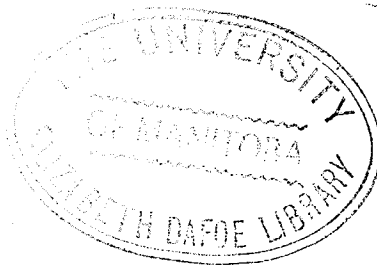POSITRON INTERACTIONS IN IONIC CRYSTALS

By

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CONTENTS

ACKNOWLEDGMENT

ABSTRACT

Two aspects of positron interactions in ionic crystals
have been investigated. First, the angular correlation of
the annihilation radiation due to positrons annihilating with
electrons in LiH crystals has been calculated. Secondly, the
positron energy gap for the first Brilloin zone in LiF crystals
has been calculated.

In the calculation of the angular correlation, the
contribution from annihilation with electrons in the hydride
ion is first obtained by treating the positron wave function
to be a linear combination of Bloch states while the crystal
potential is approximated by means of a sum of central field
potentials centred on the ion sites. The potential due to a
lithium ion is taken to be the form used by Verrall[2]. The
potential due to a hydride ion is obtained by first getting a
wave function for it, then an expression for the charge dis-
tribution is calculated, and finally the Poisson equation is
solved and the solution is then approximated by a Coulomb-
plus-Yukawa form. The result yields an angular correlation
curve 2.75 times narrower than the experimental result. An
estimate of the contributions from the annihilation with the
electrons in the lithium ion is performed and the result is
too small to affect the results for the hydride ion. In the

calculation, polarisation effects and the contributions from excited states have been neglected.

In LiF crystals, there has been, so far, no report on the existence of a τ_2- component. It is believed that if the first forbidden gap in the positron band structure overlaps the Ore gap to a great extent, it might shed some light on the absence of the τ_2- component. This positron energy gap is calculated by using a method which is very much similar to the one used by Tong[4] in the calculation of the electron gap in LiF. The result shows that the magnitude of this gap amounts only to 0.07 e.v. and its effect is too small to enable one to draw a definite conclusion as to why the τ_2- component should be absent.

CHAPTER ONE

INTRODUCTION

Following the discovery of positrons, which were predicted by Dirac's theory, a number of experiments have proved their existence. It was found that positrons and electrons are anti-particles and can annihilate one another giving rise to photon emission. The discovery of the positron led to numerous investigations of its interactions in matter. It is now generally known that a positron can annihilate with an electron in the following manners:-

(1) It can collide and annihilate in flight with an electron in a singlet state with the emission of two photons. The annihilation life time is of the order of 10^{-10} sec. in condensed matter.

(2) It can form positronium with an electron in a singlet state and then annihilate to give two photons. The mean life time of the process is 1.25×10^{-10} sec. This is known as the τ_1 - component.

The above two processes cannot be resolved experimentally. Associated with the two photon annihilation, there is observed in the condensed phase a second longer life time of the order of 10^{-9} sec. It is known as the τ_2 - component.

(3) It can form positronium with an electron in the triplet state and then annihilate to give three photons. The mean life time is 1.4×10^{-7} sec.

The τ_2- component associated with the two-photon anni-
hilation is now generally explained by the so-called "pick-
off" process. According to this, the triplet positronium formed
will be scattered continually by the material. The positron
may then annihilate with one of the electrons whose spin state
relative to it is singlet with the emission of two photons.
This explanation is discussed in detail by Wallace[1].

If the "pick-off" process is correct, then for substances
in which a τ_2- component is observed, there will be a limited
range of energies over which positronium formation will take
place. This range has come to be known as the "Ore gap".
Neamtan and Verrall[2] have verified theoretically the existence
of such a gap in LiH while Bisi et al[3] have reported the
existence of the τ_2- component in a number of ionic crystals
including LiH. Meanwhile, Tong[4] has shown that such a gap
also exists in LiF crystals but the gap does not extend down
to the ground state. So far, no report has been made in regard
to the existence of the τ_2- component in LiF. One aspect of
the present work is to seek an explanation of its absence in
LiF.

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(1) P.R. Wallace: Solid State Physics Vol.10(1960) Academic Press
(2) Neamtan and Verrall: Phys. Rev. 134, 5A (1964) Also,
     R.I.Verrall, M.Sc. Thesis, University of Manitoba (Unpublished)
(3) Bisi, Fiorentini, and Zappa: Phys. Rev. 131, 1023 (1963)
(4) E. Tong, M.Sc. Thesis, University of Manitoba (Unpublished)

Another widely investigated aspect of positrons anni-
hilating with electrons in ionic crystals is the angular
correlation of the annihilation photons. The experimental data
can be fitted with a curve consisting of a central inverted
parabola with a tail at larger angles[5]. Stewart[6] reported
in LiH a half-width whose reciprocal is 1.2Å for the angular
correlation curve. Neamtan et al[7] did a theoretical calculation
based on the assumption that the positron is tightly bound to
the hydride ion and obtained a corresponding result of 5.2Å.
Recently, Gol'danskii et al[8] were able to obtain a close fit
to the experimentally observed angular correlation curve.
However, their results are subject to some doubt. A discussion
of this will be given in Chapter 6 of this thesis. Another
aspect of this thesis is, therefore, to investigate the angular
correlation of the annihilation radiation in LiH crystals on
the assumption that the positron is in a Bloch state prior to
annihilation.

(5) G.Lang and S. deBenedetti: Phys. Rev. 108, 914 (1957)
(6) A.T. Stewart and R.H. March: Phys. Rev. 122, 75 (1961)
(7) Neamtan, Darewych, and Oczkowski: Phys. Rev. 126, 193 (1962)
(8) V.I. Gol'danskii, A.V. Ivanova and E.P. Prokop'ev: Soviet
    Physics JETP 20, 440 (1965) (English Translation)

CHAPTER TWO

THE CRYSTAL POTENTIAL IN LiH

The lithium hydride crystal is composed of positive lithium ions and negative hydride ions arranged in a regular array. It is a face-centred cubic structure. Since the crystal is an ionic one, the ion sites are relatively far apart as compared with the extent of the electron cloud around them. For the present purpose, the potential in the crystal is approximated by considering it as due to an infinite sum of contributions from the individual ion sites. Thus the potentials due to a positive and a negative ion would have to be found. These potentials can be adequately approximated by a Coulomb-plus-Yukawa form.

The potential, at a distance R, due to a positive lithium ion *was obtained* ~~has been worked out~~ by Verrall[2], according to whom it is of the following form:

$$v_1(R) = \frac{e}{R} + \frac{2e}{R} \exp(-\alpha R) \quad \ldots\ldots\ldots\ldots(2.1)$$

where $\alpha = 4.152\text{Å}^{-1}$, and e is the electronic charge.

To get the potential due to the hydride ion, the following procedures were adopted:- first, a wave function for the hydride ion was found, secondly the charge density of the electron distribution of the hydride ion was determined, and lastly the Poisson equation was solved to obtain the potential required.

The determination of the hydride ion wave function is severely restricted by the requirements that the evaluation of the integrals involved in subsequent calculations should be feasible. Besides this, it has to take into account the repulsion between the two electrons in the ion and the fact that the two electrons are identical. Darewych[9] has worked out a form of the wave function which is given by the following:-

$$\psi(r_2, r_3) = (1 + \nu' r_{23}) (e^{-(\lambda' r_2 + \mu' r_3)} + e^{-(\mu' r_2 + \lambda' r_3)}) \quad ..(2.2)$$

where r_2, r_3 are position vectors of the electrons with respect to an origin taken at the nucleus, r_{23} is the distance between the electrons, and the parameters λ', μ', ν' have the following values:-

$$\lambda' = .9033 \text{Å}^{-1}$$
$$\mu' = 2.0315 \text{Å}^{-1}$$
$$\nu' = .5898 \text{Å}^{-1}$$

However, for the present purpose, this function is not suitable because it presents severe difficulties in the evaluation of integrals arising from the angular correlation calculations. Thus, the above form is modified to the following:-

$$\psi(r_2, r_3) = (1 + \nu^2 r_{23}^2) (e^{-(\lambda r_2 + \mu r_3)} + e^{-(\mu r_2 + \lambda r_3)}) \quad ..(2.3)$$

where λ, μ, ν are a set of parameters, different from those in (2.2), to be determined.

To determine these parameters, the expectation value of the

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(9) Private communication

Hamiltonian H of the system is minimized with respect to λ, μ and ν. The values of λ, μ, ν that correspond to the best value of energy are to be used.

The Hamiltonian of the hydride ion is

$$H = -\frac{1}{K}(\nabla_2^2 + \nabla_3^2) - e^2\left(\frac{1}{r_2} + \frac{1}{r_3} - \frac{1}{r_{23}}\right) \quad \ldots \ldots (2.4)$$

$$= -\frac{1}{K}\nabla^2 - e^2 V$$

where $K = 2m/\hbar^2$, $\nabla^2 = \nabla_2^2 + \nabla_3^2$ and the subscripts 2 and 3 refer to the coordinates of the two electrons. Now, for a well-behaved function ψ, by means of Green's theorem, we have

$$\int_{\tau_\infty} \psi \nabla^2 \psi \, d\tau = -\int_{\tau_\infty} (\nabla\psi)^2 \, d\tau$$

where the integration is taken over all configuration space. Thus,

$$(\psi, H\psi) = -\frac{1}{K}\int_\tau \psi\nabla^2\psi \, d\tau - e^2\int_\tau V\psi^2 \, d\tau$$

$$= +\frac{1}{K}\int_\tau (\nabla\psi)^2 \, d\tau - e^2\int_\tau V\psi^2 \, d\tau$$

$$= \frac{1}{K}A - e^2 B \quad \ldots \ldots \ldots (2.5)$$

where $(\nabla\psi)^2 = (\nabla_2\psi)^2 + (\nabla_3\psi)^2$

$$A = \int_\tau (\nabla\psi)^2 \, d\tau$$

$$B = \int_\tau V\psi^2 \, d\tau$$

Now, $\quad \nabla_2\psi = \left(\frac{\partial}{\partial x_2}\mathbf{i} + \frac{\partial}{\partial y_2}\mathbf{j} + \frac{\partial}{\partial z_2}\mathbf{k}\right)\psi$

and $\quad \psi = \psi(r_2, r_3, r_{23})$

$$\therefore \quad \frac{\partial}{\partial x_2} = \frac{\partial\psi}{\partial r_2}\frac{\partial r_2}{\partial x_2} + \frac{\partial\psi}{\partial r_{23}}\frac{\partial r_{23}}{\partial x_2}$$

with similar expressions for $\dfrac{\partial \psi}{\partial y_2}$ and $\dfrac{\partial \psi}{\partial z_2}$.

$$\nabla_2 \psi = \frac{\partial \psi}{\partial r_2}\frac{\underline{r}_2}{r_2} + \frac{\partial \psi}{\partial r_{23}}\frac{\underline{r}_2 - \underline{r}_3}{\underline{r}_{23}}$$

and $(\nabla_2 \psi)^2 = \left(\dfrac{\partial \psi}{\partial r_2}\right)^2 + \left(\dfrac{\partial \psi}{\partial r_{23}}\right)^2 + 2\left(\dfrac{\partial \psi}{\partial r_2}\right)\left(\dfrac{\partial \psi}{\partial r_{23}}\right)\dfrac{\underline{r}_2 \cdot (\underline{r}_2 - \underline{r}_3)}{r_2 r_{23}}$

$$= \left(\frac{\partial \psi}{\partial r_2}\right)^2 + \left(\frac{\partial \psi}{\partial r_{23}}\right)^2 + \left(\frac{\partial \psi}{\partial r_2}\right)\left(\frac{\partial \psi}{\partial r_{23}}\right)\frac{r_2^2 - r_3^2 + r_{23}^2}{r_2 r_{23}}$$

$$.. (2.6)$$

Similarly, $(\nabla_3 \psi)^2 = \left(\dfrac{\partial \psi}{\partial r_3}\right)^2 + \left(\dfrac{\partial \psi}{\partial r_{23}}\right)^2 + \left(\dfrac{\partial \psi}{\partial r_3}\right)\left(\dfrac{\partial \psi}{\partial r_{23}}\right)\dfrac{r_3^2 - r_2^2 + r_{23}^2}{r_3 r_{23}}$

$$.. (2.7)$$

Thus, $(\nabla_2 \psi)^2$ and $(\nabla_3 \psi)^2$ are symmetric with respect to inter-change of r_2 and r_3, so that we have

$$A = \int (\nabla_2 \psi)^2 d^3 r_2 d^3 r_3 + \int (\nabla_3 \psi)^2 d^3 r_2 d^3 r_3$$

$$= 2\int (\nabla_2 \psi)^2 d^3 r_2 d^3 r_3 = 2\int (\nabla_3 \psi)^2 d^3 r_2 d^3 r_3 \quad .. (2.8)$$

With the form of ψ given by (2.3), one obtains

$$\frac{\partial \psi}{\partial r_2} = -(1 + \nu^2 r_{23}^2)(\lambda e^{-(\lambda r_2 + \mu r_3)} + \mu e^{-(\mu r_2 + \lambda r_3)})$$

$$\frac{\partial \psi}{\partial r_{23}} = 2\nu^2 r_{23}(e^{-(\lambda r_2 + \mu r_3)} + e^{-(\mu r_2 + \lambda r_3)})$$

$$\therefore (\nabla_2 \psi)^2 = e^{-2(\lambda r_2 + \mu r_3)}\left\{\lambda^2(1 + \nu^2 r_{23}^2)^2 + 4\nu^4 r_{23}^2 - \frac{2\nu^2\lambda(1+\nu^2 r_{23}^2)(r_2^2 - r_3^2 + r_{23}^2)}{r_2}\right\}$$

$$+ e^{-2(\mu r_2 + \lambda r_3)}\left\{\mu^2(1 + \nu^2 r_{23}^2)^2 + 4\nu^4 r_{23}^2 - \frac{2\nu^2\mu(1+\nu^2 r_{23}^2)(r_2^2 - r_3^2 + r_{23}^2)}{r_3}\right\}$$

$$+ e^{-(\lambda + \mu)(r_2 + r_3)}\left\{2\lambda\mu(1 + \nu^2 r_{23}^2)^2 + 8\nu^4 r_{23}^2 - \frac{2\nu^2(\lambda + \mu)(1+\nu^2 r_{23}^2)(r_2^2 - r_3^2 + r_{23}^2)}{r_2}\right\}$$

$$- - - - (2.9)$$

Hence the evaluation of A involves integrals of the types

$$\int r_{23}^{n} e^{-(ar_2 + br_3)} d^3r_2 \, d^3r_3 \quad , \quad \int \frac{(1 + \nu^2 r_{23}^2)(r_2^2 - r_3^2 + r_{23}^2)e^{-(ar_2 + br_3)}}{r_2} d^3r_2 \, d^3r_3$$

where n = 0,2,4.

Also, $\quad B = \int V \psi^2 \, d^3r_2 \, d^3r_3$

$$= \int (\tfrac{1}{r_2} + \tfrac{1}{r_3} - \tfrac{1}{r_{23}})(1 + \nu^2 r_{23}^2)^2 \left\{ e^{-2(\lambda r_2 + \mu r_3)} + e^{-2(\mu r_2 + \lambda r_3)} + 2e^{-(\lambda + \mu)(r_2 + r_3)} \right\} d^3r_2 \, d^3r_3$$

Thus, the integration of this term involves integrals of the

types $\quad \int r_{23}^{n} e^{-(ar_2 + br_3)} d^3r_2 \, d^3r_3 \quad , \quad \int r_{23}^{2m}(\tfrac{1}{r_2} + \tfrac{1}{r_3})e^{-(ar_2 + br_3)} d^3r_2 \, d^3r_3 .$

where n = -1,1,3 and m = 0,1,2.

Furthermore, the expectation value of H, $\langle H \rangle$, is given

by
$$\langle H \rangle = \frac{(\psi, H\psi)}{(\psi, \psi)} = \frac{\tfrac{1}{k} A - e^2 B}{C}$$

where $\quad C = (\psi, \psi) = \int (1 + \nu^2 r_{23}^2)^2 \left\{ e^{-2(\lambda r_2 + \mu r_3)} + e^{-2(\mu r_2 + \lambda r_3)} + 2e^{-(\lambda + \mu)(r_2 + r_3)} \right\} d^3r_2 d^3r_3$

which involves integrals of the type $\quad \int r_{23}^{n} e^{-(ar_2 + br_3)} d^3r_2 \, d^3r_3$

with n = 0,2,4.

Thus, the evaluation of H involves the evaluation of integrals

of the forms:-

$$\left. \begin{array}{l} \int r_{23}^{n} e^{-(ar_2 + br_3)} d^3r_2 \, d^3r_3 \\[2ex] \int r_{23}^{2m} e^{-(ar_2 + br_3)} (\tfrac{1}{r_2} + \tfrac{1}{r_3}) d^3r_2 \, d^3r_3 \\[2ex] \text{and} \int \frac{(1 + \nu^2 r_{23}^2)(r_2^2 - r_3^2 + r_{23}^2)e^{-(ar_2 + br_3)}}{r_2} d^3r_2 \, d^3r_3 \end{array} \right\} \quad \cdots\cdots\cdots\cdots (2.10)$$

with n = -1,0,1,2,3,4 and m = 0,1,2.

In the evaluation of some of these integrals, it is convenient to express the volume element $d^3r_2 d^3r_3$ in terms of r_2, r_3, r_{23} and three suitable angles. Thus, for the integration over $\underline{r_3}$, we have to take $\underline{r_2}$ as the polar axis, and referring to fig. (1), we have
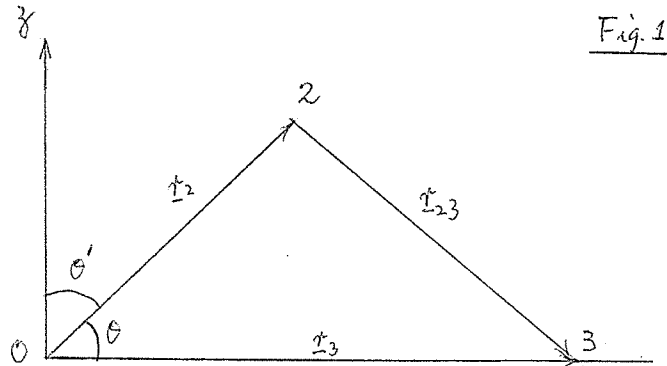

Fig. 1.

$$d^3r_2 d^3r_3 = r_2^2 \sin\theta' d\theta' dr_2 d\varphi' \, r_3^2 \sin\theta \, dr_3 d\theta d\varphi$$

in which θ', θ range from 0 to π and φ, φ' from 0 to 2π. Hence, integrating over θ', φ and φ' first, we have for integrands that do not involve the azimuthal angle,

$$d^3r_2 d^3r_3 = 8\pi^2 \, r_2^2 \, r_3^2 \sin\theta \, d\theta \, dr_2 \, dr_3 \qquad \ldots\ldots\ldots (2.11)$$

Now from the triangle o23, one obtains

$$r_{23}^2 = r_2^2 + r_3^2 - 2r_2 r_3 \cos\theta$$

$$\therefore r_{23} dr_{23} = r_2 r_3 \sin\theta \, d\theta \qquad \ldots\ldots\ldots (2.12)$$

Substituting (2.12) into (2.11), we get

$$d^3r_2 d^3r_3 = 8\pi^2 \, r_2 r_3 r_{23} \, dr_2 dr_3 dr_{23} \qquad \ldots\ldots\ldots (2.13)$$

With the aid of (2.13), one can now evaluate all the integrals involved in (2.10). A table of the integrals is given in the appendix. With the aid of these integrals, we have, after omitting the factor π^2 ,

$$A(\lambda,\mu,\nu) = \frac{2(\lambda^2+\mu^2)}{(\lambda\mu)^3} + \frac{12(\lambda^4+\mu^4)\nu^2}{(\lambda\mu)^5} - \frac{72(\lambda^2+\mu^2)\nu^4}{(\lambda\mu)^5}$$

$$- \frac{15\nu^4(\lambda^2+\mu^2)(3\lambda^4+4\lambda^2\mu^2+3\mu^4)}{(\lambda\mu)^7} + \frac{256\lambda\mu}{(\lambda+\mu)^6} - \frac{1536\nu^2}{(\lambda+\mu)^6} - \frac{64 \times 576\nu^4}{(\lambda+\mu)^8}$$

$$+ \frac{48 \times 16^2\lambda\mu\nu^2}{(\lambda+\mu)^8} + \frac{5^2 \times 4^6 \times 3\lambda\mu\nu^4}{(\lambda+\mu)^{10}} \qquad \cdots\cdots\cdots\cdots \quad (2.14a)$$

$$B(\lambda,\mu,\nu) = \frac{2(\lambda+\mu)}{(\lambda\mu)^3} + \frac{6^2(2\lambda^3+\lambda^2\mu+\lambda\mu^2+2\mu^3)}{(\lambda\mu)^5} + \frac{15\nu^4(3\lambda^5+\lambda^4\mu+2\lambda^3\mu^2+2\lambda^2\mu^3+\lambda\mu^4+3\mu^5)}{(\lambda\mu)^7}$$

$$- \frac{2(\lambda^2+3\lambda\mu+\mu^2)}{(\lambda\mu)^2(\lambda+\mu)^3} - \frac{2\nu^2(3\lambda^4+9\lambda^3\mu+11\lambda^2\mu^2+9\lambda\mu^3+3\mu^4)}{(\lambda\mu)^4(\lambda+\mu)^3} - \frac{3\nu^4(5\lambda^6+15\lambda^5\mu+21\lambda^4\mu^2+23\lambda^3\mu^3+21\lambda^2\mu^4+15\lambda\mu^5+5\mu^6)}{(\lambda\mu)^6(\lambda+\mu)^3}$$

$$+ \frac{88}{(\lambda+\mu)^5} + \frac{3488\nu^2}{(\lambda+\mu)^7} + \frac{8^2 \times 1125\nu^4}{(\lambda+\mu)^9} \qquad \cdots\cdots\cdots\cdots \quad (2.14b)$$

$$C(\lambda,\mu,\nu) = \frac{2}{(\lambda\mu)^3} + \frac{12\nu^2(\lambda^2+\mu^2)}{(\lambda\mu)^5} + \frac{15\nu^4(3\lambda^4+4\lambda^2\mu^2+3\mu^4)}{(\lambda\mu)^7}$$

$$+ \frac{128}{(\lambda+\mu)^6} + \frac{4^4 \times 24\nu^2}{(\lambda+\mu)^8} + \frac{4^5 \times 150\nu^4}{(\lambda+\mu)^{10}} \qquad \cdots\cdots\cdots\cdots \quad (2.14c)$$

It is to be noted that $A(\lambda,\mu,\nu)$, $B(\lambda,\mu,\nu)$ and $C(\lambda,\mu,\nu)$ are homogenious functions in λ, μ, ν of degress -4, -5, and -6 respectively. Thus, the expectation value of H can be minimized immediately with respect to one of the variables, say ν, and we are left with a problem involving two variables. One has

$$\langle H \rangle = \frac{\frac{1}{k}A(\lambda,\mu,\nu) - e^2 B(\lambda,\mu,\nu)}{C(\lambda,\mu,\nu)}$$

$$= \frac{\frac{\nu^2}{k}A(\frac{\lambda}{\nu},\frac{\mu}{\nu},1) - \nu e^2 B(\frac{\lambda}{\nu},\frac{\mu}{\nu},1)}{C(\frac{\lambda}{\nu},\frac{\mu}{\nu},1)}$$

Minimizing $\langle H \rangle$ with respect to ν, we get

$$y = \frac{B(1,m)}{2A(1,m)} Ke^2 = \frac{1}{a_o} \frac{B(1,m)}{A(1,m)} \quad \cdots\cdots\cdots (2.15)$$

and $\langle H \rangle_y = - \dfrac{B^2(1,m)}{4A(1,m)C(1,m)} Ke^4 = - \dfrac{B^2(1,m)}{A(1,m)C(1,m)} \dfrac{e^2}{2a_o}$ (2.16)

where $1 = \dfrac{\lambda}{\nu}$, and $m = \dfrac{\mu}{\nu}$. Thus, we need only minimize (2.16)

with respect to $1,m$ where now

$$A(1,m) = \frac{2(1^2+m^2)}{(1m)^3} + \frac{12(1^4+m^4)}{(1m)^5} - \frac{72(1^2+m^2)}{(1m)^5} + \frac{15(1^2+m^2)(31^4+41^2m^2+3m^4)}{(1m)^7}$$

$$+ \frac{2561m}{(1+m)^6} - \frac{1536}{(1+m)^6} - \frac{64 \times 576}{(1+m)^8} + \frac{48 \times 16^2 1m}{(1+m)^8} + \frac{5^2 \times 4^6 \times 31m}{(1+m)^{10}} \qquad (2.17a)$$

$$B(1,m) = \frac{2(1+m)}{(1m)^3} + \frac{6(21^3+1^2m+1m^2+2m^3)}{(1m)^5} + \frac{15(31^5+1^4m+21^3m^2+21^2m^3+1m^4+5m^5)}{(1m)^7}$$

$$- \frac{2(1^2+31m+m^2)}{(1m)^2(1+m)^3} - \frac{2(31^4+91^3m+111^2m^2+91m^3+3m^4)}{(1m)^4(1+m)^3}$$

$$- \frac{3(51^6+151^5m+211^4m^2+231^3m^3+211^2m^4+151m^5+5m^6)}{(1m)^6(1+m)^3} + \frac{88}{(1+m)^5}$$

$$+ \frac{34884}{(1+m)^7} + \frac{8^2 \times 1125}{(1+m)^9} \qquad (2.17b)$$

$$c(1,m) = \frac{2}{(1m)^3} + \frac{12(1^2+m^2)}{(1m)^5} + \frac{15(31^4+41^2m^2+3m^4)}{(1m)^7} + \frac{128}{(1+m)^6}$$

$$+ \frac{4^4 \times 24}{(1+m)^8} + \frac{4^5 \times 150}{(1+m)^{10}} \qquad (2.17c)$$

It was found that the substitutions

$$\begin{cases} 1 = x - y \\ m = x + y \end{cases}$$

and then $\begin{cases} \xi = x^2 \\ \eta = y^2 \end{cases}$

simplified the expressions to some extent. It terms of these

new variables ξ , η , (2.17a),(2.17b),(2.17c) become

$$A(\xi,\eta) = \frac{4(\xi+\eta)}{(\xi-\eta)^3} + \frac{24}{(\xi-\eta)^3} + \frac{192\xi\eta}{(\xi-\eta)^5} + \frac{156(\xi+\eta)}{(\xi-\eta)^5} + \frac{1440(\xi+\eta)\xi\eta}{(\xi-\eta)^7}$$

$$+ \frac{4}{\xi^2} - \frac{4\eta}{\xi^3} + \frac{24}{\xi^3} + \frac{156}{\xi^4} - \frac{48\eta}{\xi^4} - \frac{300\eta}{\xi^5} \qquad (2.18a)$$

$$B(\xi,\eta) = \sqrt{\xi}\left\{\frac{11}{4\xi^3} + \frac{109}{4\xi^4} + \frac{1125}{8\xi^5} + \frac{4}{(\xi-\eta)^3} - \frac{72}{(\xi-\eta)^4} + \frac{510}{(\xi-\eta)^5} + \frac{96\xi}{(\xi-\eta)^5}\right.$$

$$- \frac{1800\xi}{(\xi-\eta)^6} + \frac{1440\xi^2}{(\xi-\eta)^7} - \frac{1}{\xi(\xi-\eta)^2} + \frac{3}{\xi(\xi-\eta)^3} - \frac{9}{\xi(\xi-\eta)^4} - \frac{1}{4\xi^2(\xi-\eta)}$$

$$\left. \frac{1}{4\xi^3(\xi-\eta)^2} - \frac{3}{8\xi^2(\xi-\eta)^3}\right\} \tag{2.18b}$$

$$C(\xi,\eta) = \frac{2}{(\xi-\eta)^3} + \frac{24(\xi+\eta)}{(\xi-\eta)^5} - \frac{30}{(\xi-\eta)^7} + \frac{180(\xi+\eta)^2}{(\xi-\eta)^7} + \frac{2}{\xi^3} + \frac{24}{\xi^4} + \frac{150}{\xi^5}$$

$$\tag{2.18c}$$

The expression $-B^2(\xi,\eta)/A(\xi,\eta)C(\xi,\eta)$ was then minimized with respect to ξ, η with the aid of the I.B.M. 1620 computer. The best results obtained were

$$\lambda = .9123Å^{-1}$$
$$\mu = 2.0333Å^{-1}$$
$$\nu = .3393Å^{-1}$$

corresponding to a minimum energy of -14.14 e.v.

Experimentally, the hydride ion is a weakly bound system with a binding energy for the second electron of merely 0.7e.v. Thus, the ground state energy of such a system would be - 13.6-0.7 = -14.3 e.v. A comparison with our calculated energy shows that our value is slightly too high. However, since we are only interested in the angular correlation phenomenon which involves the participation of the system as a whole, the value we get is assumed to be good enough.

A comparison can now be made between the function we found and the one used by Darewych. To this end, we calculate the

overlap of the two functions:

$$\psi_H(r_2,r_3) = (1 \neq \nu^2 r_{23}^2)(e^{-(\lambda r_2 + \mu r_3)} + e^{-(\mu r_2 + \lambda r_3)})$$

$$\psi_D(r_2,r_3) = (1 \neq \nu' r_{23})(e^{-(\lambda' r_2 + \mu' r_3)} + e^{-(\mu' r_2 + \lambda' r_3)})$$

i.e., to see how close the integral

$$I = \frac{\int \psi_D^* \psi_H \, d^3 r_2 d^3 r_3}{\sqrt{\int |\psi_D|^2 d^3 r_2 d^3 r_3 \times \int |\psi_H|^2 d^3 r_2 d^3 r_3}}$$

is to unity. The result obtained was I = 0.99. Thus, it is
concluded that the function so chosen represents the hydride
ion fairly well.

Consider the wave function $\psi(r_2,r_3)$. If this is normalised
to unity, then $|\psi(r_2,r_3)|^2 d^3 r_2 d^3 r_3$ is the probability of
finding particle 2 in the volume element $d^3 r_2$ and finding
particle 3 in the volume element $d^3 r_3$. Integrating over $\underline{r_3}$, we
obtain that

$$\int |\psi(r_2,r_3)|^2 \, d^3 r_3$$

is the probability density for particle 2. The charge density
due to particle 2 is therefore

$$- e \int |\psi(r_2,r_3)|^2 \, d^3 r_3$$

where e is the magnitude of the electronic charge on the electron.
Since the two particles are identical, the total charge density
is
$$\rho(r_2) = - 2e \int |\psi(r_2,r_3)|^2 \, d^3 r_3$$

The potential $v_2(R)$ due to the hydride ion at distance R
is then found by solving the Poisson equation:-

$$\nabla^2 v_2(R) = - 4\pi \rho(R) \tag{2.19}$$

Now $$\rho(R) = - \frac{2e}{\pi^2 c} \int |\psi(r_2,r_3)|^2 \, d^3 r_3$$

where $\pi^2 c$ = normalisation factor of $\psi(r_2, r_3)$. Integrating, we obtained,

$$\rho(R) = -\frac{2e}{\pi^2 c} G' \qquad (2.20)$$

where $G' = 4\pi e^{-2\lambda R}\left\{\frac{2}{(2\mu)^3} + \frac{4\nu^2 R^2}{(2\mu)^3} + \frac{48\nu^2}{(2\mu)^5} + \frac{2\nu^4 R^4}{(2\mu)^3} + \frac{10}{3} \times \frac{4!\,\nu^4 R^2}{(2\mu)^5} + \frac{6!\,\nu^4}{(2\mu)^7}\right\}$

$$+ 4\pi e^{-2\mu R}\left\{\frac{2}{(2\lambda)^3} + \frac{4\nu^2 R^2}{\cdot(2\lambda)^3} + \frac{48\nu^2}{(2\lambda)^5} + \frac{2\nu^4 R^4}{(2\lambda)^3} + \frac{10}{3} \times \frac{4!\,\nu^4 R^2}{(2\lambda)^5} + \frac{6!\,\nu^4}{(2\lambda)^7}\right\}$$

$$+ 8\pi e^{-(\lambda+\mu)R}\left\{\frac{2}{(\lambda+\mu)^3} + \frac{4\nu^2 R^2}{(\lambda+\mu)^3} + \frac{48\nu^2}{(\lambda+\mu)^5} + \frac{2\nu^4 R^4}{(\lambda+\mu)^3} + \frac{10}{3} \times \frac{4!\,\nu^4 R^2}{(\lambda+\mu)^5} + \frac{6!\,\nu^4}{(\lambda+\mu)^7}\right\}$$

$$= \pi G$$

letting $v_2(R) = -\frac{e}{R} + \frac{\gamma e}{R} e^{-\beta R}$ where β, γ are parameters to be found, we have from (2.19), and (2.20)

$$\nabla^2 v_2(R) = \frac{e\gamma\beta^2}{R} e^{-\beta R} = -4\pi\rho(R)$$

$$= \frac{-4\pi(-2e)\pi G}{\pi^2 c} = \frac{8G}{c}e$$

$$\therefore \ \gamma\beta^2 e^{-\beta R} = \frac{8G}{C}R$$

Taking logarithms on both sides, we have

$$\log\left(\frac{8GR}{C}\right) = \log(\gamma\beta^2) - \beta R \qquad (2.21)$$

If the graph of log (8GR/C) vs. R is nearly a straight line, then from the intercept and slope of the line, the parameters β, γ can be found.

The best fit found was

$$\gamma = 1.84$$

$$\beta = 1.805 \text{Å}^{-1}$$

It is to be noted that the curve fitting has been done in the region $0.5 < r < 2$ Å. This should be sufficiently good because the distance between two adjacent hydride ions is about 2 Å.

Curve fitting of potential due to a hydride ion.

Slope $= -1.805$

Intercept $= 1.788$

$\therefore \quad \gamma = 1.84$

$\beta = 1.805$

$\log \left(\frac{8q}{c} R \right) \rightarrow$

R in Å $\rightarrow$
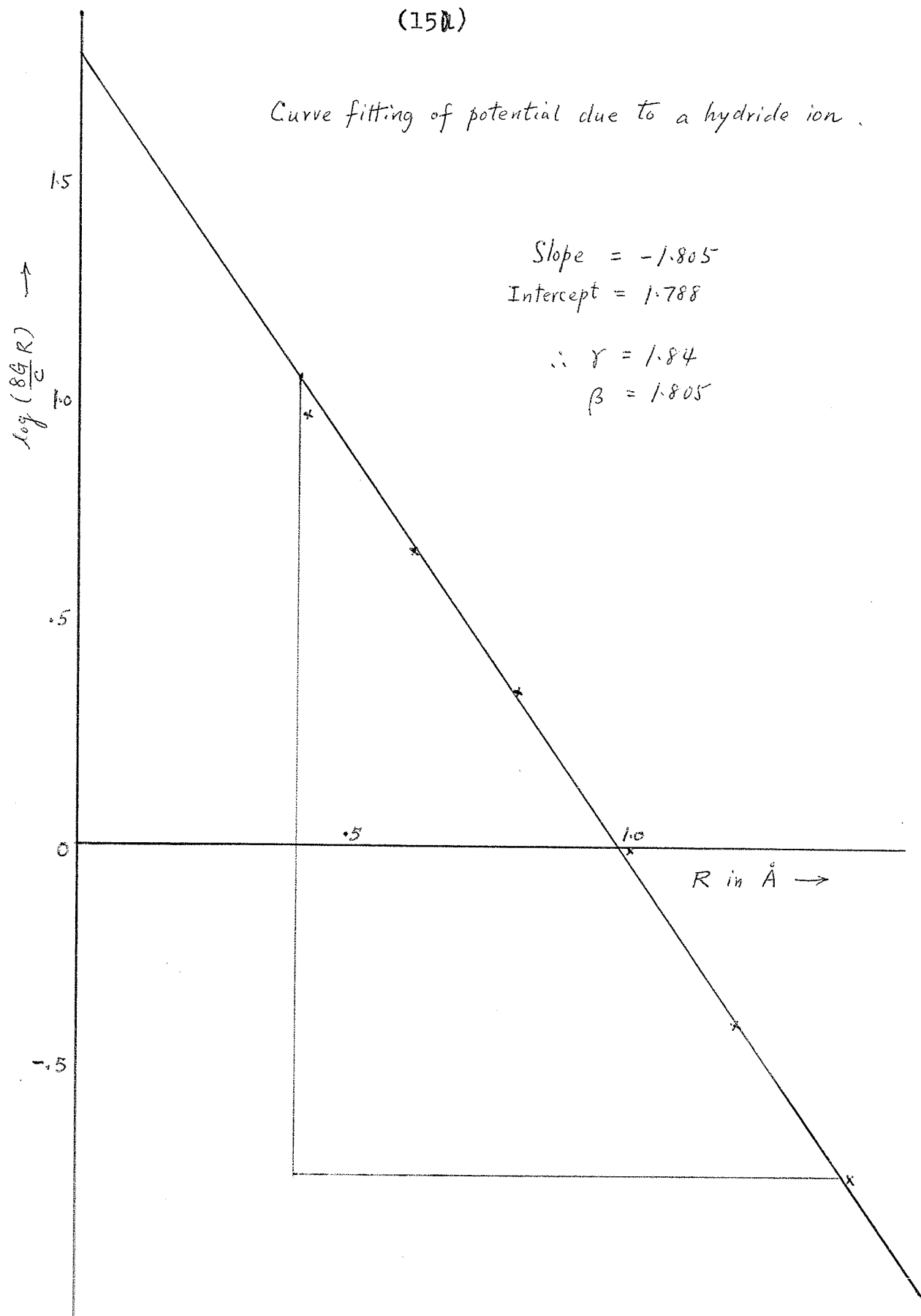
Fourier Analysis of the Crystal Potential

We will find the crystal potential as seen by a positron because we will be interested later in finding its wave function which requires a knowledge of its potential in the lithium hydride crystal. In this case, the wave function is vanishingly small around a positive ion site. In the Fourier analysis of the potential, we take the origin to be at one of the negative ion sites. The potential at a distance R is given by

$$v(\underline{R}) = \sum_j \left[v_1(\underline{R}-\underline{R}_j-\underline{a}) + v_2(\underline{R}-\underline{R}_j) \right] \qquad (2.22)$$

where $\underline{R}_j$ denotes the position vector of the jth negative ion and $\underline{a}$ is a position vector of a positive ion with respect to the origin.

Since $v(\underline{R}) = v(-\underline{R})$ and $v(\underline{R})$ is periodic, having the periodicity of the crystal, it can be Fourier analysed in the form

$$v(\underline{R}) = \sum_{\underline{K}} c_{\underline{K}} \, e^{2\pi i \underline{K} \cdot \underline{R}}$$

If S is the side of a box of volume τ_R, then we have

$$c_{\underline{K}} = \lim_{S \to \infty} \frac{1}{S^3} \int_{\tau_R} e^{-2\pi i \underline{K} \cdot \underline{R}} \, v(\underline{R}) \, d\tau_R$$

$$= \lim_{S \to \infty} \frac{1}{S^3} \int_{\tau_R} e^{2\pi i \underline{K} \cdot \underline{R}} \, v(-\underline{R}) \, d\tau_R$$

$$= \lim_{S \to \infty} \frac{1}{S^3} \int_{\tau_R} e^{2\pi i \underline{K} \cdot \underline{R}} \, v(\underline{R}) \, d\tau_R$$

$$= c_{-\underline{K}}$$

$$= \lim_{S \to \infty} \frac{1}{S^3} \int_{\tau_R} e^{-2\pi i \underline{K} \cdot \underline{R}} \sum_j \left[v_1(\underline{R}-\underline{R}_j-\underline{a}) + v_2(\underline{R}-\underline{R}_j) \right] d\tau_R$$

$$= \lim_{S \to \infty} \frac{e}{S^3} \int_{\tau_R} e^{-2\pi i \underline{K} \cdot \underline{R}} \sum_j \left[\frac{1}{|\underline{R}-\underline{R}_j-\underline{a}|} + \frac{2 \, e^{-\alpha |\underline{R}-\underline{R}_j-\underline{a}|}}{|\underline{R}-\underline{R}_j-\underline{a}|} \right.$$

$$\left. - \frac{1}{|\underline{R}-\underline{R}_j|} + \frac{1.84 \, e^{-\beta |\underline{R}-\underline{R}_j|}}{|\underline{R}-\underline{R}_j|} \right] d\tau_R \qquad (2.23)$$

Now $\displaystyle\int \frac{e^{-\beta|\underline{R}-\underline{R}_j|}}{|R-R_j|}\; e^{-2\pi i\underline{K}\cdot\underline{R}}\; d\tau_R$

$= \displaystyle\frac{e^{-\beta R}}{R}\, e^{-2\pi i\underline{K}\cdot(\underline{R}+\underline{R}_j)}\; d\tau_R$ by a shift of origin

$= \displaystyle\frac{e^{-\beta R}}{R}\, e^{-2\pi i\underline{K}\cdot\underline{R}}\; d\tau_R$ because $\underline{K}$ is a vector of the

reciprocal lattice.   (2.24a)

Also, $\displaystyle\int \frac{e^{-\alpha|\underline{R}-\underline{R}_j-\underline{a}|}}{|\underline{R}-\underline{R}_j-\underline{a}|}\; e^{-2\pi i\underline{K}\cdot\underline{R}}\; d\tau_R$

$= \displaystyle\frac{e^{-\alpha R}}{R}\, e^{-2\pi i\underline{K}\cdot\underline{R}}\; e^{-2\pi i\underline{K}\cdot\underline{a}}\; d\tau_R$ (2.24b)

To evaluate (2.23), take a coordinate system as shown in fig.2.
$\underline{I}$, $\underline{J}$, $\underline{K}$ are unit vectors in the orthogonal system.
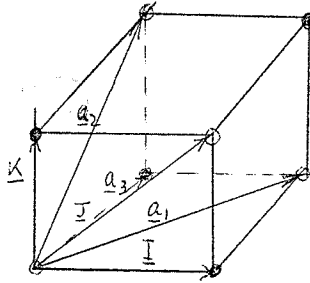
Fig. 2

• *positive ion sites*
○ *negative ion sites*

We have, $\underline{a}_1 = L(\underline{I}+\underline{J})$

$\underline{a}_2 = L(\underline{J}+\underline{K})$

$\underline{a}_3 = L(\underline{K}+\underline{I})$

∴   volume of the unit Bravais cell $= \underline{a}_1\cdot(\underline{a}_2\times\underline{a}_3) = 2L^3$.
Hence the number of vectors $\underline{R}_j$ in the summation is $s^3/2L^3$.

∴ $c_{\underline{K}} = \displaystyle\frac{e}{2L^3}\int e^{-2\pi i\underline{K}\cdot\underline{R}}\left[-\frac{1}{R} + \frac{1.84e^{-\beta R}}{R} + \frac{1}{R}\, e^{-2\pi i\underline{K}\cdot\underline{a}} + \frac{2}{R}e^{-\alpha R}\; \times \right.$

$\left. e^{-2\pi i\underline{K}\cdot\underline{a}}\; \right]\; d\tau_R$

After taking into account equations (2.24a) and (2.24b).

Now, we have $\displaystyle\int \frac{e^{-\beta R}}{R}\; e^{-2\pi i\underline{K}\cdot\underline{R}}\; d\tau_R = \frac{4\pi}{4\pi^2 K^2 + \beta^2}$

and $\int \frac{1}{R} e^{-2\pi i \underline{K} \cdot \underline{R}} \, d\tau_R = \lim_{\beta \to 0} \int \frac{e^{-\beta R}}{R} \, e^{-2\pi i \underline{K} \cdot \underline{R}} \, d\tau_R$

$$= \frac{4\pi}{4\pi^2 K^2}$$

Hence, $C_{\underline{K}} = \frac{2 e}{L^3} \left[\frac{1.84}{4\pi^2 K^2 + \beta^2} - \frac{1}{4\pi^2 K^2} + e^{-2\pi i \underline{K} \cdot \underline{a}} \left(\frac{2}{4\pi^2 K^2 + \alpha^2} + \frac{1}{4\pi^2 K^2} \right) \right]$

$$(2.25)$$

Now $\underline{a}$ is the position vector of a positive ion with respect to the origin (a negative ion site), it can be chosen as

$$\underline{a} = \tfrac{1}{2}(\underline{a}_1 + \underline{a}_2 + \underline{a}_3)$$

A general value for $\underline{a}$ would be $\underline{a} \quad \underline{R}_j$ where

$$\underline{R}_j = m_1\underline{a}_1 + m_2\underline{a}_2 + m_3\underline{a}_3$$

$$\therefore \quad \underline{a} = (m_1 + \tfrac{1}{2})\underline{a}_1 + (m_2 + \tfrac{1}{2})\underline{a}_2 + (m_3 + \tfrac{1}{2})\underline{a}_3$$

We have, furthermore, $\underline{K} = n_1\underline{b}_1 + n_2\underline{b}_2 + n_3\underline{b}_3$ where $\underline{b}_1$, $\underline{b}_2$, $\underline{b}_3$ are basis vectors of the reciprocal lattice, and are related to the $\underline{a}$'s through the relations:

$$\underline{b}_i = \frac{\underline{a}_j \times \underline{a}_k}{\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)} \qquad \text{etc.}$$

$$\therefore \quad \underline{b}_i \cdot \underline{a}_j = \delta_{ij}$$

Thus, $e^{-2\pi i \underline{K} \cdot \underline{a}} = e^{-2\pi i \, n_1(m_1 + \tfrac{1}{2}) + n_2(m_2 + \tfrac{1}{2}) + n_3(m_3 + \tfrac{1}{2})}$

$$= e^{-\pi i (n_1 + n_2 + n_3)} = (-1)^{n_1 + n_2 + n_3}$$

Further, if we express the $\underline{b}$'s in terms of the orthogonal triad $\underline{I}$, $\underline{J}$, $\underline{K}$, we get

$$\underline{b}_1 = \frac{1}{2L^3}(\underline{a}_2 \times \underline{a}_3) = \frac{1}{2L}(\underline{I} + \underline{J} - \underline{K})$$

$$\underline{b}_2 = \frac{1}{2L^3}(\underline{a}_3 \times \underline{a}_1) = \frac{1}{2L}(\underline{J} + \underline{K} - \underline{I})$$

$$\underline{b}_3 = \frac{1}{2L3}(\underline{a}_1 \times \underline{a}_2) = \frac{1}{2L}(\underline{K} + \underline{I} - \underline{J})$$

Hence $\underline{K} = \dfrac{1}{2L}\left[(n_1+n_2-n_3)\underline{I} + (n_2+n_3-n_1)\underline{J} + (n_3+n_1-n_2)\underline{K}\right]$

Letting $\underline{k} = 2\pi\underline{K}$, we have

$$k^2 = \frac{\pi^2}{L^2}\left[(n_1+n_2-n_3)^2 + (n_2+n_3-n_1)^2 + (n_3+n_2-n_1)^2\right]$$

and $\quad C_{\underline{K}} = C_{n_1 n_2 n_3} = \dfrac{2e}{L^3}\left[\dfrac{1.84}{k^2+\beta^2} - \dfrac{1}{k^2} + (-1)^{n_1+n_2+n_3}\left(\dfrac{2}{k^2+\alpha^2} + \dfrac{1}{k^2}\right)\right]$

Expressing L in units of a_o and α, β in units of a_o^{-1}, we have

$$C_{\underline{K}} = C_{n_1 n_2 \, n_3} = \frac{2\pi}{L^3}\left[\frac{1.84}{k^2+\beta^2} - \frac{1}{k^2} + (-1)^{n_1+n_2+n_3}\left(\frac{2}{k^2+\alpha^2} + \frac{1}{k^2}\right)\right]$$

in which $C_{\underline{K}}$ is expressed now in units of e/a_o.

Let $\quad N_1 = n_1 + n_2 - n_3$

$\qquad\quad N_2 = n_2 + n_3 - n_1$

$\qquad\quad N_3 = n_3 + n_1 - n_2$

$\therefore\; N_1 + N_2 + N_3 = n_1 + n_2 + n_3$.

Thus, it can be seen that N_1, N_2, N_3 are all either even or odd, and in terms of them, we get

$$C_{N_1 N_2 N_3} = \frac{2\pi}{L^3}\left[\frac{1.84}{k^2+\beta^2} - \frac{1}{k^2} + (-1)^{N_1+N_2+N_3}\left(\frac{2}{k^2+\alpha^2} + \frac{1}{k^2}\right)\right]$$

$$(2.26)$$

with $\quad k^2 = \dfrac{\pi^2}{L^2}(N_1^2 + N_2^2 + N_3^2)$.

CHAPTER THREE

WAVE FUNCTION OF POSITRON IN THE LiH CRYSTAL

Having obtained the crystal potential, we are now in a position to find the wave function of a positron moving in the field of the crystal. This wave function is needed in the calculation of the annihilation γ rays as a result of the positron interaction with an electron of the negative ion.

Let us first examine the symmetries of the crystal. Since the crystal structure is face-centred cubic, the crystal is invariant under permutations and, or separate inversions of coordinate axes in Cartesian system. That means a point in the crystal designated by the ordered triple (X,Y,Z) would under a permutation of any two and, or separate inversions of the coordinates, be transformed to a different point of the crystal lattice. Since there are 6 ways to permute 3 numbers, and two ways to choose either positive or negative from each coordinates, there are altogether 6x2x2x2 = 48 elements in the crystal group. Following Tong[4], we use the following notations to denote the generators of the group:

E	(X,Y,Z)	identity element
P_{xy}	(Y,X,Z)	element for interchange of X,Y axes
P_{yz}	(X,Z,Y)	element for interchange of Y,Z axes
P_{zx}	(Z,Y,X)	element for interchange of X,Z axes
I_x	$(-X,Y,Z)$	element for inversion of X axis
I_y	$(X,-Y,Z)$	element for inversion of Y axis
I_z	$(X,Y,-Z)$	element for inversion of Z axis

In this notation, the 48 group elements are

(X,Y,Z) (X,Z,Y) (Z,Y,X) (Y,X,Z) (Z,X,Y) (Y,Z,X)

(-X,Y,Z) (-X,Z,Y) (Z,Y,-X) (Y,-X,Z) (Z,-X,Y) (Y,Z,-X)

(X,-Y,Z) (X,Z,-Y) (Z,-Y,X) (-Y,X,Z) (Z,X,-Y) (-Y,Z,X)

(X,Y,-Z) (X,-Z,Y) (-Z,Y,X) (Y,X,-Z) (-Z,X,Y) (Y,-Z,X)

(-X,-Y,Z) (-X,Z,-Y) (Z,-Y,-X) (-Y,-X,Z) (Z,-X,-Y) (-Y,Z,-X)

(-X,Y,-Z) (-X,-Z,Y) (-Z,Y,-X) (Y,-X,-Z) (-Z,-X,Y) (Y,-Z,-X)

(X,-Y,-Z) (X,-Z,-Y) (-Z,-Y,X) (-Y,X,-Z) (-Z,X,-Y) (-Y,-Z,X)

(-X,-Y,-Z) (-X,-Z,-Y) (-Z,-Y,-X) (-Y,-X,-Z) (-Z,-X,-Y) (-Y,-Z,-X)

In his thesis, Tong has discussed the properties of this crystal symmetry group. We shall, therefore, simply state the results concerning its properties:

(1) The eigenvalues of the operators I_x, I_y, I_z and P_{xy}, P_{yz}, P_{zx} are either 1 or -1.

(2) The simultaneous eigenfunctions of all the elements of the same conjugate class in a one-dimensional representation of the group have the same eigenvalues.

Let us now come back to the physical problem. The Hamiltonian H of the system(the system of a positron moving in the crystal potential $V(r)$) is

$$H = -\tfrac{1}{2}\nabla^2 + V \qquad (3.1)$$

Note that atomic units have been used.

Since ∇^2 and V are invariant under permutations and, or separate inversions of the X,Y,Z axes in the Cartesian system, H then commutes with every element of the symmetry group. In

the case of ground state, we require maximum symmetries on the simultaneous eigenfunction of all the group elements. Thus we seek a wave function of all the group elements with eigenvalues equal to unity.

Now since the positron is moving in a periodic potential, its wave function is given by a linear combination of the Bloch type:

$$\psi = e^{i\underline{k}\cdot\underline{r}}\varphi(\underline{r})$$

with $\varphi(\underline{r})$ periodic, having the same periodicity as the crystal. For the ground state $\underline{k} = \underline{0}$, thus

$$\psi = \varphi(\underline{r}) \tag{3.2}$$

As $\varphi(\underline{r})$ is periodic in the lattice, we may Fourier analyse it in the form

$$\varphi(r) = \sum_{\underline{K}} A_{\underline{K}}\, e^{2\pi i\underline{K}\cdot\underline{r}} \tag{3.3}$$

where $\underline{K} = n_1\underline{b}_1 + n_2\underline{b}_2 + n_3\underline{b}_3$ is a vector of the reciprocal lattice, n_1, n_2, n_3 being integers.

Referring to fig.2, we see that $\underline{K}$ can be expressed in terms of the orthogonal triad $\underline{I}$, $\underline{J}$, $\underline{K}$ as

$$\underline{K} = \frac{1}{2L}\left[(n_1{+}n_2{-}n_3)\underline{I}{+}(n_2{+}n_3{-}n_1)\underline{J}{+}(n_3{+}n_2{-}n_1)\underline{K}\right] \tag{3.4}$$

$$= \frac{1}{2L}(N_1\underline{I}{+}N_2\underline{J}{+}N_3\underline{K})$$

with

$$N_1 = n_1{+}n_2{-}n_3$$
$$N_2 = n_2{+}n_3{-}n_1$$
$$N_3 = n_3{+}n_1{-}n_2$$

and it is to be noticed that N_1, N_2, N_3 are all either even or odd. Substituting (3.4) into (3.3), we get

$$\psi = \sum_{N_1 N_2 N_3} A_{N_1 N_2 N_3} \, e^{\frac{\pi i}{L}(N_1 X + N_2 Y + N_3 Z)}$$

$$= \sum_{N} A_N \, e^{\frac{\pi i}{L}(N_1 X + N_2 Y + N_3 Z)} \tag{3.5}$$

where N now denotes a set of the numbers N_1, N_2, N_3.

Having obtained the form of the function ψ, we now seek a linear combination of them to give the posiron wave function. According to Tong,[4] it is

$$\bar{\Psi} = \sum_{g} \epsilon_g g \psi \tag{3.6}$$

where ϵ_g is the eigenvalue corresponding to the eigenfunction of any group element g in the crystal symmetry group. In the present case, it equal to unity, i.e.,

$$g \bar{\Psi} = \bar{\Psi}.$$

We can rewrite (3.6) in the form

$$\bar{\Psi} = \sum_{N} A_N \chi_N$$

where $\chi_N = \sum_{g} g \, \phi_N \Big/ \Big(48 \sum_{g} \delta_{N,g(N)}\Big)^{\frac{1}{2}}$

$$\phi_N = e^{\frac{\pi i}{L}(N_1 X + N_2 Y + N_3 Z)}$$

The χ_N has been normalised to unity in this case. The convention for the summation is chosen to be $N_1 \geqslant N_2 \geqslant N_3 \geqslant 0$.

We must now determine the coefficients A_N in order to get the wave function. A total of 14 coefficients are chosen which corresponds to varying N_1, N_2, N_3 from 0 to 4, as the numbers of possible combinations are $(4,4,4)$, $(4,4,2)$, $(4,4,0)$, $(4,2,2)$ $(4,2,0)$, $(4,0,0),(3,3,3)$, $(3,3,1)$, $(3,1,1)$, $(2,2,2)$, $(2,2,0)$, $(2,0,0)$, $(1,1,1)$, and $(0,0,0)$, a total of 14.

These 14 coefficients are treated as parameters in the variation process of minimizing the expression $\mathcal{E} = \dfrac{(\Psi|H|\Psi)}{(\Psi|\Psi)}$. Now,

$$(\Psi|H|\Psi) = \sum_{N} \sum_{N'} A_N^* A_{N'} \alpha_{NN'}$$

where $\alpha_{NN'} = \dfrac{\pi^2}{2L^2}(N_1^2+N_2^2+N_3^2)\,\delta_{NN'} + \dfrac{\sum_g C_{N-g(N)}}{\left(\sum_g \delta_{N,g(N)}\right)^{\frac{1}{2}}\left(\sum_g \delta_{N',g(N')}\right)^{\frac{1}{2}}}$

$$(3.6)$$

and $\quad (\Psi|\Psi) = \sum_N |A_N|^2$

The C's are the Fourier coefficients of the crystal potential and their values are given by (2.26). Thus, the problem reduces to one of finding the extremum of $(\Psi|H|\Psi)$ subject to the condition that $(\Psi|\Psi) = 1$. We have

$$\frac{\partial}{\partial A_N^*}\left[(\Psi|H|\Psi) - \lambda(\Psi|\Psi)\right] = 0$$

or $\quad \sum_{N'} \alpha_{NN'} A_{N'} - \lambda A_N = 0 \quad$ for each N $\qquad (3.7)$

Making a convention to label the A_N as column vectors, so that (3.7) is equivalent to

$$\alpha \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ \vdots \\ \vdots \end{pmatrix} = \lambda \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ \vdots \\ \vdots \end{pmatrix}$$

$$(3.8)$$

where $\alpha = (\alpha_{NN'})$ is in fact a matrix representation of the Hamiltonian H with respect to χ_N. It is symmetric with respect to interchange of N, and N'. Equation (3.8) is equivalent to

$$H\Psi = \mathcal{E}\Psi$$

Therefore the whole problem of finding the A_N reduces to one of finding the eigenvectors of α. This process is performed with

the aid of the I.B.M. 1620 computer. The programme for such a diagonalisation and finding of eigenvectors of a symmetric matrix is available from the I.B.M. Library.

CHAPTER FOUR

ANGULAR CORRELATION OF ANNIHILATION γ RAYS IN LiH

This chapter deals with the angular correlation of the annihilation photons as a result of the singlet annihilation of the positron with an electron of the negative ion. Since the electronic clouds around the ion sites do not overlap appreciably, we can treat the annihilation from the electrons in the negative ions and those in the positive ions separately. We shall first concern ourselves with the contribution from the negative ion electrons and in a later section of this chapter, an estimate of the contribution due to the electrons in the positive ions will be given.

The wave function for the system (positron plus hydride ion) has been assumed to be a simple product of a function of the positron coordinates with a function of the coordinates of the electrons of the negative ions. If we denote the positron coordinate by $\underline{r}_1$, the electron coordinates by $\underline{r}_2$, and $\underline{r}_3$, then the spatial wave function of the system can be written as

$$\psi = g(\underline{r}_1)h(\underline{r}_2,\underline{r}_3)$$

B ecause the two electrons in the hydride ion are identical, the wave function describing the system should, for the singlet ground stat, by symmetric with respect to exchange of $\underline{r}_2$, and $\underline{r}_3$. Thus $h(r_2,r_3)$ is taken to be of the form found from Chapter2, i.e.,

$$h(r_2,r_3) = (1+\nu^2 r_{23}^2)(e^{-(\lambda r_2 + \mu r_3)} + e^{-(\mu r_2 + \lambda r_3)}) \qquad (4.1a)$$

where λ, μ, ν have been determined. Write

$h(r_2,r_3)$

$$h(\underline{r}_2,\underline{r}_3) = f(\underline{r}_2,\underline{r}_3) + f(\underline{r}_3,\underline{r}_2)$$

with $f(\underline{r}_2,\underline{r}_3) = (1+\nu^2 r_{23}^2)e^{-(\lambda r_2 + \mu r_3)}$

$f(\underline{r}_3,\underline{r}_2) = (1+\nu^2 r_{23}^2)e^{-(\mu r_2 + \lambda r_3)}$ (4.1b)

The positron wave function $g(r_1)$ is taken to be of the form found from Chapter 3. Thus,

$$g(r_1) = \sum_N A_N \chi_N$$

where $\chi_N = \sum_g g\phi_N /(48 \sum_g \delta_{N,g(N)})^{\frac{1}{2}}$ (4.1c)

$\phi_N = e^{\frac{\pi i}{L}(N_1 X + N_2 Y + N_3 Z)}$

$\therefore \quad \psi = g(\underline{r}_1)\left[f(\underline{r}_2,\underline{r}_3) + f(\underline{r}_3,\underline{r}_2)\right]$

$= f(\underline{r}_1,\underline{r}_2,\underline{r}_3) + f(\underline{r}_1,\underline{r}_3,\underline{r}_2)$ (4.1)

The Fourier transform of $f(\underline{r}_1,\underline{r}_2,\underline{r}_3)$ is

$$\varphi(\underline{p}_1,\underline{p}_2,\underline{p}_3) = (2\pi)^{-9/2}\int f(\underline{r}_1,\underline{r}_2,\underline{r}_3)\exp(-i/\hbar)(p_1 r_1 + p_2 r_2 + p_3 r_3)d^3r_1 d^3r_2 d^3r$$

Suppose ω_0 denote the vacuum state and the positron is in a "spin-up" state, then the initial state vector of the system has to take into account the creation of the positron and of two electrons corresponding to the ones in the hydride ion. Thus, we can take it to be of the form[7],

$$\omega_i = \int d^3p_1 d^3p_2 d^3p_3\, \varphi(\underline{p}_1,\underline{p}_2,\underline{p}_3)b^\dagger(\underline{p}_1,\uparrow)\left[a^\dagger(\underline{p}_2,\downarrow)a^\dagger(\underline{p}_3,\uparrow) + \right.$$
$$\left. a^\dagger(\underline{p}_3,\downarrow)a^\dagger(\underline{p}_2,\uparrow)\right]\omega_0 \quad (4.2)$$

where we have deliberately omitted the normalization factor because we shall be dealing only with the angular correlation. Thus, from now on, multiplicative constants may be omitted. In the expression, $b^\dagger$, $a^\dagger$, are the creation operators for positron and electrons; $\uparrow$ and $\downarrow$ denote spin-up and spin-down respectively.

Now the positron would annihilate with either one of the

two electrons producing two photons. The electrons that is not annihilated will be left in one of a complete set of orthonormal states. Thus, for the final state, we can take it as

$$\omega_f = \int d^3p' \; \chi(\underline{p}')a^\dagger(\underline{p}',\uparrow)c^\dagger(\underline{k},\underline{e}_1)c^\dagger(\underline{p}-\underline{k},\underline{e}_2)\,\omega_o \qquad (4.3)$$

where $(\underline{p}')$ is the Fourier transform of the state of the electron that is not annihilated. Suppose $u(\underline{r})$ is the wave function, then

$$\chi(\underline{p}') = \int d^3r \; u(\underline{r})\exp(-i/\hbar)\underline{p}'\cdot\underline{r} \qquad (4.4)$$

Furthermore, $\underline{k}$ and $\underline{p}-\underline{k}$ are the momenta of the two photons created, c is the photon creation operator, and $\underline{p}'$ is the momentum of the "left-over" electron; $\underline{e}_1$, $\underline{e}_2$ are the polarisation vectors of the two photons.

We need now the matrix element between the initial and final states. Consider equation (4.2), it consists of two terms, the first term $b^\dagger(\underline{p}_1,\uparrow)a^\dagger(\underline{p}_2,\downarrow)a^\dagger(\underline{p}_1,\uparrow)$ can be interpreted as the annihilation of the positron with electron of momentum $\underline{p}_2$. leaving an electron with momentum $\underline{p}_3$ and in spin-up state. Similarly for the term $b^\dagger(\underline{p}_1,\uparrow)a^\dagger(\underline{p}_3,\downarrow)a^\dagger(\underline{p}_2,\uparrow)$. Now the momenta involved are small, so we can replace the matrix element which normally would be a function of the momenta of the annihilating pair by its value for zero momenta.

In view of the above considerations, the matrix element is given by

$$M = M(0,0)\int d^3p' d^3p_1 d^3p_2 d^3p_3 \; \chi^*(\underline{p}') \; \varphi(\underline{p}_1,\underline{p}_2,\underline{p}_3) \times$$
$$\left[\delta^3(\underline{p}'-\underline{p}_3)\delta^3(\underline{p}-\underline{p}_1-\underline{p}_2) + \delta^3(\underline{p}'-\underline{p}_2)\delta^3(\underline{p}-\underline{p}_1-\underline{p}_3)\right] \qquad (4.5)$$

where $M(0,0)$ is the matrix element for two-photon annihilation from the singlet state of electron and positron with zero

momenta. Dropping the factor $M(0,0)$, (4.5) reduces to

$$M = \int d^3p_2 d^3p_3 \left[\chi^*(\underline{p}_3)\, \varphi(\underline{p}-\underline{p}_2,\underline{p}_2,\underline{p}_3) + \chi^*(\underline{p}_2)\, \varphi(\underline{p}-\underline{p}_3,\underline{p}_2,\underline{p}_3) \right]$$

$$= \int d^3p_2 d^3p_3 \left\{ \chi^*(\underline{p}_2)\left[\varphi(\underline{p}-\underline{p}_3,\underline{p}_2,\underline{p}_3) + \varphi(\underline{p}-\underline{p}_3,\underline{p}_3,\underline{p}_2) \right] \right\}$$

after integrations over $\underline{p}'$ and $\underline{p}_1$ and interchange of $\underline{p}_2$ and $\underline{p}_3$.
We now reintroduce the configuration space, we have,

$$\int d^3p_2 d^3p_3\ \chi^*(\underline{p}_2)\, \varphi(\underline{p}-\underline{p}_3,\underline{p}_2,\underline{p}_3)$$

$$= \int d^3p_2 d^3p_3 d^3r_1 d^3r_2 d^3r_2' d^3r_3\ u^*(\underline{r}_2') f(\underline{r}_1,\underline{r}_2,\underline{r}_3) \times$$
$$\exp\left\{ (-i/\hbar)\left[\underline{p}\cdot\underline{r}_1 + \underline{p}_2\cdot(\underline{r}_2-\underline{r}_2') + \underline{p}_3\cdot(\underline{r}_3-\underline{r}_1) \right] \right\}$$

$$= \int d^3r_1 d^3r_2 d^3r_2' d^3r_3 u^*(\underline{r}_2') f(\underline{r}_1,\underline{r}_2,\underline{r}_3)\exp\left[(-i/\hbar)\underline{p}\cdot\underline{r}_1\right]\delta^3(\underline{r}_2-\underline{r}_2')\delta^3(\underline{r}_3-\underline{r}_1$$

$$= \int d^3r_2 d^3r_3 u^*(\underline{r}_2) f(\underline{r}_3,\underline{r}_2,\underline{r}_3)\exp\left[(-i/\hbar)\underline{p}\cdot\underline{r}_3\right]$$

Similarly, $\int d^3p_2 d^3p_3\ \chi^*(\underline{p}_2)\, \varphi(\underline{p}-\underline{p}_3,\underline{p}_3,\underline{p}_2)$

$$= \int d^3r_2 d^3r_3\ u^*(\underline{r}_3) f(\underline{r}_2,\underline{r}_2,\underline{r}_3)\exp\left[(-i/\hbar)\underline{p}\cdot\underline{r}_2\right]$$

Hence, (4.6) becomes

$$M = \int d^3r_2 d^3r_3 \left\{ u^*(\underline{r}_2)\exp\left[(-i/\hbar)\underline{p}\cdot\underline{r}_3\right] f(\underline{r}_3,\underline{r}_2,\underline{r}_3) + \right.$$
$$\left. u^*(\underline{r}_3)\exp(-i/\hbar)\underline{p}\cdot\underline{r}_2\ f(\underline{r}_2,\ \underline{r}_2,\ \underline{r}_3) \right\} \qquad (4.7)$$

Summing the square of the matrix element in (4.7) over all
the final states of the surviving electron, we get, with the aid
of the closure relation for $u(\underline{r})$,

$$\sum_u |M|^2 = \int d^3r_2' d^3r_3' d^3r_2 d^3r_3 \exp\left[(i/\hbar)\underline{p}\cdot(\underline{r}_3'-\underline{r}_3)\right]\left[f(\underline{r}_3',\underline{r}_2',\underline{r}_3') + f(\underline{r}_3',\underline{r}_3',\underline{r}_2')\right]$$
$$\times \left[f(\underline{r}_3,\underline{r}_2,\underline{r}_3) + f(\underline{r}_3,\underline{r}_3,\underline{r}_2)\right]\sum_u u(\underline{r}_2')u^*(\underline{r}_2)$$

$$= \int d^3r_2' d^3r_3' d^3r_2 d^3r_3 \exp\left[(i/\hbar)\underline{p}\cdot(\underline{r}_3'-\underline{r}_3)\right]\left[f(\underline{r}_3',\underline{r}_2',\underline{r}_3') + f(\underline{r}_3',\underline{r}_3',\underline{r}_2')\right]^*$$
$$\times \left[f(\underline{r}_3,\underline{r}_2,\underline{r}_3) + f(\underline{r}_3,\underline{r}_3,\underline{r}_2)\right]\delta^3(\underline{r}_2'-\underline{r}_2)$$

$$= \int d^3r_1 d^3r_2 d^3r_3 \exp\left[(i/\hbar)\underline{p}\cdot(\underline{r}_1-\underline{r}_3)\right]\left[f(\underline{r}_1,\underline{r}_2,\underline{r}_1) + f(\underline{r}_1,\underline{r}_1,\underline{r}_2)\right]^*$$
$$\times \left[f(\underline{r}_3,\underline{r}_2,\underline{r}_3) + f(\underline{r}_3,\underline{r}_3,\underline{r}_2)\right] \qquad (4.8)$$

after integrating over $\underline{r}_2'$ and replacing $\underline{r}_3'$ by $\underline{r}_1$.

This is the basic equation for the angular correlation of the annihilation photons. To make it look symmetrical with respect to electron coordinates, we write it as

$$I = \int d^3r_1 d^3r_2 d^3r_3 \exp\left[(i/\hbar)\underline{p}\cdot(\underline{r}_2-\underline{r}_3)\right]\left[f(\underline{r}_2,\underline{r}_1,\underline{r}_2)+f(\underline{r}_2,\underline{r}_2,\underline{r}_1)\right]^*$$
$$\times \left[f(\underline{r}_3,\underline{r}_1,\underline{r}_3)+f(\underline{r}_3,\underline{r}_3,\underline{r}_1)\right] \tag{4.9}$$

where we have interchanged $\underline{r}_1$ and $\underline{r}_2$.

Now from (4.1), we have

$$\left[f(\underline{r}_2,\underline{r}_1,\underline{r}_2)+f(\underline{r}_2,\underline{r}_2,\underline{r}_1)\right]^*\left[f(\underline{r}_3,\underline{r}_1,\underline{r}_3)+f(\underline{r}_3,\underline{r}_3,\underline{r}_1)\right]$$

$$= g^*(\underline{r}_2)g(\underline{r}_3)(1+\nu^2 r_{12}^2)(1+\nu^2 r_{13}^2)\left[e^{-(\lambda r_1+\mu r_2)}+e^{-(\mu r_1+\lambda r_2)}\right] \times$$
$$\left[e^{-(\lambda r_1+\mu r_3)}+e^{-(\mu r_1+\lambda r_3)}\right]$$

$$= g^*(\underline{r}_2)g(\underline{r}_3)(1+\nu^2 r_{12}^2)(1+\nu^2 r_{13}^2)\left[e^{-(2\lambda r_1+\mu r_2+\mu r_3)}+e^{-(\lambda+\mu)r_1+\mu r_2+\lambda r_3)}\right.$$
$$\left.+ e^{-((\lambda+\mu)r_1+\lambda r_2+\mu r_3)}+e^{-(2\mu r_1+\lambda r_2+\lambda r_3)}\right] \tag{4.10}$$

But from (4.1σ),

$$g(\underline{r}) = \frac{\sum\limits_{N} A_N \sum\limits_{g} g\left[e^{\frac{\pi i}{L}(N_1 X+N_2 Y+N_3 Z)}\right]}{\left[48 \sum\limits_{g} \delta_{N,g(N)}\right]^{\frac{1}{2}}}$$

where the group element g operating on the function $e^{\frac{\pi i}{L}(N_1 X+N_2 Y+N_3 Z)}$ is the same as permuting and taking the negatives of the numbers N_1, N_2, N_3. Denoting $N_1 X+N_2 Y+N_3 Z$ as a scalar product, we have

$$g(\underline{r}) = \frac{\sum\limits_{N} A_N \sum\limits_{g} g\, e^{\frac{\pi i}{L}\underline{N}\cdot\underline{r}}}{\left[48 \sum\limits_{g} \delta_{N,g(N)}\right]^{\frac{1}{2}}} \tag{4.11}$$

$$\therefore \quad g^*(\underline{r}_2)g(\underline{r}_3) = \frac{\sum\limits_{N}\sum\limits_{N'} A_N A_{N'} \sum\limits_{g} g\left[e^{-\frac{\pi i}{L}\underline{N}\cdot\underline{r}_2}\right]\sum\limits_{g'} g'\left[e^{+\frac{\pi i}{L}\underline{N}'\cdot\underline{r}_3}\right]}{\left[48 \sum\limits_{g} \delta_{N,g(N)}\right]^{\frac{1}{2}}\left[48 \sum\limits_{g'} \delta_{N',g'(N')}\right]^{\frac{1}{2}}} \tag{4.12}$$

where g, g' operate on N, N' respectively.

The integrand in (4.9) becomes

$$\sum_N \sum_{N'} A_N^* A_{N'} \exp\left[(i/\hbar)\underline{p}\cdot(\underline{r}_3-\underline{r}_2)\right] \sum_{g,g'} g\left[e^{-\frac{\pi i}{L}\underline{N}\cdot\underline{r}_2}\right] g'\left[e^{\frac{\pi i}{L}\underline{N}'\cdot\underline{r}_3}\right] \times$$

$$(1+\nu^2 r_{12}^2)(1+\nu^2 r_{13}^2)\left[e^{-(2\lambda r_1+\mu r_2+\mu r_3)}+e^{-(\lambda+\mu)r_1+\mu r_2+\lambda r_3)}+\right.$$
$$\left. e^{-((\lambda+\mu)r_1+\lambda r_2+\mu r_3)}+e^{-(2\mu r_1+\lambda r_2+\lambda r_3)}\right]/\left[48\sum_g \delta_{N,g(N)}\right]^{\frac{1}{2}}\left[48\sum_{g'}\delta_{N',g'(N')}\right]^{\frac{1}{2}}$$

If we are dealing with a large number of crystals oriented at random which is usually the case experimentally, the above expression has to be averaged over all directions of $\underline{p}$. Two ways of performing the integration seem possible: (1) to average over all directions of $\underline{p}$ first and then perform the spatial integration, (2) to do it in the reverse order. It seems to be simpler to adopt the first procedure.

Thus we first average over all directions of $\underline{p}$. To do this, we replace the integral I by its integral over solid angles in $\underline{p}$ space divided by 4π.

$$\therefore \quad I = \frac{1}{4\pi}\int I d\Omega_p$$

The only term in I that contains $\underline{p}$ is $e^{(-i/\hbar)\underline{p}\cdot(\underline{r}_3-\underline{r}_2)}$, so we need only average this term over $\underline{p}$ and the rest is left unchanged. Hence,

$$I =\int d^3r_1 d^3r_2 d^3r_3 \frac{\sin p r_{23}}{p r_{23}}\sum_N \sum_{N'} \sum_{g,g'} e^{\frac{\pi i}{L}(\underline{N}'\cdot\underline{r}_3-\underline{N}\cdot\underline{r}_2)} \times$$

$$(1+\nu^2 r_{12}^2)(1+\nu^2 r_{13}^2)\left[e^{-(2\lambda r_1+\mu r_2+\mu r_3)}+e^{-((\lambda+\mu)r_1+\mu r_2+\lambda r_3)}+\right.$$
$$\left. e^{-((\lambda+\mu)r_1+\lambda r_2+\mu r_3)}+e^{-(2\mu r_1+\lambda r_2+\lambda r_3)}\right]/\left[48\sum_g \delta_{N,g(N)}\right]^{\frac{1}{2}}\left[48\sum_{g'}\delta_{N',g'(N')}\right]^{\frac{1}{2}}$$

$$(4.13)$$

where $r_{23}=|\underline{r}_2-\underline{r}_3|$ and the vectors N, N' are to be operated on by g and g'.

Rewriting (4.13) as

$$I = \frac{\sum\limits_{N}\sum\limits_{N'} A_N^* A_{N'} \sum\limits_{g}\sum\limits_{g'}{}'}{48\left[\sum\limits_{g}\delta_{N,g(N)}\right]^{\frac{1}{2}}\left[\sum\limits_{g'}\delta_{N',g'(N')}\right]^{\frac{1}{2}}} \int d^3r_1 d^3r_2 d^3r_3 \frac{\sin pr_{23}}{pr_{23}} e^{\frac{\pi i}{L}(\underline{N}'\cdot\underline{r}_3 - \underline{N}\cdot\underline{r}_2)}$$

$$x\ (1+\nu^2 r_{12}^2)(1+\nu^2 r_{13}^2)\left[e^{-(2\lambda r_1 + \mu r_2 + \mu r_3)} + e^{-((\lambda+\mu)r_1 + \mu r_2 + \lambda r_3)} + \right.$$
$$\left. e^{-((\lambda+\mu)r_1 + \lambda r_2 + \mu r_3)} + e^{-(2\mu r_1 + \lambda r_2 + \lambda r_3)}\right] \tag{4.13a}$$

We can now integrate (4.13a) over $\underline{r}_1$. The integral involved is

$$\mathcal{J} = \int d^3r_1\ (1+\nu^2 r_{12}^2)(1+\nu^2 r_{13}^2)\ e^{-ar_1}$$

where a is a constant. Now

$$\mathcal{J} = \int d^3r_1 e^{-ar_1} + \nu^2\int d^3r_1 r_{12}\ e^{-ar_1} + \nu^2\int d^3r_1 r_{13}\ e^{-ar_1} + \nu^4\int d^3r_1 r_{12}r_{13}e^{-ar_1}$$
$$= \mathcal{J}_1 + \nu^2\mathcal{J}_2 + \nu^2\mathcal{J}_3 + \nu^4\mathcal{J}_4$$

The first three integrals are easy to evaluate, we shall try to evaluate the fourth integral first. To integrate this, choose $\underline{r}_3$ as the polar axis (fig. 4.1)
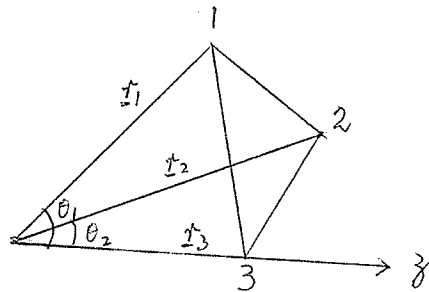

Fig. 4.1

Let $\underline{r}_1 = (r_1,\ \theta_1,\ \varphi_1) = (r_1\sin\theta_1\cos\varphi_1,\ r_1\sin\theta_1\sin\varphi_1,\ r_1\cos\theta_1)$
$\underline{r}_2 = (r_2, \theta_2, \varphi_2) = (r_2\sin\theta_2\cos\varphi_2,\ r_2\sin\theta_2\sin\varphi_2,\ r_2\cos\theta_2)$
$\underline{r}_3 = (0,0,r_3)$

We need the expression for the angle between $\underline{r}_1$ and $\underline{r}_2$ and also the angle between $\underline{r}_3$ and $\underline{r}_1$.

Now $\quad \underline{r}_1 \cdot \underline{r}_3 = r_1 r_3 \cos\theta_1$ $\qquad$ (4.14a)

$$\frac{\underline{r}_1 \cdot \underline{r}_2}{r_1 r_2} = \sin\theta_1 \cos\varphi_1 \; \sin\theta_2 \cos\varphi_2 \; \sin\theta_1 \sin\varphi_1 \sin\theta_2 \sin\varphi_2 + \cos\theta_1 \cos\theta_2$$

$$= \sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2) + \cos\theta_1 \cos\theta_2 \qquad (4.14b)$$

$\therefore$ making use of (4.14a) and (4.14b), one gets

$$\mathcal{I}_4 = \int d^3 r_1 r_{12}^2 r_{13}^2 \, e^{-ar_1} = \int\int \left\{ r_1^2 + r_2^2 - 2r_1 r_2 \left[\sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2) + \cos\theta_1 \cos\theta_2 \right] \right\}$$

$$\times (r_1^2 + r_3^2 - 2r_1 r_3 \cos\theta_1) e^{-ar_1} r_1^2 \sin\theta_1 \, dr_1 d\theta_1 d\varphi_1$$

Since $\quad \displaystyle\int_0^{2\pi} \cos(\varphi_1 - \varphi_2) d\varphi_1 = 0$

$$\int_0^{\pi} \sin\theta_1 \cos\theta_1 d\theta_1 = 0$$

$$\therefore \quad \mathcal{I}_4 = \int (r_1^2 + r_2^2)(r_1^2 + r_3^2) e^{-ar_1} r_1^2 \sin\theta_1 \, dr_1 d\theta_1 d\varphi_1$$

$$+ \int (r_1^2 e^{-ar_1} \sin\theta_1 \cos^2\theta_1 \cos\theta_2 \cdot 4 r_1^2 r_2 r_2 \, dr_1 d\theta_1 d\varphi_1$$

$$= 4\pi \int_0^\infty (r_1^2 + r_2^2)(r_1^2 + r_3^2) \, e^{-ar_1} r_1^2 dr_1 + \frac{16\pi}{3} \cos\theta_2 \int_0^\infty r_1^4 r_2 r_3 e^{-ar_1} \, dr_1$$

But $\quad \cos\theta_2 = \dfrac{r_2^2 + r_3^2 - r_{23}^2}{2 r_2 r_3}$

$$\therefore \quad \mathcal{I}_4 = 4\pi \int_0^\infty (r_1^2 + r_2^2)(r_1^2 + r_3^2) r_1^2 e^{-ar_1} \, dr_1 + \frac{8\pi}{3}(r_2^2 + r_3^2 - r_{23}^2) \int_0^\infty r_1^4 e^{-ar_1} \, dr_1$$

$$= 4\pi \left[\frac{6!}{a^7} + (r_2^2 \; r_3^2) \frac{4!}{a^5} + r_2^2 r_3^2 \frac{2!}{a^3} \right] + \frac{8\pi}{3}(r_2^2 + r_3^2 - r_{23}^2) \frac{4!}{a^5}$$

$\mathcal{I}_2$ can be evaluated by choosing $\underline{r}_2$ to be the polar axis.

Thus $\quad \underline{r}_1 = (r_1, \theta_1, \varphi_1)$

$\qquad \underline{r}_2 = (0, 0, r_2)$

$$\therefore \mathcal{I}_2 = \int (r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_1) r_1^2 \sin\theta_1 \, e^{-ar_1} \, dr_1 d\theta_1 d\varphi_1$$

$$= 4\pi \int_0^\infty r_1^2 (r_1^2 + r_2^2) e^{-ar_1} \, dr_1 = 4\pi \left[\frac{4!}{a^5} + r_2^2 \frac{2!}{a^3} \right]$$

Similarly, $\mathcal{I}_3 = 4\pi \left[\dfrac{4!}{a^5} + r_3^2 \dfrac{2!}{a^3} \right]$

and $\mathcal{J}_1 = 4\pi \dfrac{2!}{a^3}$

$\therefore \quad \mathcal{J} = 4\pi \dfrac{2!}{a^3} + 4\pi\nu^2\left[\dfrac{4!}{a^5} + r_2^2 \dfrac{2!}{a^3}\right] + 4\pi\nu^2\left[\dfrac{4!}{a^5} + r_3^2 \dfrac{2!}{a^3}\right] +$

$4\pi\nu^4\left[\dfrac{6!}{a^7} + (r_2^2 \ r_3^2)\dfrac{4!}{a^5} + r_2^2 r_3^2 \dfrac{2!}{a^3}\right] + \dfrac{8\pi\nu^4}{3}(r_2^2 \ r_3^2 - r_{23}^2)\dfrac{4!}{a^5}$

$= 8\pi\left(\dfrac{1}{a^3} + \dfrac{24\nu^2}{a^5} + \dfrac{360\nu^4}{a^7}\right) + 8\pi(r_2^2 \ r_3^2)\nu^2\left(\dfrac{1}{a^3} + \dfrac{20^2}{a^5}\right)$

$- 8\pi\nu^4 r_{23}^2 \dfrac{8}{a^5} + 8\pi\nu^4 r_2^2 r_3^2 \dfrac{1}{a^3} \quad .$

Thus, I is now of the form,

$$I = \dfrac{\sum_N \sum_{N'} A_N^* A_{N'} \sum_g \sum_{g'}}{48\left[\sum_g \delta_{N,g(N)}\right]^{\frac{1}{2}}\left[\sum_{g'} \delta_{N',g'(N')}\right]^{\frac{1}{2}}} \int d^3r_2 d^3r_3 \ \dfrac{\sin pr_{23}}{pr_{23}} \ e^{\frac{\pi i}{L}(\underline{N}'\cdot\underline{r}_3 - \underline{N}\cdot\underline{r}_2)}$$

$$\times \ e^{-(br_2 + cr_3)}$$

where b, c are constants. We have now 4 types of integrals involved, namely,

(1) $\displaystyle\int \dfrac{\sin pr_{23}}{pr_{23}} \ e^{\frac{\pi i}{L}(\underline{N}'\cdot\underline{r}_3 - \underline{N}\cdot\underline{r}_2) - br_2 - cr_3} \ d^3r_2 d^3r_3$

(2) $\displaystyle\int \dfrac{\sin pr_{23}}{pr_{23}} \ e^{\frac{\pi i}{L}(\underline{N}'\cdot\underline{r}_3 - \underline{N}\cdot\underline{r}_2) - br_2 - cr_3}(r_2^2 + r_3^2) d^3r_2 d^3r_3$

(3) $\displaystyle\int \dfrac{\sin pr_{23}}{pr_{23}} \ e^{\frac{\pi i}{L}(\underline{N}'\cdot\underline{r}_3 - \underline{N}\cdot\underline{r}_2) - br_2 - cr_3} \ r_{23}^2 \ d^3r_2 d^3r_3$

(4) $\displaystyle\int \dfrac{\sin pr_{23}}{pr_{23}} \ e^{\frac{\pi i}{L}(\underline{N}'\cdot\underline{r}_3 - \underline{N}\cdot\underline{r}_2) - br_2 - cr_3} \ r_2^2 r_3^2 \ d^3r_2 d^3r_3$

An exact evaluation of these integrals is not practical. We note that the values of A_N is largest when $\underline{N} = (0,0,0)$, and

(35)

decreases very rapidly as N_1, N_2, N_3 increases. In fact, only the first few terms need be considered. In all of the integrals involved, we have ultimately to multiply them by the product $A_N^* A_{N'}$, and then perform the summation. A glance of the table for the first five coefficients of A_N shows that the products with one factor equal to $A_{(0,0,0)}$ are much larger than any other products.

$A_{N'}^* A_{N'}$ \\ $A_N^* A_N$	A_{222}	A_{220}	A_{200}	A_{111}	A_{000}
A_{222}	.0001	.0003	.0009	-.001	-.009
A_{220}	.0003	.0009	.0027	-.003	-.027
A_{200}	.0009	.0027	.0081	-.009	-.081
A_{111}	-.001	-.003	-.009	.01	.09
A_{000}	-.009	-.027	-.081	.09	.81

Table showing products of $A_N^* A_{N'}$

Furthermore, all the integrals decrease as the length of the vector (N_1, N_2, N_3) increases and the value is largest for $\underline{N}$ or $\underline{N}' = \underline{0}$. Thus, it is quite reasonable to consider those integrals with either $\underline{N}$ or $\underline{N}'$ equal to zero.

An obvious method to perform the integration is, of course, to expand $\sin pr_{23}/pr_{23}$ in terms of a power series and then perform the integration term by term. But it was found that the resulting series so formed is a slowly convergent one. Thus, we shall adopt the former procedure and in a later section indicate the error involved in such an approximation.

Hence, we set $\underline{N} = \underline{0}$ in all of the above integral types. All of them can be evaluated if we express the volume element $d^3r_2 d^3r_3$ in terms of three lengths and three suitable angles[10]. The results of integrations are:

$$(1) = \int \frac{\sin pr_{23}}{pr_{23}} e^{\frac{\pi i}{L}(\underline{N}' \cdot \underline{r}_3 - \underline{N} \cdot \underline{r}_2) - br_2 - cr_3} \, d^3r_2 d^3r_3$$

$$= (8\pi)^2 \frac{bc}{\alpha^2 \gamma \delta}$$

$$(2) = \int \frac{\sin pr_{23}}{pr_{23}} e^{\frac{\pi i}{L}(\underline{N}' \cdot \underline{r}_3 - \underline{N} \cdot \underline{r}_2) - br_2 - cr_3} (r_2^2 + r_3^2) \, d^3r_2 d^3r_3$$

$$= (8\pi)^2 \frac{12bc\,\beta}{\alpha^4 \gamma \delta} + (8\pi)^2 \frac{2bc\,\epsilon}{\alpha^2 \gamma^3 \delta^3}$$

$$(3) = \int \frac{\sin pr_{23}}{pr_{23}} e^{\frac{\pi i}{L}(\underline{N}' \cdot \underline{r}_3 - \underline{N} \cdot \underline{r}_2) - br_2 - cr_3} r_2^2 r_3^2 \, d^3r_2 d^3r_3$$

$$= (8\pi)^2 \frac{24bc\,\beta\epsilon}{\alpha^4 \gamma^3 \delta^3}$$

$$(4) = \int \frac{\sin pr_{23}}{pr_{23}} e^{\frac{\pi i}{L}(\underline{N}' \circ \underline{r}_3 - \underline{N} \cdot \underline{r}_2) - br_2 - cr_3} r_{23}^2 \, d^3r_2 d^3r_3$$

$$= (8\pi)^2 \frac{12bc\,\beta}{\alpha^4 \gamma \delta} + (8\pi)^2 \frac{32bcp^2(\frac{\pi^2}{L^2}N'^2 - p^2 - c^2)}{\alpha^2 \gamma^3 \delta^3} + (8\pi)^2 \frac{2bc\,\epsilon}{\alpha^2 \gamma^3 \delta^3}$$

where
$$\alpha = b^2 + p^2$$
$$\beta = b^2 - p^2$$
$$\gamma = c^2 + (p - \frac{\pi}{L} N')^2$$
$$\delta = c^2 + (p + \frac{\pi}{L} N')^2$$
$$\epsilon = 6c^6 + 6c^4(p^2 + \frac{\pi^2}{L^2}N'^2) - 9c^2(p^2 - \frac{\pi^2}{L^2}N'^2)^2 - 6[(p^2 + \frac{\pi^2}{L^2}N'^2)x$$

$$(p^2 - \frac{\pi^2}{L^2}N'^2)^2] + c^2[(p + \frac{\pi}{L}N')^4 + (p - \frac{\pi}{L}N')^2 + (p - \frac{\pi}{L}N')^4]$$

---

[10] See Chapter 2 equation (2.13)

All of these integrals involve$\not$ only the length of (N_1', N_2', N_3') and because $g'(|N'|) = |N'|$, $g'(|N'|^2) = |N'|^2$, we have for the summation over g and g', simply a factor of 48x48 because there are 48 elements in the group.

Having evaluated the integrals, we can now perform the summation over N and N'. For this, a total of five coefficients were chosen corresponding to the vectors $(0,0,0)$, $(1,1,1)$, $(2,0,0)$, $(2,2,0)$ and $(2,2,2)$. The expression for which the summation is to be performed is given in the appendix. The summation is performed with the aid of the I.B.M. 1620 computer.

Results

The following table shows the results obtained for different values of p. In this calculation, the common multiplicative factor of $(8\pi)^3/48$ has been omitted.

p ($\mathring{A}^{-1}$)	Integral (total contribution) (arbitrary units)	Values from different values of N.				
		(0,0,0)	(1,1,1)	(2,0,0)	(2,2,0)	(2,2,2)
0.0	12.37	12.35	.06	-.03	-.01	-.001
0.1	11.39	11.37	.06	-.03	-.005	-.0007
0.2	8.98	8.96	.05	-.03	-.005	-.0007
0.3	6.22	6.21	.046	-.02	-.004	-.0006
0.4	3.95	3.94	.04	-.02	-.003	-.0005
0.5	2.41	2.40	.03	-.02	-.003	-.0004
0.6	1.48	1.46	.025	-.01	-.002	-.0003
0.7	0.93	0.92	.02	-.01	-.002	-.0003
0.8	0.61	0.60	.017	-.009	-.001	-.0002
0.9	0.42	0.41	.015	-.008	-.001	-.0002
1.0	0.30	0.30	.013	-.007	-.001	-.0002

A graph showing the angular correlation as a function of p shows a value of p at half height equal to $3.1 \mathring{A}^{-1}$. If we fit the

(37a)

ANGULAR CORRELATION CURVE FOR H⁻ ELECTRONS

Half-height occurs at $p = .31 \text{Å}^{-1}$
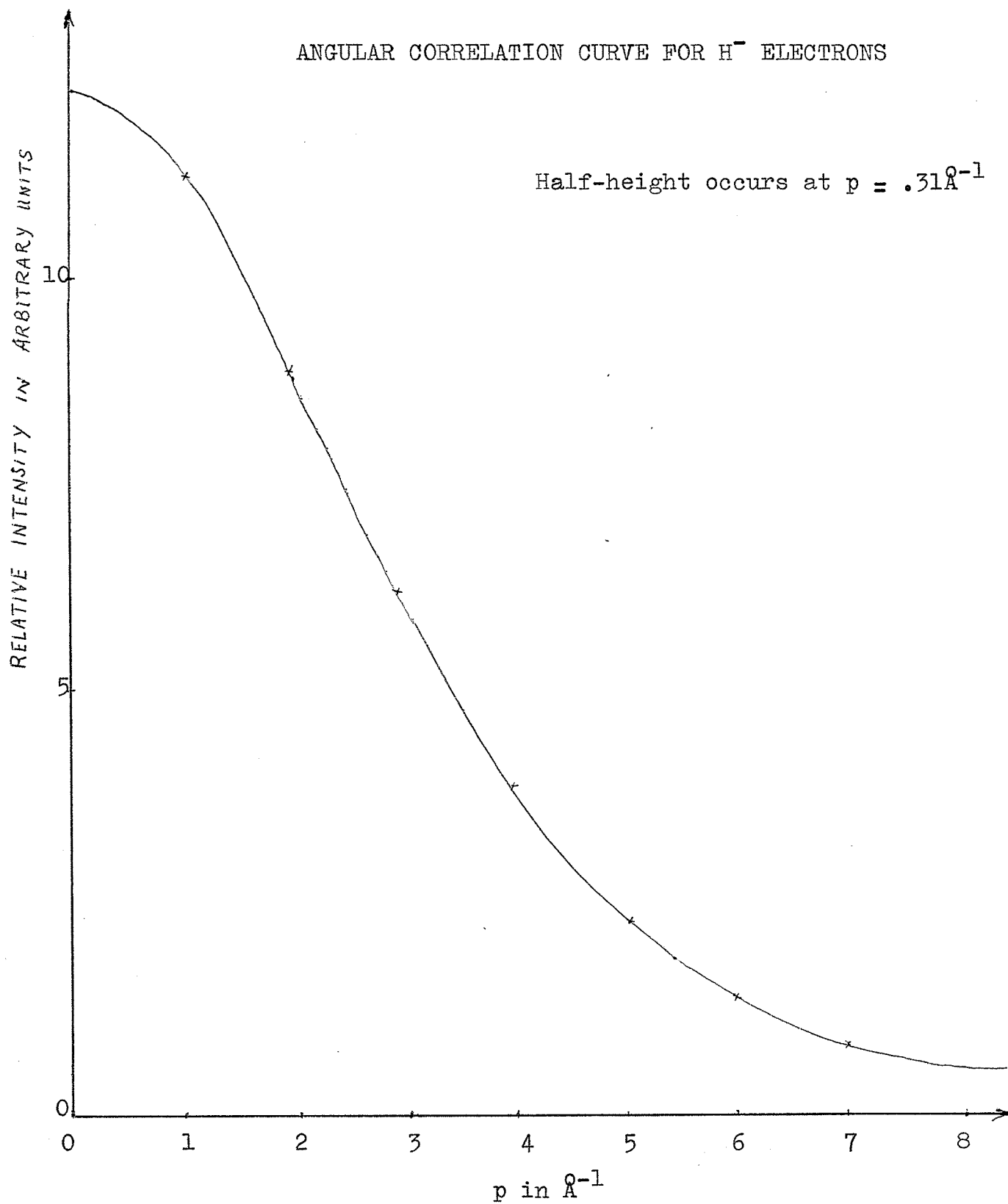
peak of the graph with an inverted parabola of the form

$$y = 1 - \tfrac{1}{2}b^2 p^2$$

we get at half height $b = 1/p$. In our case, $b = 3.3$ Å.

Estimation of Error

The error introduced by the neglect of coefficients for $N > (2,2,2)$ is assumed to be negligible since the product $A_N^* A_{N'}$ is very small as compared with the rest. Thus, normally for each value of p the result consists of a summation of 25 terms as there are 5 coefficients altogether. In the calculation we have set $N = 0$, so the summation becomes only a sum of 5 terms. Since the expression is symmetrical with respect to N and N', we have in fact obtained the summation as a sum of 9 terms. Thus we would like to account for the effect of the remaining 16 terms. That is, the terms with the 4 sets of products

$$A_{222}A_{222} \ , \quad A_{222}A_{220} \ , \quad A_{222}A_{200} \ , \quad A_{222}A_{111}$$

$$A_{220}A_{222} \ , \quad A_{220}A_{220} \ , \quad A_{220}A_{200} \ , \quad A_{220}A_{111}$$

$$A_{200}A_{222} \ , \quad A_{200}A_{220} \ , \quad A_{200}A_{200} \ , \quad A_{200}A_{111}$$

$$A_{111}A_{222} \ , \quad A_{111}A_{220} \ , \quad A_{111}A_{200} \ , \quad A_{111}A_{111}$$

In order to do this, we assume the integrals corresponding to the 4 products in each set be equal to one with $\underline{N'} = \underline{0}$. This maximizes the estimate of error because the integral with $\underline{N'} = \underline{0}$ has the largest value. Thus for the point $p = 0$, the absolute

error is $\quad -\cdot 0008\sqrt{48}\sqrt{6}\left(\frac{\cdot 0001}{\sqrt{6}\sqrt{6}} + \frac{\cdot 0003}{\sqrt{6}\sqrt{4}} + \frac{\cdot 0009}{\sqrt{6}\sqrt{8}} + \frac{-\cdot 001}{\sqrt{6}\sqrt{6}} \right) - \cdot 0052\sqrt{48}\sqrt{6}\left(\frac{\cdot 0003}{\sqrt{6}\sqrt{6}} + \frac{\cdot 0009}{\sqrt{6}\sqrt{4}} + \frac{\cdot 0027}{\sqrt{6}\sqrt{8}} - \frac{\cdot 03}{\sqrt{6}\sqrt{6}} \right)$

$-\cdot 0314\sqrt{48}\sqrt{6}\left(\frac{\cdot 0009}{\sqrt{6}\sqrt{6}} + \frac{\cdot 0027}{\sqrt{6}\sqrt{4}} + \frac{\cdot 0081}{\sqrt{6}\sqrt{8}} - \frac{\cdot 009}{\sqrt{6}\sqrt{6}} \right) + \cdot 06\sqrt{48}\sqrt{6}\left(-\frac{\cdot 001}{\sqrt{6}\sqrt{6}} - \frac{\cdot 003}{\sqrt{6}\sqrt{4}} - \frac{\cdot 009}{\sqrt{6}\sqrt{8}} + \frac{\cdot 01}{\sqrt{6}\sqrt{6}} \right)$

which is negligible compared with 12.37. Similarly, we can calculate the error for the other points. It can be seen that

the error involved is actually negligible.

Effect of the electrons in the Li ions

We can get a rough estimate of the effect of the Li ion
electrons on the angular correlation. Since the first term in the
wave function for the positron is very big compared with the rest,
we shall try to estimate the effect by taking only this term
for the wave function of positron. For the wave function of the
Li ion, we use a function obtained by *a* variational method, namely,

$$\psi_{Li} = e^{-\alpha(r_2 + r_3)}$$

where $\alpha = Z'/a_0$ and Z' is the effective charge on the ion as
found from *the* variational method. It is equal to 2.69 . a_0 is the
first Bohr radius. Thus $\alpha = 5.08 \mathring{A}^{-1}$.

To get the expression describing this effect, we go back
to equation (4.9). After averaging over all directions of $\underline{p}$, we
get

$$I_{Li} = A_{000}^2 \int d^3r_1 d^3r_2 d^3r_3 \frac{\sin pr_{23}}{pr_{23}} \left[2e^{-\alpha(r_1+r_2)}\right]\left[2e^{-\alpha(r_1+r_3)}\right] \tag{4.15}$$

In order to compare the results, we have to normalised ψ_{Li} to
the same constant as the ψ_H. Thus, setting $(\psi_H, \psi_H) = (\psi_{Li}, \psi_{Li})$
We have the normalisation constant K for ψ_{Li} given by

$$K^2 \int e^{-2\alpha(r_3 \, r_2)} d^3r_2 d^3r_3 = \frac{\pi^2 K^2}{\alpha^6} = (\psi_H, \psi_H) = \pi^2 \times \frac{.0017777}{.3393^6}$$

$$\therefore \quad K^2 = \alpha^6 \times 1.16$$

Furthermore we have to put back the constant that has been
dropped in the case of the hydride ion. Taking all these facts
into account, (4.15) becomes

$$I_{Li} = \frac{24 \times .99^2 \times 1.16\alpha^5}{(\alpha^2 + p^2)^4}$$

This expression has a central maximum at $p = 0$ equal to approximately 0.2 and has the half width occurring at $p = 2.04\text{Å}^{-1}$. Comparing this result with the one for the hydride ion, it is seen that the effect due to the electrons of the Li ions can be neglected.

CHAPTER FIVE

POSITRON ENERGY AT THE BOUNDARIES OF THE FIRST BRILLOIN ZONE IN LiF

The method and mathematical expressions used in this calculation are very similar to those in Tong's thesis[4]. Thus, the wave function of the positron in the LiF crystal is assumed to be a combination of Bloch states of the form

$$\psi_{\underline{k}} = e^{i\underline{k}\cdot\underline{r}}\varphi(\underline{r}) \qquad (5.1)$$

where $\varphi(\underline{r})$ has the periodicity of the lattice. (5.1) is the eigenfunction with eigenvalue $E_{\underline{k}}$ satisfying the equation

$$H\psi_{\underline{k}} = E_{\underline{k}}\psi_{\underline{k}}$$

in which H is the Hamiltonian of the system of a positron moving in the field of the crystal, $\underline{k}$ is the wave vector ending on the surface of the first Brilloin zone.

We now seek the trial wave function. It must have the same periodicity as the crystal and must be ~~invariant under the~~ a simultaneous eigenfunction ~~operations of every~~ of all the group elements. Thus, as is in Tong's thesis, we take it to be of the form

$$\overline{\psi} = \sum_{\mathcal{N}} A_{\mathcal{N}} \sum_{g} \epsilon_g \, g\left[e^{\left[\frac{\pi i}{L}(\mathcal{N}_1 X + \mathcal{N}_2 Y + \mathcal{N}_3 Z)\right]} \right]$$

$$\overline{\psi} = \sum_{\mathcal{N}} A_{\mathcal{N}} \chi_{\mathcal{N}}$$

where $\mathcal{N}_1$, $\mathcal{N}_2$, $\mathcal{N}_3$ are half intergers, $\mathcal{N}$ is a set of them, and ϵ_g is the eigenvalue of the group element.

The symmetry properties at the bottom and top of the first Brilloin zone are different. At these boundaries, the value of ϵ_g

take on the following values[11].

$$\epsilon_g = \begin{cases} 1 & \text{for inversions} \\ 1 & \text{for permutations} \end{cases}$$

and
$$\epsilon_g = \begin{cases} 1 & \text{for inversions} \\ -1 & \text{for permutations} \end{cases}$$

We now need the average value of the Hamiltonian H. It is

given by $\mathcal{E} = \langle H \rangle = \dfrac{(\bar{\Psi}|H|\bar{\Psi})}{(\bar{\Psi}|\bar{\Psi})}$

with $(\bar{\Psi}|H|\bar{\Psi}) = \sum_N \sum_{N'} A_N^* A_{N'} (\chi_N|H|\chi_{N'})$

$$= \sum_N \sum_{N'} A_N^* A_{N'} \alpha_{NN'}$$

where $\alpha_{NN'} = \dfrac{\pi^2}{2L^2}(N_1^2 + N_1^2 + N_1^2)\delta_{NN'} + \dfrac{\sum_g \epsilon_g C_{N-g(N')}}{\left[\sum_g \epsilon_g \delta_{N,g(N)}\right]^{\frac{1}{2}}\left[\sum_g \epsilon_g \delta_{N',g(N')}\right]^{\frac{1}{2}}}$

and the C_N are the Fourier coefficients of the crystal potential in

LiF. Furthermore,

$$(\bar{\Psi}|\bar{\Psi}) = |A_N|^2$$

We can now minimize $\mathcal{E} = \dfrac{(\bar{\Psi}|H|\bar{\Psi})}{(\bar{\Psi}|\bar{\Psi})}$ with respect to the

parameters A_N^*. Our problem is the same as to find the extremum

of $(\bar{\Psi}|H|\bar{\Psi})$ subject to the condition $(\bar{\Psi}|\bar{\Psi}) = 1$. Thus, we have

$$\frac{\partial}{\partial A_N^*}\left[(\bar{\Psi}|H|\bar{\Psi}) - \lambda(\bar{\Psi}|\bar{\Psi})\right] = 0 \quad \text{for each } N$$

and so $\sum_N \alpha_{NN'} A_{N'} - \lambda A_N = 0 \quad \text{for each } N \quad (5.2)$

Following the same procedures as in Chapter 3, we make a convention

to label A_N as a column vector so that (5.2) becomes

$$\alpha \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ \vdots \end{pmatrix} = \lambda \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ \vdots \end{pmatrix}$$

where α is the matrix $\alpha_{NN'}$. It is symmetrical with respect to

---

(11) Jones: Theory of Brilloin Zones and Electronic States in
crystals Chapter 3. (North Holland Publishing Company,
Amsterdam)

N and N'. The problem thus reduces to one of diagonlaizing $\mathscr{K}$. The smallest eigenvalue gives the minimum energy. Such a diagonalization was performed with the aid of the I.B.M. 1620 computer.

Results

The results of calculation give a value for $\mathcal{E}$ at the boundaries of the first Brilloin zone equal to 1.088 and 1.093 a.u. of energy. This gives a gap of 0.005 a.u. of energy which is 0.07 e.v.

Since the crystal on the whole is electrically neutral, the average value of the crystal potential over space would be zero. Thus, the correction due to shift of origin of the crystal potential is

$$V_{shift} = \lim_{S \to \infty} \frac{1}{S^3} \int V \, d\tau_R$$

$$= c_{000}$$

$$= \frac{2\pi}{L^3} \left[\frac{2}{\alpha^3} + \frac{4.7}{\beta^2} \right]$$

$$= 12.08 \text{ e.v.}$$

For the case of positron, the true energy is then $\dfrac{(\Psi|H|\Psi)}{(\Psi|\Psi)}$ - 12.08e.v. Thus the energies at the boundaries are 2.72 and 2.79 e.v.

(44)

CHAPTER SIX

DISCUSSIONS AND CONCLUSIONS

The angular correlation of the annihilation γ rays in LiH crystals as a result of positron interaction with electrons in the hydride ion has been calculated. The graph of angular correlation as a function of momentum gives a width at half height equal to 0.31Å^{-1}. If the peak of the graph is fitted with an inverted parabola of the form $y = 1 - \frac{1}{2}b^2p^2$, then at half height we get a value of $b = 3.3\text{Å}$. This has to be compared with the experimental value of 1.2Å by Stewart[6] and the theoretical value of 5.2Å by Neamtan et al[7].

Gol'danskii et al[8] in a recent paper have reported that in LiH a close fit to the experimental angular correlation curve is achieved. They used a self-consistent field method to calculate the wave function of the system and obtained for the ground state an energy of the e^+H^- system to be -1.335 a.u. Neamtan et al[7], however, obtained a value of -1.517 a.u. by using a variational procedure. This means that the result of Gol'danskii et al is 2.48 e.v. higher than that obtained by Neamtan et al. However, the results which Neamtan et al obtained is an upper bound , and the big difference in the energies indicates that the wave function used by Gol'danskii et al cannot be a very accurate description of the system.

The present result, in unit of Å^{-1}, is however, 2.75 narrower by a factor of ~~times narrower~~ than

the experimental value. This can be attributed to many factors.
First, the contributions from the electrons of the lithium ions
have been neglected. However, as can be seen from the estimate
obtained in Chapter 4, its effect is small as far as the half
width is concerned, because the amplitude of the central maximum
of the angular correlation curve is very much smaller than in
the case of the hydride ion. Its contribution is significant
only at large values of momenta. Thus, one can regard the con-
tribution to the angular correlation as ~~arises~~ arising solely from the
positrons interacting with the electrons in the negative ion.

Polarisation effects as well as the annihilation from
excited states have also been neglected. These effects would tend
to increase the energy and momentum of the system and as a
result, the angular correlation curve would be widened.

A remark about the positron wave function is in order. It
is to be noted that the constant term in the expansion is large
compared with the rest of the terms. Furthermore, the function
does not seem to vanish at any point in the crystal lattice.
This is not at all too unreasonable because, after all, the
potential of the crystal was Fourier analysed and only a finite
number of terms have been taken. Thus, the Coulomb term is no
longer present and so we do not necessarily require the wave
function to vanish.

It is interesting to see what is the average energy of the
positron if we just take the first five coefficients in the
expansion and then compare it with the value obtained when all

the 14 coefficients were used. To this end, we pick out the
corresponding 5x5 matrix in the matrix representation of the
Hamiltonian. Thus we have the average energy equal to

$$
(-.01,-.03,-.09,.1,.99)
\begin{pmatrix}
8.8 & .75 & .53 & -.40 & .23 \\
.75 & 6.6 & .86 & -.66 & .37 \\
.53 & .86 & 3.7 & -.67 & .42 \\
-.40 & -.66 & -.67 & 3.4 & -.41 \\
.23 & .37 & .42 & -.41 & .53
\end{pmatrix}
\begin{pmatrix}
-.01 \\
-.03 \\
.09 \\
.1 \\
.99
\end{pmatrix}
$$

which is .431 a.u. This has to be divided by the length of the
vector (-.01,-.03,-.09,.1,.99) which turns out to be .99. Thus
the average energy is .431 a.u. and the value obtained from
I.B.M. computer using 14 coefficients is .429 a.u. Thus, it is
seen that the approximation which we introduced in the evaluation
of the angular correlation in Chapter 4 is justifiable.

The positron energies at the boundaries of the first
Brilloin zone in LiF have been found to be 2.72 and 2.79 e.v.
respectively making a gap of .07 e.v. The relation of this energy
gap to the Ore gap in the crystal is shown in the following
figure:-

Figure showing the positron gap and the Ore gap
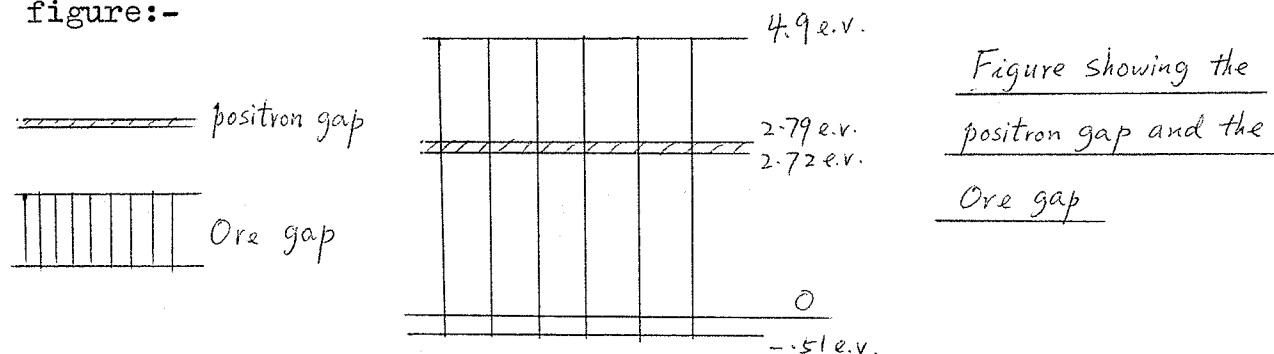
It is seen that the positron gap falls within the Ore gap but is
so narrow as to have little effect. Thus, no definite conclusion
can be drawn as to why the τ_2- component in LiF should be absent.

APPENDIX 1

Table of the Integrals occurred in (2.10)

1. $\displaystyle\int e^{-(ar_2 + br_3)}\, d^3r_2 d^3r_3 = \frac{64\pi^2}{(ab)^3}$

2. $\displaystyle\int e^{-(ar_2 + br_3)}\, r_{23}^{-1}\, d^3r_2 d^3r_3 = \frac{32\pi^2(a^2 + 3ab + b^2)}{(ab)^2(a+b)^3}$

3. $\displaystyle\int e^{-(ar_2 + br_3)}\, r_{23}\, d^3r_2 d^3r_3 = \frac{64\pi^2(3a^4 + 9a^3b + 11a^2b^2 + 9ab^3 + 3b^4)}{(ab)^4(a+b)^3}$

4. $\displaystyle\int e^{-(ar_2 + br_3)}\, r_{23}^2\, d^3r_2 d^3r_3 = \frac{48\cdot(4\pi)^2(a^2 + b^2)}{(ab)^5}$

5. $\displaystyle\int e^{-(ar_2 + br_3)}\, r_{23}^3\, d^3r_2 d^3r_3 = \frac{12(8\pi)^2(5a^6 + 15a^5b + 21a^4b^2 + 23a^3b^3 + 21a^2b^4 + 15ab^5 + 5b^6)}{(ab)^6(a+b)^3}$

6. $\displaystyle\int e^{-(ar_2 + br_3)}\, r_{23}^4\, d^3r_2 d^3r_3 = 48\times 30(4\pi)^2\left(\frac{1}{a^7b^3} + \frac{4}{3a^5b^5} + \frac{1}{a^3b^7}\right)$

7. $\displaystyle\int e^{-(ar_2 + br_3)}\left(\frac{1}{r_2} + \frac{1}{r_3}\right) d^3r_2 d^3r_3 = \frac{32\pi^2(a+b)}{(ab)^3}$

8. $\displaystyle\int e^{-(ar_2 + br_3)}\left(\frac{1}{r_2} + \frac{1}{r_3}\right) r_{23}^2\, d^3r_2 d^3r_3 = \frac{3(8\pi)^2(a+b)}{(ab)^4} + \frac{6(8\pi)^2(a^3 + b^3)}{(ab)^5}$

9. $\displaystyle\int e^{-(ar_2 + br_3)}\left(\frac{1}{r_2} + \frac{1}{r_3}\right) r_{23}^4\, d^3r_2 d^3r_3 = 60\times(8\pi)^2\left(\frac{3}{a^2b^7} + \frac{1}{a^3b^6} + \frac{2}{a^4b^5} + \frac{2}{a^5b^4} + \frac{1}{a^6b^3} + \frac{3}{a^7b^2}\right)$

10. $\displaystyle\int e^{-(ar_2 + br_3)}\frac{1}{r_2}(1 + \nu^2 r_{23}^2)(r^2 - r^2 + r_{23}^2)\, d^3r_2 d^3r_3$

$$= \frac{384\pi^2}{a^4b^3} + 120\times 64\pi^2\nu^2\left(\frac{1}{a^4b^5} + \frac{1}{a^6b^3}\right)$$

APPENDIX   2

Fourier Coefficients for the wave function of positron in LiH

Coefficient	Value at minimum energy
A_{444}	$-.00073540$
A_{442}	$-.00223532$
A_{440}	$-.00199524$
A_{422}	$-.00500601$
A_{420}	$-.00721032$
A_{400}	$-.00560202$
A_{333}	$-.00016465$
A_{331}	$-.00046848$
A_{311}	$-.00012355$
A_{222}	$-.01143770$
A_{220}	$-.03196170$
A_{200}	$-.09282904$
A_{111}	$.10410818$
A_{000}	$.98958393$

APPENDIX 3

Expression for angular correlation over which summation is to be performed

The Expression is $\dfrac{1}{\left[\sum\limits_{g}\delta_{N,g(N)}\right]^{\frac{1}{2}}\left[\sum\limits_{g}\delta_{N',g(N')}\right]^{\frac{1}{2}}} \times E$ where

$$E = RA\left(\frac{1}{WA^2 \cdot WE \cdot WG}\right) + RB\left(\frac{1}{WB^2 \cdot WF \cdot WH}\right) + RC\left(\frac{1}{WB^2 \cdot WE \cdot WG} + \frac{1}{WA^2 \cdot WF \cdot WH}\right)$$

$$+ RD\left(\frac{6\,WC}{WA^4 \cdot WE \cdot WG} + \frac{WM}{WA^2 \cdot WE^3 \cdot WG^3}\right) + RE\left(\frac{6\,WD}{WB^4 \cdot WF \cdot WH} + \frac{WK}{WB^3 \cdot WF^3 \cdot WH^3}\right)$$

$$+ RF\left(\frac{6\,WD}{WB^4 \cdot WE \cdot WG} + \frac{6\,WC}{WA^4 \cdot WF \cdot WH} + \frac{WM}{WB^2 \cdot WE^3 \cdot WG^3} + \frac{WK}{WA^2 \cdot WF^2 \cdot WH^3}\right)$$

$$- \frac{RG \cdot p^2(WL \cdot W - WA)}{WA^3 \cdot WE^2 \cdot WG^2} - \frac{RH \cdot p^2(WL \cdot W - WB)}{WB^3 \cdot WF^2 \cdot WH^2} - RI\, p^2\left(\frac{WL \cdot W - WA}{WB^3 \cdot WE^2 \cdot WG^2} + \frac{WL \cdot W - WB}{WA^3 \cdot WF^2 \cdot WH}\right)$$

$$+ RJ \cdot \frac{WC \cdot WM}{WA^4 \cdot WE^3 \cdot WG^3} + RK \cdot \frac{WD \cdot WK}{WB^4 \cdot WF^3 \cdot WH^3} + RL\left(\frac{WD \cdot WM}{WB^4 \cdot WE^3 \cdot WG^3} + \frac{WC \cdot WK}{WA^4 \cdot WF^3 \cdot WA^3}\right)$$

with $RA = \mu^2\left(\dfrac{1}{8\lambda^3} + \dfrac{24\nu^2}{32\lambda^5} + \dfrac{360\nu^4}{128\lambda^7}\right)$, $RB = \lambda^2\left(\dfrac{1}{8\mu^3} + \dfrac{24\nu^2}{32\mu^5} + \dfrac{360\nu^4}{128\mu^7}\right)$

$RC = \lambda\mu\left(\dfrac{1}{(\lambda+\mu)^3} + \dfrac{24\nu^2}{(\lambda+\mu)^5} + \dfrac{360\nu^4}{(\lambda+\mu)^7}\right)$, $RD = 2\nu^2\left(\dfrac{1}{8\lambda^3} + \dfrac{12\nu^2}{32\lambda^5}\right)$

$RE = 2\nu^2\left(\dfrac{1}{8\mu^3} + \dfrac{12\nu^2}{32\mu^5}\right)$, $RF = 2\lambda\mu\nu^2\left(\dfrac{1}{(\lambda+\mu)^3} + \dfrac{12\nu^2}{(\lambda+\mu)^5}\right)$

$RG = \dfrac{8\mu^2\nu^4}{\lambda^5}$, $RH = \dfrac{8\lambda^2\nu^4}{\mu^5}$, $RI = \dfrac{3\mu\lambda\nu^4}{(\lambda+\mu)^3}$, $RJ = \dfrac{3\mu^2\nu^4}{\lambda^3}$

$RK = \dfrac{3\lambda^2\nu^4}{\mu^3}$, $RL = \dfrac{24\lambda\mu\nu^4}{(\lambda+\mu)^3}$; $W = N_1^2 + N_2^2 + N_3^2$, $WN = \sqrt{W}$.

$WA = \mu^2 + p^2$, $WB = \lambda^2 + p^2$, $WC = \mu^2 - p^2$, $WD = \lambda^2 - p^2$,

$WE = \mu^2 + (p - WL \times WLN)^2$, $WF = \lambda^2 + (p - WL \times WLN)^2$, $WG = \mu^2 + (p + WL \times WLN)^2$

$WH = \lambda^2 + (p + WL \times WLN)^2$, $WI = p^2 + WL \times W$, $WJ = p^2 - WL \times W$,

$WK = 6\lambda^6 + 6\lambda^4 WI - 9\lambda^2 WJ^2 + \lambda^2(4WI^2 - WJ^2) - 6WI \times WJ^2$

$WM = 6\mu^6 + 6\mu^4 WI - 9\mu^2 WJ^2 + \mu^2(4WI^2 - WJ^2) - 6WI \times WJ^2$

$WL = \pi^2/2.043^2$, $WLN = \pi/2.043$, $\lambda = .9123$, $\mu = 2.0333$, $\nu = .3393$.

SUPPLEMENT

The following supplement gives a list of the computer programmes used in this thesis. We shall give below a short explanatory note to each of them.

Explanatory notes

Programme 1

In this programme, we vary the two variables ~~occurred~~ *occurring* in the expression $\dfrac{-B^2(\xi, \eta)}{A(\xi,\eta)C(\xi,\eta)}$, where $A(\xi, \eta)$, $B(\xi, \eta)$, $C(\xi, \eta)$ are given by equations (2.18a), (2.18b) and (2.18c), independently. That is, we first keep one variable fixed and vary the other until an extremum value in energy is obtained. Then we keep this variable at the value which corresponds to an energy extremum and vary the other variable in the same fashion. This procedure is done by means of a "Sense Switch" statement.

Programme 2

The logic in this programme is straight-forward.

Programme 3

This programme is very much similar to the one used by Tong[4] in the calculation of the Fourier Coeffiecients of the Crystal Potential in LiF. The factor $(-1)^{N_1 + N_2 + N_3}$ is taken cared of by means of an "IF" statement.

Statements 3, 16, and 17 take care of the range of the summation. The results are being punched out.

Programme 4

This programme is the same as the one used by Tong in the calculation of matrix elements of positron in LiF. The programme for the diagonalization and finding of eigenvectors is available from I.B.M. library.

Programme 5

The logic in the summation process is straight forward. Here the sum $\sum_{j} \delta_{N, g(N)}$ has been calculated before-hand, for the values of N_1, N_2, N_3 used.

Programme 1

Programme for the variation of ,   in the expression

```
  1 FORMAT (F14.8, F14.8)
 10 FORMAT (E14.8, E14.8, E8.2)
  4 FORMAT (E14.8, E14.8, E8.2)
    DIMENSION A(4), B(5), C(2), D(31), E(31), F(31), G(31)
 11 IF (SENSE SWITCH 2)20,21
 20 READ 4, P,Q,R
    GO TO 2
 21 READ 10, S,T,U
  2 DO 5 I = 1,31
    XI = I
    IF (SENSE SWITCH 1)200,210
200 X = P (XI-16.)*R*P
    Y = Q (XI-16.)*R*Q
    GO TO 22
210 X = S+(XI-16.)*U*T
    Y = T+(XI-16.)*U*S
 22 Z = X-Y
    A(1) = 4.*(X+Y)/(Z*Z*Z)+24./(Z*Z*Z)+192.*X*Y/(Z*Z*Z*Z*Z)
    A(2) = 1440.*X*Y*(X+Y)/(Z*Z*Z*Z*Z*Z*Z)+4.*(X*X)-4.*Y/(X*X*X)
    A(3) = 24./(X*X*X)+156./(X*X*X*X)-48.*Y/(X*X*X*X)
           -300.*Y/(X*X*X*X*X)
    A(4) = 156.*(X+Y)/(Z*Z*Z*Z*Z)
    B(1) = 11./(4.*X*X*X)+109./(4.*X*X*X*X)+1125./(8.*X*X*X*X*X)
    B(2) = -72./(Z*Z*Z*Z)+510./(Z*Z*Z*Z*Z)+96.*X/(Z*Z*Z*Z*Z)
           +4./(Z*Z*Z)
    B(3) = -1800.*X/(Z*Z*Z*Z*Z*Z)+1440.*X*X/(Z*Z*Z*Z*Z*Z*Z)
           -1./(X*X*X)
    B(4) = 3./(X*Z*Z*Z)-9./(X*Z*Z*Z*Z)-1./(4.*X*X*Z)
    B(5) = 1./(4.*X*X*Z*Z)-3./(8.*X*X*Z*Z*Z)
    C(1) = 2./(Z*Z*Z)+24.*(X Y)/(Z*Z*Z*Z*Z)+150./(Z*Z*Z*Z*Z)
           +2./(X*X*X)
    C(2) = 720.*X*Y/(Z*Z*Z*Z*Z*Z*Z)+24./(X*X*X*X)+150./(X*X*X*X*X)
    D(I) = A(1)+A(2)+A(3)+A(4)
    E(I) = B(1)+B(2)+B (3)+B(4)+B(5)
    F(I) = C(1)+C(2)
    G(I) = 13.6*E(I)*E(I)*X/(D(I)*F(I))
  5 PUNCH 1,X,Y,G(I)
    PAUSE
    GO TO 11
    END
```

Programme 2

Curve fitting, expression (2.21)

```
1 FORMAT (E8.2, 10X, E11.5)
  G = .0017777/((.3393)**6.)
  X = .9123
  Y = 2.0333
  Z = .3393
2 DO 3 I = 1,7
  XI = I
  R = .4 (XI-1.)*.2
  W = X+Y
  A1 = 1./(4.*Y*Y*Y)+Z*Z*R*R/(2.*Y*Y*Y)+3.*Z*Z/(2.*Y*Y*Y*Y*Y)
  A2 = Z*Z*Z*Z*R*R*R*R/(4.*Y*Y*Y)+5.*Z*Z*Z*Z*R*R/(2.*Y*Y*Y*Y*Y)
  A3 = 45.*Z*Z*Z*Z/(8.*Y*Y*Y*Y*Y*Y*Y)
  E1 = 2/*X*R
  A = (A1+A2+A3)*4.*EXP(-E1)
  B1 = 1./(4.*X*X*X)+Z*Z*R*R/(2.*X*X*X)+3.*Z*Z/(2.*X*X*X*X*X)
  B2 = Z*Z*Z*Z*R*R*R*R/(4.*X*X*X)+5.*Z*Z*Z*Z*R*R/(2.*X*X*X*X*X)
  B3 = 45.*Z*Z*Z*Z/(8.*X*X*X*X*X*X*X)
  E2 = 2.*Y*R
  B = (B1+B2+B3)*4.*EXP(-E2)
  C1 = 2./(W*W*W)+4.*Z*Z*R*R/(W*W*W)+48.*Z*Z/(W*W*W*W*W)
  C2 = 2.*Z*Z*Z*Z*R*R*R*R/(W*W*W)+80.*Z*Z*Z*Z*R*R/(W*W*W*W*W)
  C3 = 720.*Z*Z*Z*Z/(W*W*W*W*W*W*W)
  E3 = W*R
  C = (C1+C2+C3)*8.*EXP(-E3)
  H = A+B+C
  P = 8.*H*R/G
  Q = LOG(P)
3 PRINT 1,R,Q
  PAUSE
  END
```

Programme 3

Fourier Coefficients of Crystal Potential in LiH
Expression (2.26)

```
 1 FORMAT (I1,I1,I1,F12.8)
   DIMENSION B(4)
   ALPHA = (4.152*0.5292)**2.
   BETA = (1.805*0.5292)**2/
   XL = 2.043/0.5292
   XK = 8.0
   XJ = 8.0
   XI = 8.0
 7 A = XI*XI+XJ*XJ+XK*XK
   C = (A*3.14159*3.14159)/(XL*XL)
   B(1) = 2./(C+ALPHA)
   B(2) = 1.84/(C+BETA)
   N = XI+XJ+XK
   IF (N-(N/2)*2)8,8,9
 8 B(4) = B(1)+B(2)
   GO TO 10
 9 B(4) = B(2)-B(1)-2./C
10 B(3) = 4.*3.14159*B(4)/(XL*XL*XL)
   I = XI
   J = XJ
   K = XK
   IJ = I+J
   JK = J+K
   IF (IJ-(IJ/2)*2)2,2,3
 2 IF (JK-(JK/2)*2)4,4,3
 4 PUNCH 1,I,J,K,B(3)
 3 XK = K-1
   IF (XK)16,7,7
16 XJ = J-1
   XK = XJ
   IF (XJ)17,7,7
17 XI = I-1
   XJ = XI
   XK = XI
   IF (XI)18,7,7
18 PAUSE
   END
```

Programme   4

Matrix elements for the ground state of e^{+} in LiH

This programme is the same as the one used by Tong[4] for the calculation of matrix elements for the ground state of e^{+} in LiF. The only change made here is to replace the corresponding parameters for LiH.

Programme   5

Summation of the angular correlation expression as given

in Appendix 3

```
  9 FORMAT (I1,I1,I1,E14.8)
  1 FORMAT (F4.1,10X,F4.1,F4.1,F4.1,E14.8)
    DIMENSION X(3),C(3,3,3)
    WL = 3.14159*3.14159/(2.043*2.043)
    WLN = 3.14159/2.043
    T = .9123
    U = 2.0333
    V = .3393
    Z = 2.9456
    RA1 = U*U*(1./(8.*T*T*T)+3.*V*V/(4.*T*T*T*T*T))
    RA2 = U*U*45.*V*V*V*V/(16.*T*T*T*T*T*T*T)
    RA = RA1+RA2
    RB1 = T*T*(1./(8.*U*U*U)+3.*V*V/(4.*U*U*U*U*U))
    RB2 = T*T*45.*V*V*V*V/(16.*U*U*U*U*U*U*U)
    RB = RB1+RB2
    RC1 = T*U*(1./(Z*Z*Z)+24.*V*V/(Z*Z*Z*Z*Z))
    RC2 = T*U*360.*V*V*V*V/(Z*Z*Z*Z*Z*Z*Z)
    RC = RC1+RC2
    RD =.25*U*U*V*V*(1./(T*T*T)+3.*V*V/(T*T*T*T*T))
    RE =.25*T*T*V*V*(1./(U*U*U)+3.*V*V/(U*U*U*U*U))
    RF =2.*T*U*V*V*(1./(Z*Z*Z)+12.*V*V/(Z*Z*Z*Z*Z))
    RG = 8.*V*V*V*V*U*U/(T*T*T*T*T)
    RH = 8.*V*V*V*V*T*T/(U*U*U*U*U)
    RI = 256.*T*U*V*V*V*V/(Z*Z*Z*Z*Z)
    RJ = 3.*V*V*V*V*U*U/(T*T*T)
    RK = 3.*V*V*V*V*T*T/(U*U*U)
    RL = 24.*V*V*V*V*T*U/(Z*Z*Z)
  3 READ 9,I,J,K,G
    I = I+1
    J = J+1
    K = K+1
    C(I,J,K) = G
    IF(K-1)130,130,3
130 IF(J-1)131,131,3
131 IF(I-1)132,132,3
132 CONTINUE
    A=0.0
    Q=48.
    QN = SQRTF(Q)
  8 X(1) = 2.0
    X(2) = 2.0
    X(3) = 2.0
  7 IF(X(1)-X(2))10,11,10
 10 IF(X(2)-X(3))12,13,12
 11 IF(X(1)-X(3))14,15,14
```

```
12 IF(X(3))16,17,16
13 IF(X(2))17,19,17
14 IF(X(3))17,18,17
15 IF(X(1))20,21,20
16 S = 1.0
   GO TO 22
17 S = 2.0
   GO TO 22
18 S = 4.0
   GO TO 22
19 S = 8.0
   GO TO 22
20 S = 6.0
   GO TO 22
21 S = 48.0
22 SN = SQRTF(S)
   LX = X(1)
   MX = X(2)
   NX = X(3)
   L = LX+1
   M = MX+1
   N = NX+1
   W = X(1)*X(1)+X(2)*X(2)+X(3)*X(3)
   WN = SQRTF(W)
   WA = U*U+A*A
   WB = T*T+A*A
   WC = U*U-A*A
   WD = T*T-A*A
   WE = U*U+(A-WN*WLN)*(A-WN*WLN)
   WF = T*T+(A-WN*WLN)*(A-WN*WLN)
   WG = U*U+(A+WN*WLN)*(A+WN*WLN)
   WH = T*T+(A+WN*WLN)*(W+WN*WLN)
   WI = A*A+WL*W
   WJ = A*A-WL*W
   WK1 =6.*T*T*T*T*T*T+6.*T*T*T*T*WI-9.*T*T*WJ*WJ
   WK2 =T*T*(4.*WI*WI-WJ*WJ)-6.*WI*WJ*WJ
   WK = WK1+WK2
   WM1 =6.*U*U*U*U*U*U+6.*U*U*U*U*WI-9.*U*U*WJ*WJ
   WM2 =U*U*(4.*WI*WI-WJ*WJ)-6.*WI*WJ*WJ
   WM = WM1+WM2
   P1 =RA*(1./(WA*WA*WE*WG))+RB*(1./(WB*WB*WF*WH))
   P2 =RC*(1./(WB*WB*WE*WG)+1./(WA*WA*WF*WH)
   P3 =RD*(6.*WC/(WA*WA*WA*WA*WE*WG)+WM/(WA*WA*WA*WE*WE*WE*WG*WG*WG))
   P4 =RE*(6.*WD/(WB*WB*WB*WB*WF*WH)+WK/(WB*WB*WB*WF*WF*WF*WH*WH*WH))
   P5 =RF*(6.*WD/(WB*WB*WB*WB*WE*WG)+6.*WC/(WA*WA*WA*WA*WF*WH)
   P6 =RF*(WM/(WB*WB*WE*WE*WE*WG*WG*WG)+WK/(WA*WA*WF*WF*WF*WH*WH*WH))
   P7 =-RG*A*A*(WL*W-WA)/(WA*WA*WA*WE*WE*WG*WG)
   P8 =-RH*A*A*(WL*W-WB)/(WB*WB*WB*WF*WF*WH*WH)
   P9 =-RI*A*A*(WL*W-WA)/(WB*WB*WB*WE*WE*WG*WG)
   P10 =-RI*A*A*(WL*W-WB)/(WA*WA*WA*WF*WF*WH*WH)*WF*WH)
   P11 =RJ*WC*WM/(WA*WA*WA*WA*WE*WE*WE*WG*WG*WG)
```

```
P12 = RK*WD*WK/(WB*WB*WB*WB*WF*WF*WF*WH*WH*WH)
P13 = RL*WD*WM/(WB*WB*WB*WB*WE*WE*WE*WG*WG*WG)
P14 = RL*WC*WK/(WA*WA*WA*WA*WF*WF*WF*WH*WH*WH)
PP1 =P1+P2+P3+P4+P5+P6+P7
PP2 =P8+P9+P10+P11+P12+P13+P14
P = (PP1+PP2)*48.*48.*C(L,M,N)*C(1,1,1)
P = P/(QN*SN)
PUNCH 1,A,X(1),X(2),X(3),P
X(3) = X(3)-2.0
IF(X(3))24,7,7
24 X(2) = X(2)-2.0
X(3) = X(2)
IF (X(2))25,7,7
25 X(1) = X(1)-1.0
X(2) = X(1)
X(3) = X(1)
IF (X(1))26,7,7
26 A = A+0.1
IF (A-1.2)8,8,29
29 PAUSE
END
```