limit $\eta \to 0$ is taken after all transition rates are calculated. We write

$$\chi_{S(i)} = \frac{1}{\sqrt{N!}} \sum_{P}{}' (-1)^P P \chi_i \equiv \frac{1}{\sqrt{N!}} \sum_{P}{}' (-1)^P \chi_{P(i)} \qquad (10)$$

(where again χ_i is the unsymmetrized initial state and $\chi_{P(i)}$ is the P permutation of the coordinates of that state). Further from

$$H_i \chi_i = E_i \chi_i$$

we obtain on multiplying by P

$$H_{P(i)} \chi_{P(i)} = E_i \chi_{P(i)}$$
$$H_{P(i)} \equiv P H_i P^{-1}$$

Now

$$\frac{i\eta}{E_i + i\eta - H} \chi_{P(i)} = \frac{1}{E_i + i\eta - H} \left[i\eta + E_i - H_{P(i)} \right] \chi_{P(i)}$$
$$= \frac{1}{E_i + i\eta - H} \left[i\eta - E_i - H + V_{P(i)} \right] \chi_{P(i)}$$
$$= \left\{ 1 + \frac{1}{E_i + i\eta - H} V_{P(i)} \right\} \chi_{P(i)}$$

Substituting this into 10 we find

$$\psi^{+}_{S(i)} = \frac{1}{\sqrt{N!}} \sum_{P}{}' (-1)^P \psi^{+}_{P(i)} \qquad (11a)$$

$$\psi^{+}_{P(i)} = \left(1 + \frac{1}{E_i + i\eta - H} V_{P(i)} \right) \chi_{P(i)} \qquad (11b)$$

So we find that each permuted state satisfies its own Lippman Schwinger equation and the total amplitude equation 11a is the sum of the amplitude for each permutation with the phase specified by the Pauli principle.

We now transform equation 11 so that we can obtain a rearrangement amplitude. To do this we first use the identity for two operators A and B

$$\frac{1}{A}-\frac{1}{B}=\frac{1}{A}(B-A)\frac{1}{B}=\frac{1}{B}(B-A)\frac{1}{A}$$

to obtain

$$\frac{1}{E_i+i\eta-H}-\frac{1}{E_i+i\eta-H_{Q(f)}}=\frac{1}{E_i+i\eta-H_{Q(f)}}V_{Q(f)}\frac{1}{E_i+i\eta-H}$$

where we used

$$H=H_f+V_f=QH_fQ^{-1}+QV_fQ^{-1}=H_{Q(f)}+V_{Q(f)}$$

Then equation 11b becomes

$$\psi^+_{P(i)}=\chi_{P(i)}+\frac{1}{E_i+i\eta-H_{Q(f)}}V_{P(i)}\chi_{P(i)}+\frac{1}{E_i+i\eta-H_{Q(f)}}V_{Q(f)}\left[\psi^+_{P(i)}-\chi_{P(i)}\right]$$

$$\psi^+_{P(i)}=\frac{i\eta}{E_i+i\eta-H_{Q(f)}}\chi_{P(i)}+\frac{1}{E_i+i\eta-H_{Q(f)}}V_{Q(f)}\psi^+_{P(i)} \qquad (12)$$

Using equation 12 in 11 we obtain

$$\psi^+_{S(i)}=\frac{1}{\sqrt{N}}\sum_P{}'(-1)^P\left\{\frac{i\eta}{E_i+i\eta-H_{Q(f)}}\chi_{P(i)}e^{-iE_it}+\frac{1}{E_i+i\eta-H_{Q(f)}}V_{Q(f)}\psi^+_{P(i)}e^{-i(E_i+i\eta)t}\right\} \qquad (13)$$

By putting 11 in this form it is clear that we can obtain the amplitude for a transition to a particular eigenstate contained in the channel

Q(f). That is the propagator (Green's function) for this channel

$$\frac{1}{E_i + i\eta - H_{\alpha(f)}}$$

was explicitly extracted. In equation 13 we have turned the potential on adiabatically so there is no . scattered wave as t → − ∞. We are using this damping device only for convenience. Both a wave packet treatment and the method of Gellman and Goldberger is given in reference 1 for obtaining the transition rates or cross sections. A time independent treatment is given by 2. The transition probability given by 13 is

$$P(i\to f) = |< \chi'_{\zeta(f)}(t), \psi^{+}_{\zeta(i)}(t) >|^2$$

since our states we normalized to unity. We then find

$$P(i\to f) = e^{2\eta t} |< \chi'_{\zeta(f)}(t), \psi^{scatt}_{\zeta(i)}(t) >|^2$$

where Ψ^{scatt} is the second term in 13. The first vanishes in the limit $\eta \to 0$ if $\langle \chi_{\alpha(f)}, \chi_{\zeta(i)} \rangle$ is finite. This is clear on physical grounds if we suppose these states are really wave packets and well separated. A mathematical proof is discussed in reference 2. The transition rate is

$$\frac{dP(i\to f)}{dt} = 2\eta\, e^{2\eta t} \left| \langle \chi'_{\zeta(f)}, \psi^{S}_{\zeta(i)} \rangle \right|^2$$

Using equation 13 we get

$$\langle \chi_{\zeta(f)}, \psi^{S}_{\zeta(i)} \rangle = \frac{1}{N!} \sum_{PQ} (-1)^{P+Q} \frac{1}{E_f + i\eta - E_i} \langle \chi_{Q(f)}, V_{Q(f)} \psi^{+}_{P(i)} \rangle$$

So

$$\dot{P}_{if} = \frac{dP_{if}}{dt} = \lim_{\eta \to 0} \frac{\eta}{(E_f - E_i)^2 + \eta^2} \left| T_{fi} \right|^2$$

Using

$$\lim_{\eta \to 0} \frac{2\eta}{x^2 + \eta^2} = 2\pi\, \delta(x)$$

we find

$$\dot{P}_{if} = 2\pi \left| T_{fi} \right|^2 \delta(E_f - E_i)$$

where

$$T_{fi} \equiv \frac{1}{N!} \sum_{PQ}{}' (-1)^{P+Q} \langle \chi_{Q(f)}, V_{Q(f)} \psi^{+}_{P(i)} \rangle$$

$$T_{fi} = \frac{1}{N!} \sum_{PQ}{}' (-1)^{P+Q} \langle Q^{-1} Q \chi_f, V_f\, Q^{-1} P \psi^{+}_{i} \rangle$$

Let $Q^{-1}P = R$ then

$$T_{fi} = \frac{1}{N!} \sum_R{}' (-1)^R \langle \chi_f , V_f \psi^+_{R(i)} \rangle \sum_a{}' 1$$

$$T_{fi} = \sum_p{}' (-1)^P \langle \chi_f , V_f \psi^+_{P(i)} \rangle \qquad (15)$$

This is the post form for the scattering amplitude. It says propagate the $P^{\underline{th}}$ permutation of the initial state. Then the amplitude is governed by the final state interaction. All the permutations on the initial state are taken and the amplitudes summed coherently with proper phases.

We shall spare the reader further tedium and simply note that the prior form of the transition matrix can be shown to be ( )

$$T_{fi} = \sum_Q{}' (-1)^Q \langle \psi^{(-)}_{Q(f)} , V_i \chi_i \rangle \qquad (16)$$

Under the condition that $(E_f = E_i)$ and,

$$\psi_f^{(-)} = \chi_f + \frac{1}{E_f - i\eta - H_f} V_f \psi_f^{(-)}$$

We are now in a position to obtain the Born approximation for capture. However, there is one important step we must take.

One of the classic difficulties with the capture problem is the following. Consider for concreteness protons on hydrogen. Then we find that formally the proton-proton interaction contributes to the capture rate. This occurs because of the non orthoginality between the initial and final states. This is rather surprising since the proton proton interaction exerts a force on the electron only indirectly through recoil. In fact Brinkinan and Kramers(3) neglected it on physical in their calculation of capture from Hydrogen in the Bern approximation. However, Jackson and Schiff(4) showed that they could lower the cross section closer to the experimental result by including the proton-proton interaction. This apparent contradiction has been answered by many workers in atomic physics including Butes, Guerjoy and Mittleman. What we do essentially is remove elastic scattering first. We shall follow Mittleman(3) in writing

$$\psi_{c_i}^{+} \equiv \pi_i \psi_i^{(+)}$$

where π_i is a projection operator onto the elastic channel. From

$$\psi_i^{(+)} = \chi_i + \frac{1}{E_i + i\eta - H_i} V_i \psi_i^{(+)}$$

we get

$$\psi_{c_i}^{+} = \chi_i + \frac{1}{E_i + i\eta - H_i} \pi_i V_i \psi_i \qquad (17)$$

But ψ_{c_i} by definition is the elastic scattering state so it should satisfy

$$\psi_{c_i}^{+} = \chi_i + \frac{1}{E_i + i\eta - H_i} U_i \psi_{c_i}^{+} \qquad (18)$$

where U_i is an appropriate optical potential which produces this elastic scattering. From 17 and 18 we get

$$\pi_i \, V_i \, \psi_i^{+} = U_i \, \psi_{c_i}^{+} \qquad (19)$$

But if we consider the scattering in the two potentials U_i and $V_i - U_i$ we find$^{(1)}$

$$T_{fi} = T_{fi}^{\text{elastic}} + \sum_{Q}{}' (-1)^{Q} \langle \psi_{Q(f)}^{(-)}, (V_i - U_i) \, \psi_{c_i}^{+} \rangle \qquad (20)$$

and this is equivalent to the scattering in V_i. Since T_{fi}^{elastic} is zero for capture we find on using '9 in 20

$$T_{fi} = \sum_{G}{}' (-1)^{Q} \langle \psi_{Q(f)}^{(-)}, [V_i, \pi_i] \, \psi_i^{(+)} \rangle \qquad (21)$$

where $[A, B] \equiv AB - BA$ and we get further

$$T_{fi}^{\text{BORN}} = \sum_{G}{}' (-1)^{Q} \langle \chi_{Q(f)}, [V_i, \pi_i] \, \chi_i \rangle \qquad (22)$$

In our case V_i is the interaction of the proton with the N electron solid and

$$\pi_i = |\gamma_1(1)\rangle\langle\gamma_1(1)| \cdots |\gamma_N(N)\rangle\langle\gamma_N(N)|$$

We note that the terms in the potential V_i which do not contain electron coordinates commute with π_i and therefore do not contribute to the T matrix. So for V_i we need consider only

$$\sum_{j=1}^{N_1}{}' \frac{Z_1 e^2}{|\vec{R}-\vec{r}_j|}$$

in evalutating equation 22.

We consider first

$$\sum_{Q}{}'(-1)^{Q} \left\langle \chi_{Q(F)}, \left[\frac{-Z_1 e^2}{|\vec{R}-\vec{r}_1|}, \Pi_i\right] \chi_i \right\rangle \tag{23}$$

The direct term of equation 23 reads

$$\left\langle P_f \frac{M}{m+M} \varphi_b, \left[\frac{-Z_1 e^2}{|\vec{R}-\vec{r}_1|}, \Pi_{k_1}(\vec{r}_1)\right] P_i \gamma_{k_1}(\vec{r}_1) \right\rangle$$

where the spin inner product has been taken and for example

$$\left| \frac{M}{m+M} P_f \varphi_b \right\rangle = \frac{1}{\sqrt{\Omega}} e^{i \frac{M}{m+M} \vec{P}_f \cdot \vec{R}} \varphi_b(\vec{r}_1-\vec{R})$$

and in equation 24 the integration is over $\vec{R}$ and $\vec{r}$. The only other terms that can contribute to 23 are the exchange terms

$$\sum_{j=2}^{N/2}{}' \left\langle P_f \frac{M}{m+M} \varphi_b(\vec{r}_2-\vec{R}) \gamma_{k_j}(\vec{r}_1) \left[\frac{-Z_1 e^2}{|\vec{r}_1-\vec{R}|}, \Pi_{k_1}(\vec{r}_1)\right] P_i \gamma_{k_1}(\vec{r}_1) \gamma_{k_j}(\vec{r}_2) \right\rangle$$

Further if we consider any of the other potentials for example

$$\frac{-Z_1 e^2}{|\vec{r}_2-\vec{R}|}$$

i.e. the ones that contain coordinates other than $\vec{r}_1$, we find that the direct term of equation 23 reads

$$\left\langle P_f \frac{M}{m+M} \varphi_b(\vec{r}_1-\vec{R}) \gamma_{k_2}(r_2) \left[\frac{-Z_1 e^2}{|r_2-R|}, \Pi_{k_2}(r_2)\right] P_i \gamma_{k_1}(\vec{r}_1) \gamma_{k_2}(r_2) \right\rangle$$

This is the difference of two identical terms and so vanishes. The exchange term would read

$$\langle \vec{P}_f \frac{M}{m+M}\, \tilde{\varphi}_b(\vec{r}_2-\vec{R})\gamma_{k_2}(r_1)\left[\frac{-Z_1e^2}{|\vec{r}_2-\vec{R}|}, \Pi_{k_2}(\vec{r}_2)\right]P_i\,\gamma_{k_1}(\vec{r}_1)\gamma_{k_2}(\vec{r}_2)\rangle$$

and vanishes since the orbitals γ_j are orthoginal. So for all potentials other than the interaction between the proton and electron 1 the transition matrix vanishes. This should not be surprising since potentials that do not contain the coordinate $\vec{r}_1$ cannot exert forces on electron one.

Putting the above together we get for the Born approximation to the transition matrix

$$T_{fi}^{B} = \int d^3R\, d^3r_1 \frac{e^{-i\vec{P}_f\cdot\frac{M}{m+M}\vec{R}}}{\sqrt{\Omega}} e^{-i\vec{P}_f\cdot\frac{m}{m+M}\vec{r}_1}\varphi_b^*(\vec{r}_1-\vec{R})\left(\frac{-Z_1e^2}{|r_1-R|}\right)\frac{e^{i\vec{P}_i\cdot\vec{R}}}{\sqrt{\Omega}}\gamma_{k_1}(\vec{r}_1)$$

$$-\int d^3R\, d^3r_1\, d^3r_2 \frac{e^{-i(\vec{P}_f\frac{M}{m+M}-\vec{P}_i)\cdot\vec{R}}}{\sqrt{\Omega}} e^{-i\vec{P}_f\frac{m}{m+M}\cdot\vec{r}_1}\varphi_b^*(\vec{r}_1-\vec{R})\gamma_{k_2}(\vec{r}_2)\gamma_{k_1}^*(\vec{r}_1)\frac{-Z_1e^2}{|\vec{r}_1-\vec{R}|}\gamma_{k_1}(r_1)$$

$$-\sum_{j=2}^{N/2}\int d^3R\, d^3r_1\, d^3r_2 \frac{e^{-i(\vec{P}_f\frac{M}{m+M}-\vec{P}_i)\cdot\vec{R}}}{\Omega} e^{-i\vec{P}_f\cdot\vec{r}_1\frac{m}{m+M}}\varphi_b^*(\vec{r}_2-\vec{R})\gamma_{k_j}(\vec{r}_2)\gamma_{k_1}^*(\vec{r}_1)\frac{(-Z_1e^2)}{|\vec{r}_1-\vec{R}|}\cdot\gamma_{k_1}(r_1)$$

The first two terms are the direct reactions, the last term is the exchange reaction. Only one term of the exchange reaction survived since the second term of the commutator in 23 vanishes for the exchange term. In the above result for T_{fi}^{B} the second term corresponds to the interproton potential.

It is advantageous to write T_{fi}^{B} above in a more condensed notation

$$T_{fi}^{B} = \frac{1}{\Omega}\Big\{\langle \vec{P}_f \tfrac{M}{m+M} \,|\, \langle \tilde{\varphi}_b V \gamma_{k_1}\rangle_{\vec{R}} \,|\, \vec{P}_i\rangle - \langle \vec{P}_f \tfrac{M}{m+M} \,|\, \langle \tilde{\varphi}_b \gamma_{k_1}\rangle_{R} \langle \gamma_{k_1} V \gamma_{k_1}\rangle_{\vec{R}} \,|\, \vec{P}_i\rangle$$

$$- \sum_{j=2}^{N_1}{}' \langle \vec{P}_f \tfrac{M}{m+M} \,|\, \langle \tilde{\varphi}_b \gamma_{k_j}\rangle_{\vec{R}} \langle \gamma_{k_j} V \gamma_{k_1}\rangle \,|\, \vec{P}_i \rangle \Big\} \qquad (25)$$

where V is the potential between electron and proton which in spatial coordinates $-Z_1 e^2/|r-R|$, $\tilde{\varphi}_b$ is the final electron bound state boosted by its translational velocity which in spatial coordinates is $e^{i\vec{p}_f \cdot \frac{m}{m+M}\vec{r}}\,\varphi_b(r_1-R)$. The bracket $\langle\ ,\ \rangle_R$ means the inner product which is an integral over $\vec{r}$ still depends upon R and the outer bracket is the Fourier transform

$$\int d^3R\ e^{-i\left(\vec{P}_f \frac{M}{m+M} - \vec{P}_i\right)\cdot\vec{R}}\ \langle\ ,\ \rangle_{\vec{R}}$$

We note that the last two terms in equation 25 can be written

$$\langle \vec{P}_f \tfrac{M}{m+M} \,|\, \sum_{j=1}^{N_1}{}' \langle \tilde{\varphi}_b \gamma_{k_j}\rangle_R \langle \gamma_{k_j} V \gamma_{k_1}\rangle \,|\, \vec{P}_i \rangle$$

From the resolution of the identitiy

$$1 = \sum_{\vec{k}}{}' |\gamma_{\vec{k}})(\gamma_{\vec{k}}| = \Big(\sum_{k<k_F}{}' + \sum_{k>k_F}{}'\Big) |\gamma_{\vec{k}})(\gamma_{\vec{k}}|$$

where $\vec{k}_F$ is a vector to the Fermi surface, we find for the last two terms in 25

$$\langle \vec{P}_f \tfrac{M}{m+M} \,|\, \langle \tilde{\varphi}_b , \Big(1-\sum_{k>k_F}{}' |\gamma_k\rangle\langle\gamma_k| V |\gamma_{k_1}\rangle_{\vec{R}} \,|\, \vec{P}_i \rangle$$

Adding this to the first term in equation 25 we get

$$T_{fi}^{B} = \langle \vec{P}_f \tfrac{M}{m+M} \,|\langle \varphi_b , \sum_{k>k_F}{}' \gamma_k\rangle\langle\gamma_k , V \gamma_{k_1}\rangle_{\vec{R}} \,|\, \vec{P}_i \rangle \qquad (26\,a)$$

or

$$T_{fi}^{B} = \langle \vec{P}_f \tfrac{M}{m+M} \,|\, \langle \varphi_b \,(1-P_0)\, V\gamma_{k_1}\rangle_{\vec{R}} \,|\, \vec{P}_i \rangle \qquad (26\,b)$$

$$P_0 \equiv \sum_{k<k_F}{}' |\gamma_{\vec{k}}\rangle\langle\gamma_{\vec{k}}|$$

Expression 26 a says that an electron in the orbital state (Block State) $\vec{k}_1$ is scattered out of the Fermi sea into another Block State by its interaction with the proton. The overlap of this latter state with the final bound state of interest is the amplitude for the process in $P_f \frac{M}{m+M} - P_i$ space. The expression 26 b says that the potential kicks an electron into a final bound state which is orthogonal to all the initial filled states. The $\left(P_f \frac{M}{m+M} - P_i\right)$ transform is then taken. The orthogonality more clearly expressed by 26 b has been built into the theory by the use of the commutators above. These results, 26 (a) and 26 (b) while intuitively satisfying, follow from the use of both the antisymmetrization of the scattering state and the commutator formalism of Mittleman. It was for this reason that we laboriously derived the scattering amplitude taking into account autisymmetrization.

In the calculations that follow we shall drop the term P_0. The error we introduce is of order

$$\langle \tilde{\varphi}_b , \gamma_{\vec{k}} \rangle = \int \varphi_b^{*} (\vec{r}_1 - \vec{R}) e^{-i \vec{P}_f \cdot \frac{m}{m+M} \cdot \vec{r}} e^{i \vec{k} \cdot \vec{r}} \, d^3 r \qquad ; k < k_F$$

This matrix element measures the overlap between the final state boosted by the electron's transitional momentum in that state and a free state of the order of a Fermi momentum. If our final pair has an energy of the order of an MeV we expect this overlap to be small. Specifically

$$\langle \tilde{\varphi}_b , \gamma_{\vec{k}} \rangle = \frac{1}{(2\pi)^3} \int d^3p \, d^3r \, e^{i \vec{p} \cdot \vec{R}} \hat{\varphi}_b (\vec{p}) e^{-i \left(\vec{p} + \vec{P}_f \frac{m}{m+M} \right) \vec{r}} e^{i \vec{k} \cdot \vec{r}}$$

$$= \frac{1}{(2\pi)^3} \int e^{i \left(\vec{p} - \vec{P}_f \frac{m}{m+M} \right) \vec{R}} \hat{\varphi}_b^{*} \left(\left| \frac{\vec{P}_f m}{m+M} - \vec{p} \right| \right) e^{i (\vec{k} - \vec{p}) \vec{r}}$$

$$= e^{i \left(\vec{k} - \vec{P}_f \frac{m}{m+M} \right) \cdot \vec{R}} \hat{\varphi}_b^{*} \left(\left| \frac{\vec{P}_f m}{m+M} - \vec{k} \right| \right)$$

Now $\hat{\varphi}_b$ goes to zero for[†]

$$\left|\frac{\vec{P}_f m}{m+M} - \vec{k}\right| \gg \frac{1}{a_0}$$

and so this matrix element $\langle \varphi_b \, V_b \rangle$ is negligible for

$$P_f > 10^3 k_F$$

But for an MeV proton

$$P_f \sim 10\,(10^3 k_F)$$

and so this is satisfied in our case. So we shall drop the second term in 26 b and our Born-Brinkman-Kramers amplitude becomes

$$T_{fi}^{B} = \frac{1}{\Omega}\int d^3r_1\, d^3R\; e^{-i(\vec{P}_f \frac{m}{m+M} - \vec{P}_i)\cdot\vec{R}}\, e^{-i\vec{P}_f \frac{m}{m+M}\vec{r}_1}\, \varphi_b^*(\vec{r}_1-\vec{R})\frac{(-Z_1e^2)}{|\vec{r}_1-\vec{R}|}\,\chi_1(\vec{r}_1)$$

We now chang to $\vec{r}_1$ and $\vec{r}_1{}'$ as the independent variable rather than $\vec{r}_1$, $\vec{R}$. With the substitution

$$\vec{R} = \vec{r}_1 - \vec{r}_1{}'$$

we get

$$T_{fi}^{B} = \frac{1}{\Omega}\left(\int d^3r\, e^{-i(\vec{P}_f-\vec{P}_i)\cdot\vec{r}}\,\chi_k(\vec{r})\right)\left(-Z_1e^2\int d^3r'\, e^{i(\frac{M}{m+M}\vec{P}_f-\vec{P}_i)\vec{r}\,'}\,\frac{\varphi_b^*(r')}{r'}\right)$$

[†] Only capture with 1S or 2S will be necessary.

Defining

$$\gamma_k(p) = \int d^3r \; e^{-i\vec{p}\cdot\vec{r}} \, \gamma_k(\vec{r}) \qquad (27a)$$

$$\Phi(p) = \int d^3r \; e^{-i\vec{p}\cdot\vec{r}} \left(-\frac{z_1 e^2}{r} \varphi_b(r) \right) \qquad (27b)$$

we obtain for the capture from the state $\vec{k}$

$$|T_{fi}^B|^2 = \frac{1}{\Omega^2} \, |\gamma_k(\vec{P}_f - \vec{P}_i)|^2 \, \left| \Phi\left(\frac{M}{m+M}\vec{P}_f - \vec{P}_i \right) \right|^2 \qquad (28)$$

We will then use this with

$$\dot{P}_{fi} = 2\pi \, |T_{fi}^B|^2 \, \delta(E_f - E_i)$$

in

$$\dot{P} = \Big\langle \sum_{\substack{\text{final} \\ \text{States}}}' \dot{P}_{fi} \Big\rangle_{\substack{\text{Average of} \\ \text{initial spins}}}$$

to obtain the rate

$$\dot{P} = \sum_{\vec{k}, \vec{P}_f, \sigma_f}' \dot{P}_{fi} \qquad (29)$$

since the spin average is unity.

5.3 Capture of a Valence Electron

In this section we consider the capture of valence electrons by the stripped atom. That is we are interested in the rate of increase of electronic density bound to the incident proton. At first we might try a free electron model for the valence electrons. This will not work since a proton cannot capture a free electron. Capture is possible only if there is a deviation from plane wave motion for the electron. This deviation will be supplied by the lattice interaction with the electron. Since we are interested in an order of magnitude for this rate we shall use the simplest approach possible by using an effective mass approximation to account for the lattice.

First we convince ourselves that a free electron cannot be captured by a proton. We look at the transition rate derived in section 5.2,

$$\frac{dP}{dt} = 2\pi \frac{2}{\Omega} \int \frac{d^3P_f}{(2\pi)^3} \sum_{k<k_F}{}' \left|\gamma_k(\vec{P}_f - \vec{P}_i)\right|^2 \left|\Phi\left(\frac{m}{m+M}\vec{P}_f - \vec{P}_i\right)\right|^2 \delta(E_f - E_i) \tag{1}$$

where Ω is the volume of the solid and γ_k is a free electron or in the general case a Block State. If we write

$$\gamma_k(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{\Omega}} \tag{2}$$

we find that

$$\gamma_k(\vec{P}_i - \vec{P}_f) = \sqrt{\Omega}\, \delta_{k,\vec{P}_i - \vec{P}_f} \tag{3}$$

so that the argument of the delta functions in equation 1

$$E_i - E_f = \left(\frac{p_i^2}{2M} + \frac{k^2}{2m} \right) - \left(\frac{p_f^2}{2(m+M)} - W \right)$$

must be evaluated at $\vec{k} = \vec{p}_f - \vec{p}_i$, so

$$E_i - E_f = \frac{M}{2(m)(m+M)} \left\{ \left(\vec{p}_f - \frac{m+M}{M} \vec{p}_i \right)^2 + \frac{2m(m+M)}{M} W \right\}$$

Therefore the rate becomes

$$\frac{dP}{dt} = 2\pi \cdot 2 \quad \frac{2m(m+M)}{M} \int d^3\beta \, \left| \Phi\left(\frac{M}{m+M} \vec{\beta} \right) \right|^2 \delta(\beta^2 - \beta_0^2) \tag{4}$$

where

$$\vec{\beta} \equiv \vec{p}_f - \frac{m+M}{M} \vec{p}_i \tag{5a}$$

$$\beta_0^2 = \frac{2m(m+M)}{M} W \tag{5b}$$

Since W > 0 for any bound state[+] we see that the delta functions in 4 can never be satisfied and so P vanishes. This result comes from the fact that energy and momentum cannot be conserved simultaneously for this capture of a free electron. This can be seen in even a more compelling way be viewing the collision of a free electron and proton in their center of mass frame. Then the total initial momentum in that frame is zero by definition and the total energy is greater than zero. After the pair sticks

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[+] Since −W is the ionization energy.

together their centers of mass must remain at rest to conserve momentum and therefore the pair has no translational energy. But to be in a bound state their relative energy must be less than zero and so energy cannot be conserved.

We would like to obtain in this section an estimate of the magnitude of the capture rate from the valence band. We shall assume we have a simple metal at absolute zero with a narrow band such as one of the alkali metals. Therefore we shall represent the electron in the state $\vec{k}$ by the energy relation

$$\epsilon(\vec{k}) = \frac{1}{2m^*} k^2 \qquad (6)$$

where m^* is called the effective mass. That the dynamics of an electron in a lattice can be represented by a single number, m^*, or in more complicated cases by a tensor, is a well known solid state approximation. The reader will find a discussion of this approximation in reference 6 where it is further shown that the representation in equation 3 is apt. This follows both from the features of the energy bands and the fact that the Fermi surface is nearly spherical. This approximation need not be pushed too far. It will however give us an order of magnitude for the capture rate. For more complex metals or more exact solutions we might turn to a perturbation treatment for the state of the valence electron. However, the rate is then a second order process and does not lead to a simple treatment.

The relationship 3 follows from the one-electron Schroedinger equation

$$\frac{-\nabla^2}{2m^*}\chi_{\vec{k}}(\vec{r}) = \epsilon(k)\chi_{k}(\vec{r})$$

where the constant background potential has been set to zero. Then

$$\chi_{k}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{\Omega}}$$

so

$$\chi_{\vec{k}}(\vec{P}) = \sqrt{\Omega}\,\delta_{\vec{k},\vec{P}} \tag{7}$$

The argument of the delta function in equation 1 then becomes

$$E_i - E_f - \left[\frac{P_i^2}{2M} + \frac{1}{2m^*}(\vec{P}_f - \vec{P}_i)^2\right] - \left[\frac{P_f^2}{2(m+M)} - W\right] \tag{8}$$

We should note that the final energy does not contain the effective mass m^* but rather the base mass m. We understand that after being captured the active electrons response to the lattice has changed radically. The dynamics of this interaction is now contained in the number W characterizing the eigenvalue of the bound state. Obtaining this number has been one of the primary results of this investigation. We shall return to it in the next chapter, however, it should be abundently clear already that the interaction of the electron with the lattice in this final state is contained in W. We now, being guided by the results of the free electron case, from the vector

$$\vec{\beta} = \vec{P}_f - \left(\frac{m+M}{M-\Delta}\right)\vec{P}_i \tag{9}$$

where

$$\Delta = m^{*} - m \tag{10}$$

Substituting 9 into 8 and then 8 and 7 into 1, we get for $|\vec{P}_1 - \vec{P}_f| > k_F$

$$dP/dt = 0 \tag{11a}$$

and for $|\vec{P}_1 - \vec{P}_f| < k_F$

$$\frac{dP}{dt} = 2 \frac{2m^{*}(m+M)}{(M-\Delta)} \int \frac{d^3\beta}{(2\pi)^3} \left|\Phi\left(\frac{M}{m+M}\vec{\beta}\right)\right|^2 \delta(\beta^2 - \beta_0^2) \tag{11b}$$

where

$$\beta_0^2 = \frac{2m^{*}(m+M)}{(M-\Delta)} \left(\frac{P_i^2}{2}\frac{\Delta}{M(M-\Delta)} - W\right) \tag{12}$$

We assume that the replacement

$$|\Phi(\vec{\beta})|^2 \rightarrow |\Phi(|\vec{\beta}|)|^2 \tag{13}$$

can be made. For s states this is clearly true as can be seen by looking at equation 5.2 (27b). For non-s states we take a sum over final azmuthal quantum number. It is then not hard to prove that the replacement in 13 holds for the sum over azmuthal quantum numbers. With the understanding that for non-s states $|\Phi|^2$ is a sum over azmuthal quantum numbers equation 11 becomes

$$\frac{dP}{dt} = \frac{2m^{*}(m+M)}{M-\Delta} \frac{\beta_0}{(2\pi)^2} \left|\Phi\left(\frac{M}{m+M}\beta_0\right)\right|^2 \int d\cos\alpha \tag{14}$$

where we used

$$\delta(x^2-c^2) = \frac{1}{2|c|}\,\delta(x-c) + \frac{1}{2|c|}\,\delta(x+c)$$

and

$$\cos\alpha = \hat{P}_i \cdot \hat{P}_f \tag{15}$$

We note that according to 12 the rate need not vanish since β_0^2 can be greater than zero. We first assume that this is so. Then the rates is given by 14 with the angle α integrated over the region shown in figure 17. This constraint on α follows from the definition 9 and the condition for equation 11a.[+] From figure 17 we deduce the limits for the α integral,

$$\cos\alpha_{MAX} = \mu_{MIN} = -1$$

$$\cos\alpha_{MIN} = \mu_{MAX} = k_F^2$$

where

$$\mu = \cos\alpha$$

Then we find for the transition rate

$$\frac{dP}{dt} = \frac{2\,m^*(m+M)}{M-\Delta}\,\frac{\beta_0}{(2\pi)^2}\left|\Phi\left(\frac{M}{m+M}\beta_0\right)\right|^2 (\text{phase space factor}) \tag{16a}$$

[+] We are assuming the Fermi surface is on a sphere.

$$\begin{pmatrix}\text{phase space}\\ \text{factor}\end{pmatrix} = \begin{cases} 0 & \text{for } k_F < \left|\frac{m^*}{M-\Delta} P_i - \beta_0\right| \\[2ex] \dfrac{k_F^2 - \left(\beta_0 - \frac{m^*}{(M-\Delta)} P_i\right)^2}{2\beta_0 \frac{m^*}{M-\Delta} P_i} & \text{for } \left|\frac{m^*}{M-\Delta} P_i - \beta_0\right| < k_F < \left|\frac{m^*}{M-\Delta} P_i + \beta_0\right| \\[2ex] 2 & \text{for } k_F > \left|\frac{m^*}{M-\Delta} P_i + \beta_0\right| \end{cases} \tag{16b}$$

with the further understanding that the rate vanishes for $|\vec{P}_1 - \vec{P}_f| > k_F$ and $\beta_0^2 < 0$. The first condition in 16b comes about from the separation of the spheres in figure 17. The value $\left|\left(\frac{m^*}{M-\Delta} P_1 - \beta_0\right)\right|$ thus corresponds to the minimum k_F or the minimum electronic density for which the solid can support capture.

Since the total capture cross section is given by the capture rate divided by the incident flux we find

$$\sigma_T = \frac{\mathring{P}}{V/\Omega}$$

where again V is the velocity of the incident proton. Using 16a we find

$$\sigma_T \sim \Omega$$

so the cross section per particle in the solid becomes

$$\bar{\sigma} = \frac{\sigma_T}{N} \sim \frac{1}{\rho} \tag{17}$$

where $\rho = N/\Omega$, N being the number of electrons. We pointed out that the rate vanishes for all ρ below some minimum density and so the cross section 17 is finite as the density goes to zero (in fact it vanishes). The fact that the cross section vanishes follows from the separation of the two circles in figure 17 when ρ and therefore k_F becomes small enough. However we might wonder about the finite temperature case. For there the Fermi surface does not cut off sharply and so the two circles never really separate. It might then seem that the rate will not vanish and so equation 17 would imply that the cross section blows up as the density vanishes. This is certainly not the case and it can be shown that equation 17 remains finite as the density goes to zero in the finite temperature case. We remark that the solution lies in the fact that as the density goes to zero so does the temperature. The exact details will not be gone into here.

We conclude this section with a discussion of the order of magnitude of the transition rate. First we consider the order of magnitude of Δ necessary for the capture process to go. We note the condition $\beta_0^2 > 0$ implies that

$$\frac{p_i^2}{2M(M-\Delta)} - W \geqslant 0$$

or

$$\Delta \geqslant \frac{M^2 W}{p_i^2 + MW} \simeq \frac{1}{2}\frac{MW}{E} \tag{18}$$

The approximately equals sign in 18 holds when

$$\frac{p_i^2}{2M} = E \gg W$$

which is easily satisfied in all cases of interest to us. For an MeV pair the inequality 18 implies that Δ must be greater than 10^{-2}. Therefore we conclude that Δ must be positive and must differ appreciably from zero.

We note that Δ can be negative. In fact, F.S. Ham in reference 7 calculates the ratios m^*/m for the alkali metals. This turns out at k=0 to be less than one for the alkalies beginning with sodium.

Under the condition that Δ is positive at some k we note that 16b implies that for the reaction to go we also need

$$\beta_0 \sim \frac{m^*}{(M-\Delta)} P_i$$

This becomes for an MeV pair and $\Delta/M << 1$

$$\beta_0 \sim 10 \qquad \text{Rydberg units}$$

From the definition 12 of β_0 we see that this is satisfied for $\Delta \sim 1$. This means that $m^*/m \sim 2$ which is not easily satisfied for the alkali metals. However even under the circumstances that $\beta_0 \sim 10$ holds we see that the capture rate becomes

$$\mathring{P} \sim 10^{-6}$$

In the next chapter we shall see that the ionization rate is of order 10^{-1} to 10^{-2}. So we need not consider this rate at the velocities of interest to us.

5.4 Capture from the Cores

As the proton channels it interacts with the atoms in its immediate neighborhood and can capture electrons from these atoms. For example in its motion along $\langle 0,0,1 \rangle$ in sodium the situation would look like figure 13. The proton of charge Z_1 maintains a fixed impact parameter $\vec{b}$ with all the cores shown. A is the lattice constant. The cores themselves for the case of sodium say consist of a nucleus of charge eleven units surrounded by electrons in orbitals. The orbitals except for the valence band are treated as if the sodium atom were in free space. Slater[8] points out that this is an extremely good approximation for the inner orbitals. They consist of two 1s electrons, two 2s electrons and six 2p electrons. We should point out that the capture rate dies off exponentially with b and so we are justified in neglecting all but the first set of cores of the solid. We shall show the exact dependence later. We are interested in capture into the longest lived states which turn out essentially to be a combination of 1s and 2s states. This combination also depends strongly on Z_1 as is shown in Chapter 6.

It is clear that the capture rate is best approached using an impact parameter formalism since $|b|$ is fixed. In this approximation the protons motion is fixed and only the active electrons dynamics is considered. We have gone through great detail in section 5.1 to obtain the scattering amplitude in the wave treatment taking account of all formal properties. We showed that in the Born approximation the capture proceeds as if the other electrons were not present when the velocity is high enough. This entailed neglecting the second term in the commutator in equation 5.2 (22). Now the impact parameter Born approximation yields the same cross section as the wave treatment in the limit $m/M \to 0$. Therefore we need not go through the gory details again which pleases the writer probably more than the reader. For a detailed treatment of the impact parameter, see Mittleman.[5] We shall treat the capture as a one electron problem.

We shall not go into great detail for this problem since this work can be found in other places. The only difference is that in our calculation we must keep the impact parameter fixed rather than integrate over it. However, this changes the calculations very little. According to Mittleman[5] the Born approximation for capture is

$$C(\vec{b}) = -i\int_{-\infty}^{+\infty} dt \int \phi_f^*(\vec{r})\, e^{i\Delta_f} \left(-\frac{2Z_1}{x}\right) \phi_i(\vec{x})\, e^{-i\epsilon_i t}\, d^3x \tag{1}$$

where the coordinates X is from the sodium core to the electron and r is from the moving proton to the electron. ϕ_1 and ϕ_f are the initial and final states and

$$\Delta_f = \left(\epsilon_f - \frac{\vec{V}\cdot\vec{r}}{2} + \frac{V^2}{4}\right) t \tag{2}$$

takes account of the linear motion of the electron at velocity $\vec{V}$ in the final captures state (see section 5.2). If we define

$$\Phi_i(\vec{k}) = \int d^3r\, e^{-i\vec{k}\cdot\vec{r}}\, \frac{\phi_i(x)}{x} \tag{3a}$$

$$\hat{\phi}_f(\vec{k}) = \int d^3r\, e^{-i\vec{k}\cdot\vec{r}}\, \phi_f(\vec{r}) \tag{3b}$$

then using 2 and 3 in 1 we get

$$C(\vec{b}) = \frac{-2Z_1 i}{V} \int \frac{d^{(2)}k_\perp}{(2\pi)^2}\, e^{i\vec{k}_\perp\cdot\vec{b}}\, \hat{\phi}_f^*\!\left(\vec{k}_\perp, \frac{\Delta - V^2/4}{V}\right) \Phi_i\!\left(k_\perp, \frac{\Delta + V^2/4}{V}\right) \tag{4}$$

where we have used

$$\vec{k} = \vec{k}_\perp + k_z \hat{v}$$

With 4 it is straight forward to calculate all the amplitudes of interest. For example, we will describe the orbitals of sodium by using a device due to Slater.[9] According to this preciption the sodium radial orbitals are described by

$$R_{1S}^{Na} = A(1S)\, e^{-Z_{1S}\, r} \tag{5a}$$

$$R_{2S}^{Na} = A(2S)\, r e^{-Z_{2S}\, r/2} = R_{2P} \tag{5b}$$

where the values of the effective change is given by "Slater's rules"[9]

$$Z_{1S} = 10.7$$
$$Z_{2S} = 6.85$$

The normalization constants are

$$A(1S) = 2(Z_{1S})^{3/2}$$
$$A(2S) = \frac{1}{2\sqrt{6}}(Z_{2S})^{5/2}$$

We shall consider two capture rates; from 1s to 1s and then 2P ± 1 to 1 s. The other rates involve just a bit more work but are no different in kind.

For s states the Fourier amplitudes are invariant under rotation in

$k_\perp$ space and so 4 becomes

$$C(b) = \frac{-2Z}{V} i \int_0^\infty \frac{dk\,k}{(2\pi)} J_0(kb)\, \hat{\phi}_f^*\left(k_\perp, \frac{\Delta - v^2/4}{V}\right) \Phi_i\left(k_\perp, \frac{\Delta + v^2/4}{V}\right) = C(b) \tag{6}$$

The Fourier transforms in 6 for the 1s orbital of hydrogen is

$$\hat{\phi}_{1s}(\vec{k}) = 2(Z_1)^{3/2} \sqrt{4\pi}\; \frac{-\partial}{\partial\gamma}\left(\frac{1}{k^2+\gamma^2}\right)_{\gamma = Z_1}$$

and for 1s orbital of sodium multiplied by $1/X$ is

$$\Phi_{1s}(k) = A(1s)\sqrt{4\pi}\left(\frac{1}{k^2+(Z_{1s})^2}\right)$$

Using this 6 becomes when $\Delta << v^2/4$

$$C_{1s,1s} = \frac{i A(1s)}{V} 8 Z_1^{5/2}\left(-\frac{\partial}{\partial\gamma}\right)\int_0^\infty dk\, \frac{k J_0(kb)}{B}\left\{\frac{1}{k^2+\frac{v^2}{16}+Z_{1s}} - \frac{1}{k^2+\frac{v^2}{16}+\gamma^2}\right\}_{\gamma = Z_1}$$

where

$$B = \gamma^2 - (Z_{1s})^2$$

Using the definition[10] of the Bessel function of imaginary argument

$$K_0(az) = \int_0^\infty dt\, \frac{t J_0(at)}{t^2+z^2}$$

we get

$$C_{1s\to 1s} = \frac{i\, 8 A(1s)}{V} Z_1^{5/2} \; \frac{-\partial}{\partial\gamma} I(\gamma)\Big|_{\gamma = Z_1} \tag{8a}$$

where

$$I(\gamma) = \frac{1}{\gamma^2 - (Z_{1s})^2}\left[K_0\left(b\sqrt{Z_{1s}^2 + (V/4)^2}\right) - K_0\left(b\sqrt{\gamma^2 + (V/4)^2}\right)\right] \tag{8b}$$

All other transition are of the form 8a and 8b except different K functions appear as well as more derivatives. We note the exponential decrease of 8a with the impact parameter as was stated earlier.

There is one capture rate here that vanishes due to symmetry. The capture from 2p m=±1 into an s state cannot go due to cancellation of amplitudes. To see this we find that the Fourier transform 3a

$$\Phi_i(\vec{k}) = \Phi_i(k, \theta_k, \varphi_k)$$

is proportional to $e^{i\varphi_k}$. Then we would have the capture amplitude proportional to

$$\int_0^{2\pi} \frac{d\varphi_k}{2\pi} e^{ik_\perp b\cos(\varphi_k-\varphi_b)} e^{i\varphi_k}$$

as can be seen from 4. φ_b is the azmuthal location of the projectile relative to an arbitrary axis (see figure 13). Substituting $\varphi_k - \varphi_b = \varphi$ above we find that the capture amplitude is proportional to

$$e^{i\varphi_b}$$

But if we add the amplitudes for the capture from each of the four sites in figure 13, for this particular orbital of sodium, we find the total amplitude is proportional to

$$\sum_{n=0}^{3} e^{in\frac{\pi}{2}}$$

Therefore we see that the total amplitude vanishes due to symmetry.

We point out that the capture cross section go like E^{-6} where E is the energy of the proton. This is negligible in comparison to the ionization rate as we shall see.

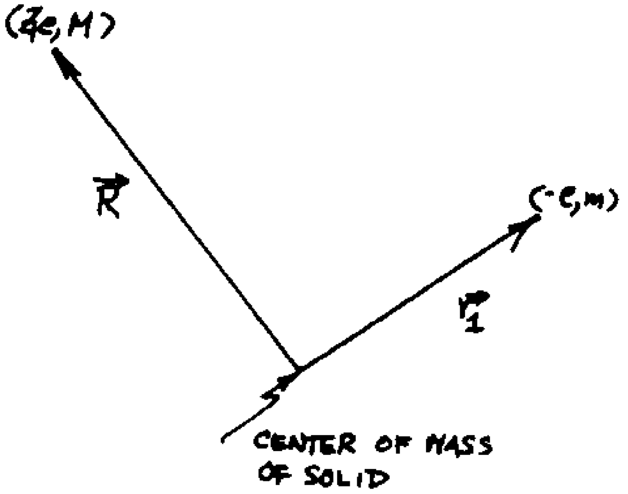

Fig. 16a

Prior Coordinates in Capture

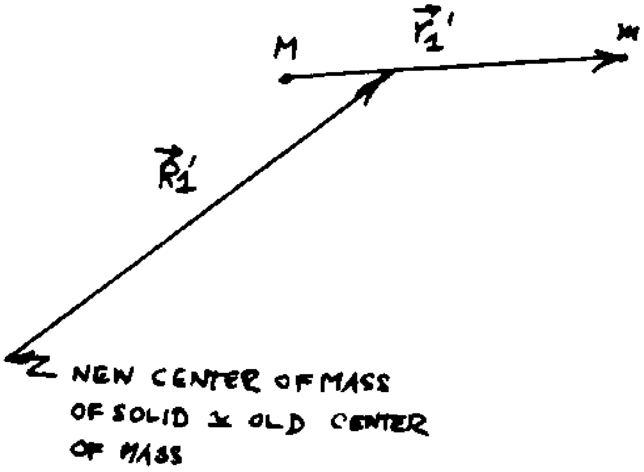

Fig. 16b

Post Coordinates in Capture

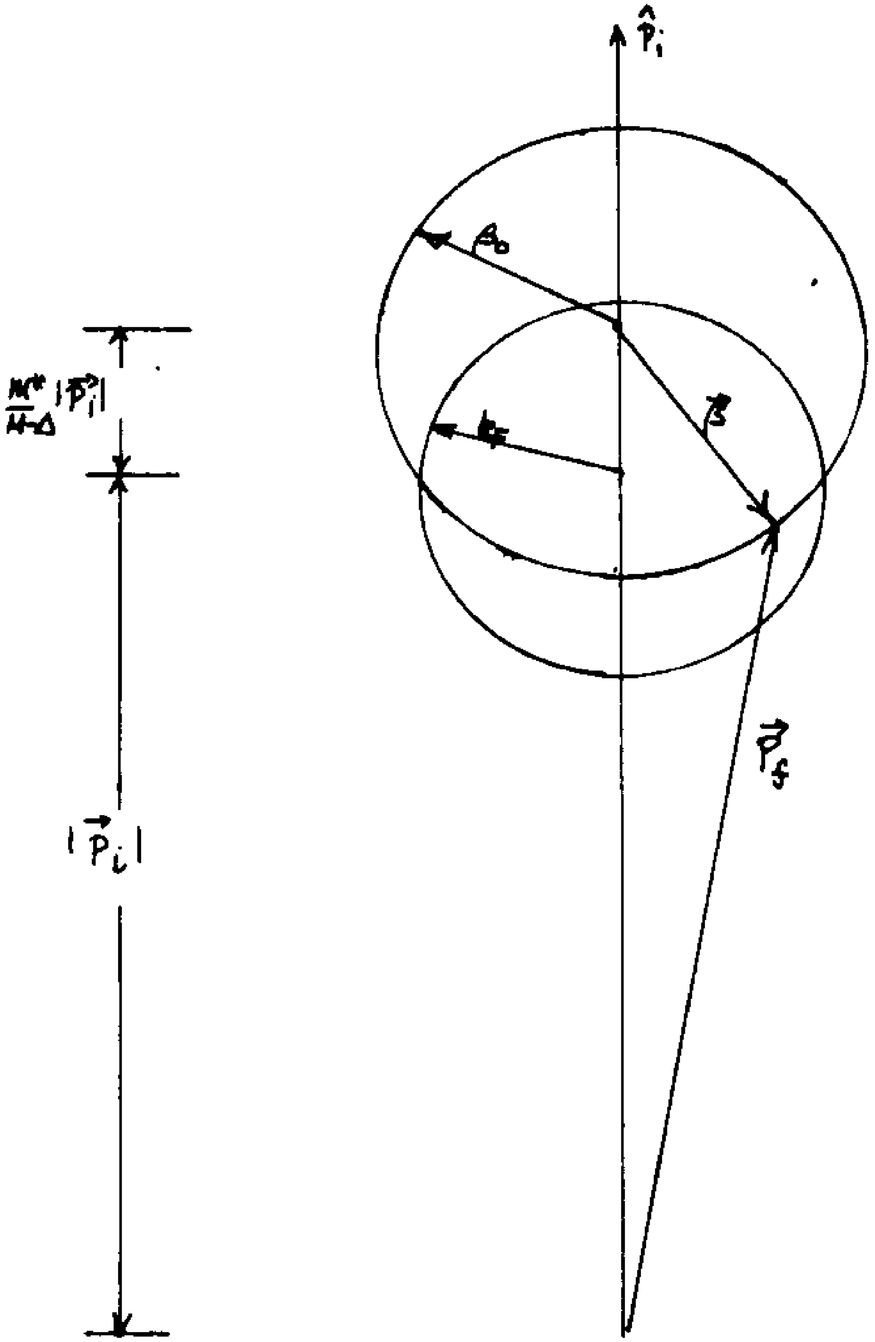

Fig. 17

Integration Limits for Capture

References Chapter 5

1. M.L. Goldberger and K.M. Watson, "Collision Theory", John Wiley and Sons (1964).
2. M.H. Mittleman, Notes.
3. H.C. Brickman and H.A. Kramers, Proc. Acad. Sci. Amsterdam, 33, 973 (1930).
4. J.D. Jackson and H. Schiff, Phys. Rev. 89, 359 (1953).
5. M.H. Mittleman, Phys. Rev. 122, 1930 (1961).
6. M. Ziman, "Electrons and Phonons", Oxford University Press (1960).
7. F.S. Ham, Phys. Rev. 128, 82 (1962).
8. J.C. Slater, "Quantum Theory of Molecules and Solids", Vol. 2 McGraw Hill, New York (19).
9. J.C. Slater, "Quantum Theory of Atomic Structure", Vol. 1 McGraw Hill, New York (1960).
10. I.S. Gradshteynad, I.W. Ryzhik, "Tables of Integral Series and Products", Academic Press, New York and London (1965).

Chapter 6

Numerical Results

6.1 Introduction

In this section we discuss some numerical computations for the states of channeling hydrogen. In the second section we discuss briefly the computational techniques used. In the third section we discuss the numerical results for the channeling of hydorgen in a sodium crystal as a specific example. In particular the penetration depth as a function of the charge on the proton, the screening parameter for the solid and the velocity of the pair is presented. We shall refer to the screening parameter often in this chapter. It is the quantity thatappears in the exponential for the Bohr type potential.

The value of λ given by the expression $\sqrt{1+Z_2^{2/3}}$ is called the Bohr screening parameter λ_b. It is approximately 2.5[†] for sodium. Often the screening length λ_b which is the inverse of λ_b is used in literature.

6.2 Numerical Results

In chapter 4 we derived the matrix elements for both the static potential and the polarization potential in a hydrogenic basis set. In particular the static potential was left in the form of a series given by equation 4.4 (14d). The terms in the series contained two double

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[†] In inverse Bohr radii

The terms in the series contained two double integrals denoted by J_1, equation 4.4(14b) and J_2, equation 4.4(14C). For convenience we write J_1 again

$$J_1 = \int_0^\infty dz\, P_{LM}\left(\frac{z}{\sqrt{1+z^2}}\right) h_l\left(\lambda\rho_g\sqrt{1+z^2}\right) \int_0^{\sqrt{1+z^2}} dr\, r^2 R_{n'l'}(\rho_g r) R_{nl}(\rho_g r) j_l(\lambda\rho_g r) \tag{1}$$

The double integral of equation 1 cannot be done analytically. Therefore, we must resort to numerical techniques. These techniques include the following: the outer quadrature is accomplished by using 10 point Gaussian-Laguerre integration. The sample points of the integrand are not uniformly spaced. Rather they are chosen to that the integral will yield a correct result for a polynomial up to degree nineteen.(1) At each sample point the integrand must be evaluated. Thus at each sample point the inner integration is done using a 10-point Gaussian quadrature scheme. This technique is also used for the integral J_2 although since the limits of the outer integral are not $(0, \infty)$ the Gaussian-Laguerre technique cannot be used. Instead two 10-point Gaussian quadratures are used. The particular computer codes for these integrals were taken from reference 1 although clearly changes were made to adopt them for this double integration. The accuracy of the integrals were considered in the following way. The matrix element for the static potential in the ground state, $\langle 1S | V_S | 1S \rangle$ was evaluated using 24 point double precision Gaussian guadrature, using the above 10 point integrations which are single precision and finally by analytic evaluation. The analytic integration is accomplished by using a Fourier integral representation for the static potential. Earlier we used an expansion in spherical harmonics which led to the integrals J_1 and J_2. This Fourier analysis method becomes prohibitively difficult for the matrix elements for higher states, particularly off diagnol ones. Further, its form made numerical analysis more difficult than expressions J_1 and J_2. The results with the screening parameter chosen as one are

= .259516 for 10 point single precision

= .259169 for 24 point double precision

= .259819 for analytic

From this we shall infer that a maximum of three place accuracy holds for 10 point single precision work. We have used single precision throughout our numerical computations because the accuracy is acceptable and the computation times are then within reason. The generation of the functions needed in the integrals is straightforward and we will not discuss it any further. Lastly, the term $C(L, l_1, m_1, l_2, m_2)$ in 4.4(14d) which is proportional to a Clebsch-Gordon coefficient is evaluated by the summation given in equations 2 through 9 in Appendix 4A.

Once the matrix elements are found we can then diagnolize the Hamiltonian 4.4 (10a). The numerical techniques used were basically Jacobi's method which searches the matrix for those elements larger than some minimum value and annihilates them by orthogonal transformation. This method although not particularly fast is very stable. Further, the Hamiltonian matrix turns out to be rather sparse and so the diagnolization time is a minor fraction of the total computation time. The code used for the diagnolization was again taken from reference 1. The full set of eigen values and eigen vectors are obtained using this code.

6.3 Numerical Results

The programs were run for $Z_1 = 2$ and $Z_1 = 1$ where again Z_1 is the number of units of charge of the incident proton. For each of these various values of the screening parameter were computed. These were run without the polarization potential. The state of lowest finding relative to the proton is the subject of table II. We shall refer to this quantity as the binding energy, remembering that it is the expectation value of the vacuum hydrogen Hamiltonian taken between the ground state for hydrogen in the solid. In table II we also give the 1S and 2S amplitudes for this ground state as well as the binding energy for various values of Z_1 and λ. The number of states used in the basis is also given. The computations were run on an IBM 360/50 and the running times were four minutes for a 14x14 matrix and fifteen minutes fora 30x30mat rix, most of which were consumed in evaluating the matrix elements. The last two lines in table II are the results of the diagnolization of the Hamiltonian with the polarization potential present.

We first note that the case $Z_1 = 2$ is of little interest since for the range of screening shown, the pair sees little of the lattice. Next we note that our remarks about the importance of the polarization potential are borne out. For the case of V=20 (Rydberg units) the electron gas is no longer effective in determining the binding of the pair. At V=10 the state of lowest energy rather than being a distrubed S state seems to have developed out of a $3d_o$ state. This does not follow from table II but rather from the details of the numerical computation. The importance of states rich in p and d character is thus reflected in the state of lowest binding. Because of the asymmetry of the polarization potential in the longitudnal direction, these states become important and thus the potential tends to elongate the atom in this direction. The fact that the binding to the proton is larger than the value without the polarization potential reflecting the oscillating character of the potential. However, this should be a clue that we should not take the results too seriously, for the polarization potential in the dipole approximation, is sampling the atom in regions less than a Bohr radius. But in such a region the granular structure of the electron gas becomes evident. Thus plasma waves for wavelengths less than a Bohr radius care not well-defined.

We have really pusched the calculation beyond its range of validity.

In returning to the static potential, we note that the matrix elements are independent of energy. Further, if we look at the binding energy versus the screening parameter, we see that the binding decreases smoothly for the interval for λ from one to one-third. That is, up to a screening length of $3\lambda_b$, the binding energy is relatively insensitive to the screening parameter λ. After this for smaller values of λ the binding energy begins to oscillate, showing a strong dependence on screening parameter.

As we continue to make λ even smaller, the states begin to take on the character of the states we obtained for λ equal to one. This is shown clearly on the graph of binding energy versus screening parameter, graph I.

We shall try to explain the pheonomena shown on graph I which at first seems somewhat bizarre! Particularly the result that a λ becomes than 1/6 the lattice seems to wipe itself out. The system seems to undergo the following behavior. The lattice is gradually brought into the problem by relaxation of the size of λ below unity. State 2S, 3S and $3d_o$ are mixed in gradually as we see in table II and graph II. Then for λ of the order of 1/3, the binding energy begins to oscillate. This oscillation for the most part can be correlated with table I and graph II. For example the local peak in the binding energy at $\lambda = 3/12$ can be understood as being caused by the presence of less 2s and consequently more 1S amplitude relative to the surrounding aplitudes. After these oscillations the system returns to almost totally 1S character as the lattice parameter is lowered below 1/6.

The fact that the system returns to 1S character can be understood in the following way. The overlap between any two different hydrogen states vanishes of the potential is constant. We shall show that for $\lambda = 1/12$ or $\lambda = 1/24$ that the potential is constant. If we write the static potential as

$$\overline{V_S} = \sum_{\text{Strings}}{}' \int_{-\infty}^{+\infty} dz \, \frac{e^{-\lambda|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} \tag{2}$$

where

$$\vec{r} = (\vec{r}_\perp, z')$$
$$\vec{R} = (\vec{R}_\perp, \vec{z})$$

then on performing the integration in 2 we find

$$\overline{V_S} = \sum_{S}{}' K_0(\lambda |\vec{r}_\perp - \vec{R}_\perp|)$$

where K_0 is a Bessel function of imaginary argument$^{(2)}$. According to Watson[(2)] we can write

$$K_0(\lambda|\vec{r}_\perp - \vec{R}_\perp|) = 2\sum_{m=0}^{\infty}{}' K_m(\lambda R_\perp) I_m(\lambda r_\perp) e^{im\phi} \qquad (3)$$

which holds for $r_\perp < R_\perp$. I_m and K_m are Bessel functions of imaginary argument and integer order[(2)]. ϕ is the angle between the two vectors in the argument of K_0. In our computation of the matrix for V_s we used a basis set up through n=3 and n=4 where n is the principle quantum number of hydrogen. For these sets it is clear that the only terms in 3 that can couple the 1S state of any other in the set is

$$2K_0(\lambda R_\perp) I_0(\lambda r_\perp) \qquad (4)$$

We note that for small λ, that is $\lambda R_\perp < 1$, this potential varies slowly over the dimensions of the hydrogen atom. In fact suppose λ = 1/24 and let us calculate the ratio of the 1S, 2S coupling of the potential to its 1S expectation value, which is

$$R = \frac{\langle 2S|\bar{V}|1S\rangle}{\langle 1S|\bar{V}|1S\rangle} = \lambda^2 \langle 2S|\rho^2|1S\rangle \qquad (5)$$

where we used the expansion of I_0 for small arguments[(2)]

$$I_0(x) = 1 + \frac{1}{2}x^2 + \ldots \qquad (6)$$

Putting 6 in 5 and using

$$r_\perp = r\cos\theta$$

we get

$$\mathcal{R} \simeq \frac{1}{2}\left(\frac{1}{10}\right)^2 \int_0^{a_0} R_{2S}\ R_{1S}\, r^4\, dr$$

$$\mathcal{R} \simeq .8 \times 10^{-2}$$

Therefore, we conclude that there is negligible coupling between the 1S and 2S states. Clearly if we look at higher couplings the above expansion of I_0 will no longer hold. In fact for high n states the expansion (3) no longer holds. However, for high n states the coupling decreases due to the exponential decrease of the ground state. This is amply reflected in the negligible change in the binding energy as we increase the basis size (see table II). Thus we conclude that as λ goes to zero the binding approachs the vacuum value of hydorgen. What we have shown is that I_0 is relatively flat for very small values of its argument. The region of very small values of the screening parameter is not much physical interest however since our understanding of the lattice precludes such highly charged bare cores. Further the Bohr potential is not well-defined for these values. If we want to use large values for the screening parameter, we must then replace the Bohr potential by a sum of Yukowa like potentials. For example we could have a separate term for each shell of the core.

We would also like to consider the lifetime or penetration depth of a channeling pair. This penetration depth D is related to the lifetime

T by the relation

$$D = V.T. \tag{8}$$

The lifetime T is related to the inverse ionization rate by equation 4.2 (12). To find D we begin with the equation for the ionization rate 3.4 (10)

$$\frac{dI}{dt} = n_e V \frac{2\pi e^4}{m V^2} \left\{ \frac{1}{I_0} - \frac{1}{E_0} \right\} \tag{7}$$

where

$$E_o = \frac{1}{2} m V^2$$

and I_o is the ionization potential (negative binding energy) of the pair. If we assume that $\dot{I}$ arises from close collions, then the rate is proportional to the local density n_e which we take as

$$n_e = \sum_{\vec{R}}{}' \frac{\int d^3r \, |\psi(\vec{r})|^2 \, \rho_{Na}(\vec{r}-\vec{R})}{\int d^3r \, |\psi(\vec{r})|^2}$$

where ψ is the ground state of the pair and ρ_{Na} is the density of sodium located at the site R. The major contribution to this will come from the average term in the sodium density when the pair is located at mid-channel. This average term is just the valence electron density, and we shall consider N_e to be this.

From the expression derived in section 4.2 equation 12

$$\frac{dI}{dt} = \frac{1}{\tau} = \Gamma \tag{9}$$

Using 7 and 9 and the condition $E_0 >> I_0$ we find

$$T = \frac{mV}{n_e 2\pi e^4} I_0$$

and using 8 we get

$$D \approx \frac{1}{(n_e a_0)^3} \frac{1}{4\pi} \left(\frac{m}{M}\right) \left(E/Ryd\right) \left(I_0/Ryd\right) \tag{10}$$

If we consider D as a function of λ then we must have

$$I_0 \to 1 \text{ as } \lambda \to \infty$$

so

$$D(\infty) \simeq 10^2$$

if we consider an MeV pair. Therefore, we can write

$$\frac{D(\lambda)}{D(\infty)} = I_0(\lambda)$$

and the penetration depth is proportional to the ionization potential.

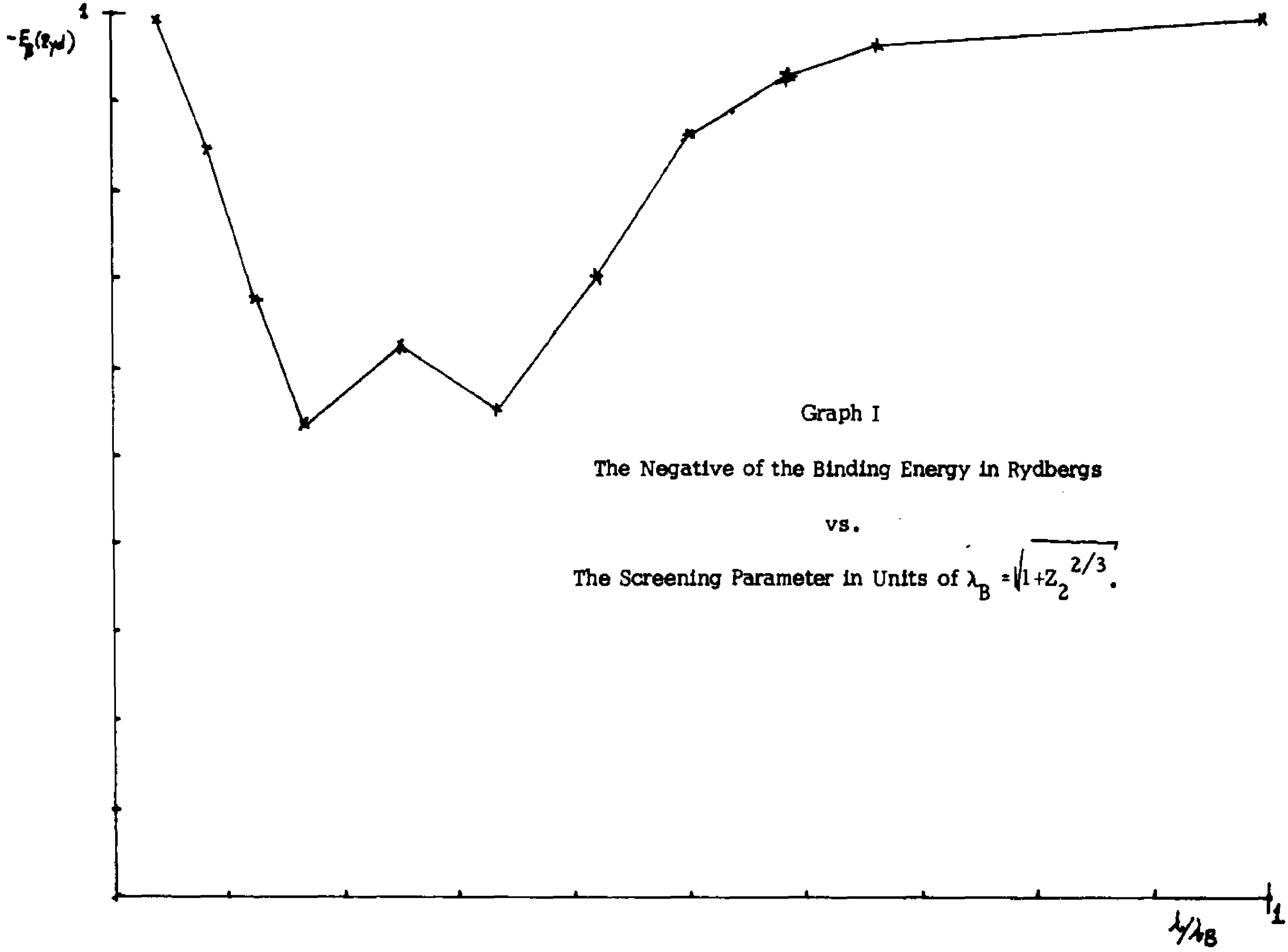
To attempt to measure D or the form of the state of greatest binding does not seem possible, at least directly. If we could do this, we might then use the results to obtain λ. The reason that states cannot be observed directly is that when the atom emerges from the crystal surface, effects may wash out any bulk effects and make measurement impossible. When the surface effects are calculated, then we could be able to obtain information about the internal states, but surface calculations are by no means easy. A direct probe of the interior might be attempted, but we notice immediately that processes such as radiative transitions would not be observable since the lifetimes of the states are too small. Placing the solid in a magnetic field would attenuate the neutral component due to Lorentz ionization and the forcing of the electron into region of high solid density. However, we again do not know whether the surface will mask their effects.

The calculations that might be performed next follow rather directly from the work discussed here. The path of the proton could be deformed and the calculations redone. That is we would be taking into account the slow oscillation of the proton. Also the velocity can be lowered to increase the importance of both collective effects and capture rates. This would necessitate a more careful examination of the polarization potential. Two other areas can be studied. First, the inclusion of a truly self-consistant calculation; and, second, a study of the oscillating character of the binding energy with screening parameter. The first course of study would allow direct loss of flux since we could be dealing with a non-hermitian potential. Thus the state vector lengths would be stretched or compressed during diagnolization. This might entail large computation times. The second course of study might give us more information on the nature of the internal states of the pair.

Number of States	λ (units of λ_B)	Z_1	a_{1s}	a_{2s}	$-E_B$ (Rydbergs)
14	1/3	2	.999	.027	$.399 \times 10^1$
30	1	2	.999	.003	$.399 \times 10^1$
30	1/3	1	.642	.748	.560
30	1/12	1	.896	−.431	.850
14	1	1	.998	−.063	.999
14	2/3	1	.979	−.189	.966
14	7/12	1	.956	−.278	.934
14	3/6	1	.898	−.421	.866
14	5/12	1	.780	−.606	.703
14	1/3	1	.636	−.754	.551
14	3/12	1	.743	.414	.629
14	1/6	1	.669	.423	.534
14	3/24	1	.766	.573	.678
14	1/12	1	.898	−.430	.852
14	1/24	1	.996	−.087	.994
14^+	1/3	1	.744	.516	.645
14^{++}	1/3	1	.635	−.753	.549

Table II

CHANNELED STATES. (a_{1s} and a_{2s} are the amplitudes of 1s and 2s in the state of lowest binding with binding energy given by E_B $\lambda = 1+Z_2^{2/3}$

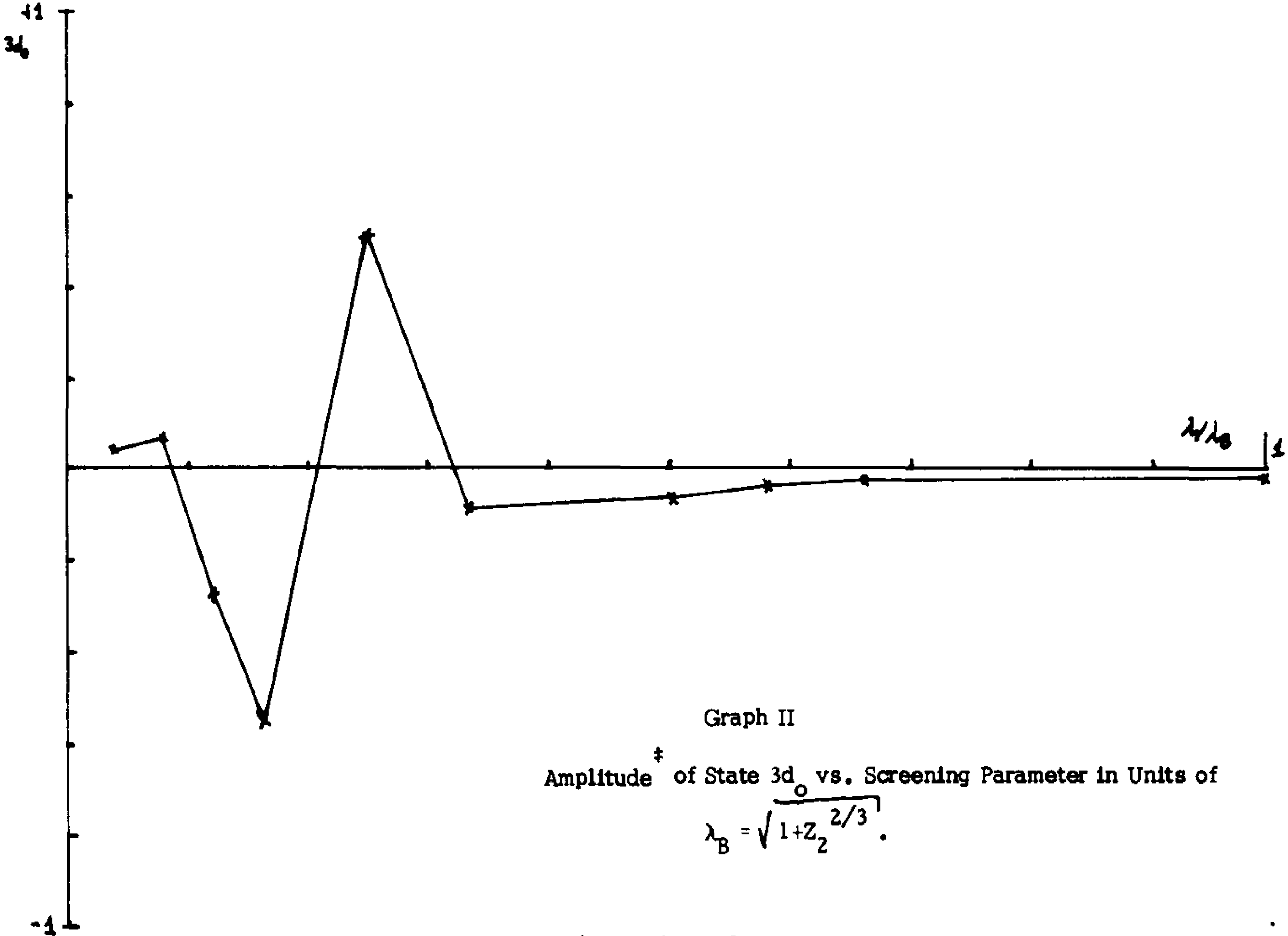


Graph I

The Negative of the Binding Energy in Rydbergs

vs.

The Screening Parameter in Units of $\lambda_B = \sqrt{1+Z_2^{2/3}}$.



Graph II

Amplitude[‡] of State $3d_o$ vs. Screening Parameter in Units of

$$\lambda_B = \sqrt{1+Z_2^{2/3}}.$$

‡ Phase taken relative to 1s.

References Chapter 6

1. I.B.M. System/360 Scientific Subroutine Package Version III, I.B.M. Publications, White Plains, N.Y. (1970)

2. G. N. Watson, "A Treatise in the Theory of Bessel Function" 2nd Edition, Cambridge University Press (1966)