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MÖSSBAUER GAMMA-RAY DIFFRACTION.

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Dedicated to Aenne and Chris, my parents, and Mr. and Mrs

F. J. Patrick.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>II</td>
<td>RESONANT SCATTERING</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td>A. Single Nucleus</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td>B. Multi Nuclei System</td>
<td>12</td>
</tr>
<tr>
<td></td>
<td>C. Phonon Effects</td>
<td>18</td>
</tr>
<tr>
<td>III</td>
<td>INTERFERENCE BETWEEN AND ELECTRONIC SCATTERING</td>
<td>19</td>
</tr>
<tr>
<td></td>
<td>A. Electronic Scattering</td>
<td>19</td>
</tr>
<tr>
<td></td>
<td>B. Interference Between Nuclear and Electronic Scattering</td>
<td>27</td>
</tr>
<tr>
<td>IV</td>
<td>DYNAMICAL THEORY OF MÖSSBAUER DIFFRACTION</td>
<td>49</td>
</tr>
<tr>
<td></td>
<td>A. Scattering From a Plane Layer</td>
<td>49</td>
</tr>
<tr>
<td></td>
<td>B. Multilayer Crystal-Dynamical Theory of Mössbauer Scattering</td>
<td>58</td>
</tr>
<tr>
<td></td>
<td>(i) Off Bragg</td>
<td>67</td>
</tr>
<tr>
<td></td>
<td>(ii) Bragg Scattering</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td>(a) Isotropic Resonant Scattering</td>
<td>72</td>
</tr>
<tr>
<td></td>
<td>(b) Isotropic Mössbauer Scattering</td>
<td>77</td>
</tr>
<tr>
<td></td>
<td>(c) Polarized Ferromagnetic</td>
<td>92</td>
</tr>
<tr>
<td></td>
<td>(d) Antiferromagnetic Scattering</td>
<td>95</td>
</tr>
<tr>
<td></td>
<td>(iii) Louie Diffraction - Bormann Transmission</td>
<td>98</td>
</tr>
<tr>
<td></td>
<td>(iv) Grazing Incidence</td>
<td>101</td>
</tr>
<tr>
<td>V</td>
<td>ACKNOWLEDGEMENTS</td>
<td>106</td>
</tr>
<tr>
<td>REFERENCES</td>
<td></td>
<td>107</td>
</tr>
<tr>
<td>APPENDIX</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
I. INTRODUCTION

One of the most powerful methods which has been employed to gain an understanding of the properties of solids has been to study the scattering of waves from solids, such as x-ray and neutron diffraction. With the discovery of the Mössbauer effect it has become of interest to investigate the possibility of gamma-ray diffraction experiments using Mössbauer radiation incident on a crystal containing the resonant nuclei. As we will see, the nuclear scattering amplitude is dependent upon the magnetic and vibrational properties of the crystal and can be varied rapidly by passing through resonance. Mössbauer scattering should therefore offer an excellent method for studying various solid state properties. Also by substituting Mössbauer atoms into substances such as organic molecules and changing the nuclear scattering amplitude by Doppler shifting the incident radiation, one could obtain much more information about the molecular structure than can be obtained by x-ray techniques.

The primary difficulty with doing scattering experiments with the resonant radiation is that the absorption cross sections are orders of magnitude larger than the scattering cross sections, so that little scattering would be expected. For example, for non Zeeman split Fe$^{57}$, the absorption cross section is

$$\sigma_a = 2\pi x_0^2 \left( \frac{2I+1}{2J+1} \right) \left( \frac{e^{-\frac{1}{2} \lambda^2 \Delta^2 / \sigma^2}}{(\Delta^2 + \sigma^2)^{3/2}} \right) = 1.1 \times 10^{-6}$$

at resonance, while the elastic scattering cross section at resonance is

$$\sigma_e = (\sigma_a^e / \sigma_a) \sigma_a = 5.3 \times 10^{-4}$$  (1)

It is for this reason that almost all Mössbauer experiments so far carried out have been absorption experiments. However, we will see that near Bragg angles, because of the interactions of the resonant nuclei, the effective coherent elastic scattering widths are greatly enhanced over that of a single nucleus, with a consequent suppression of inelastic and absorptive processes. These width enhancements cause either high $\gamma$-ray reflection or high transmission. Various aspects of the width enhancement have been discussed semiclassically in references\textsuperscript{2, 3}. These modes of excitation correspond to the superradiant states of Dicke which occur in gamma-ray emission\textsuperscript{4, 5}. 
The general quantum equations that we derive are valid for any type of Mössbauer transitions (e.g., MI, E2, etc.). For concreteness in working out the optics of a Mössbauer system, we take Fe$^{57}$ as a typical example. The Fe$^{57}$ Mössbauer transition is particularly convenient. This is a M1 nuclear transition which produces a 14.4 KeV Mössbauer gamma-ray. The wavelength of 86A is well suited for diffraction experiments. In figure (1) we show the level diagram for Fe$^{57}$ imbedded in a ferromagnetic Fe$^{56}$ lattice:

Fig. 1. Level diagram of Fe$^{57}$ imbedded in ferromagnetic Fe$^{56}$. The six possible magnetic dipole transitions produce 14.4 KeV gamma-rays which are polarized. $\tilde{E}_{(x)}$ ($\Delta m = \pm 1$), $\tilde{E}_{(0)}$ ($\Delta m = 0$).

The width of the excited $\frac{3}{2}$ state is $\gamma = 4.9 \times 10^{-9}$ e.v. with corresponding lifetime $\tau = 1.4 \times 10^{-7}$ sec. The separation of the two ground states is $g_0 = 1.9 \times 10^{-7}$ e.v., and for the excited states $g_1 = 1.1 \times 10^{-7}$ e.v. The internal conversion coefficient is $\alpha = 27^\circ$ and the radiative width is $\gamma = \gamma / (1 + \alpha) = 4.6 \times 10^{-9}$ e.v. Diagram (b) gives the unpolarized hyperfine pattern with the relative intensities (squares of Clebsch-Gordon coefficients involved).

In addition to ferromagnetic Fe$^{57}$, Fe$^{57}$ imbedded in Fe$_2$O$_3$ is antiferromagnetic with slightly larger values of $g_0$, $g_1$, and Fe$^{57}$ imbedded in stainless steel is unsplit, isotropic (magnetically disordered state). We will consider the optics of these three systems.

*) There is some discrepancy on this value. Cambel and Bernstein$^{(7)}$ and others use $\alpha = 15$. 
Before deriving the correct quantum expressions governing resonant optics, it is useful to summarize the classical treatment of single atom scattering, and the non resonant quantum approximation in order to gain insight into the corrections necessary.

Non-resonant scattering can be treated very easily both classically and quantum mechanically. The classical model is the scattering light by an oscillator with characteristic frequency \( \omega_0 \). The force equation is
\[
\ddot{x} + \omega_0^2 x = \frac{\hbar^2}{m} \frac{\vec{E}_0 \cdot \vec{E}}{\omega_0^2 - \omega^2} e^{-i\omega t}
\]
which has the solution
\[
\vec{x} = \frac{\vec{E}_0 \cdot \vec{E}}{(\omega_0^2 - \omega^2)} e^{-i\omega t}
\]

The emitted radiation field with transverse polarization \( \hat{e} \) is
\[
\hat{e} \cdot \vec{E}_{rad} = \hat{e} \cdot \frac{\vec{E}_0 \cdot \vec{E}}{k^2} \frac{n \times (n \times \vec{x})}{(k - \omega t)}
\]
\[
= \left( \frac{\epsilon_0^2}{m c^2} \right) \left( \frac{\omega_0^4 - \omega^4}{\omega_0^2 - \omega^2} \right) \left( \frac{\hat{e} \cdot \vec{E}_0 \cdot \vec{E}}{k} \right) \left( \delta(k - \omega t) \right)
\]
which gives the intensity distribution
\[
I(\theta) = \left( \frac{\hbar^2}{k^2} \right) \left( \frac{\epsilon_0^2}{m c^2} \right) \left( \frac{\omega_0^4 - \omega^4}{\omega_0^2 - \omega^2} \right) \sin^2 \theta d\alpha
\]
\[
I = \left( \frac{\hbar^2}{k^2} \right) \left( \frac{\epsilon_0^2}{m c^2} \right) \left( \frac{\omega_0^4 - \omega^4}{\omega_0^2 - \omega^2} \right)
\]

In quantum mechanics, the non-resonant scattering can be treated by time dependent perturbation theory. The Dirac relativistic Hamiltonian for a particle in a potential \( v \), interacting with radiation is
\[
H = (\vec{p} + \vec{e} \cdot \vec{v} + m\beta) - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} (\alpha_R \gamma^r e^{ikx} + \alpha_L \gamma^l e^{-ikx}) + \Sigma_{k = 1}^N \alpha_k \gamma^k
\]
\[
= H_{atom} + H_{int} + H_{rad}
\]

For scattering from the \( |K\rangle \) to the \( |K'\rangle \) state, the following absorption and emission processes contribute:

**Emission:** \( \langle a; \cdots; m_{k-1}, m_k, m_{k+1}; | H | a; \cdots; m_{k-1}, m_k, m_{k+1} \rangle \) = \( \frac{\sqrt{2 \omega_k}}{\sqrt{\omega_0^2 - \omega^2}} \langle \alpha e^{-ikx} | a; \cdots; m_{k-1}, m_k, m_{k+1} \rangle \)

**Absorption:** \( \langle m; \cdots; m_{k-1}, m_k, m_{k+1}; | H | a; \cdots; m_{k-1}, m_k, m_{k+1} \rangle \) = \( \frac{\sqrt{2 \omega_k}}{\sqrt{\omega_0^2 - \omega^2}} \langle \alpha_e e^{ikx} | m; \cdots; m_{k-1}, m_k, m_{k+1} \rangle \)

**Absorption:** \( \langle a; \cdots; m_{k-1}, m_k, m_{k+1}; | H | a; \cdots; m_{k-1}, m_k, m_{k+1} \rangle \) = \( \frac{\sqrt{2 \omega_k}}{\sqrt{\omega_0^2 - \omega^2}} \langle \alpha_e e^{-ikx} | m; \cdots; m_{k-1}, m_k, m_{k+1} \rangle \)

**Emission:** \( \langle m; \cdots; m_{k-1}, m_k, m_{k+1}; | H | a; \cdots; m_{k-1}, m_k, m_{k+1} \rangle \) = \( \frac{\sqrt{2 \omega_k}}{\sqrt{\omega_0^2 - \omega^2}} \langle \alpha e^{ikx} | m; \cdots; m_{k-1}, m_k, m_{k+1} \rangle \)
The amplitude for the scattering process in lowest order is then

\[ M_{aa} = \frac{e^2}{2\sqrt{2}\hbar} \sum_m \left[ \hat{\mathcal{E}}_m \hat{\mathcal{E}}^{*}_m \right] \text{Re} \left[ \frac{\hat{\mathcal{E}}_m \hat{\mathcal{E}}^{*}_m}{E_a - K' - E_m} \right] \]

By Fermi's golden rule the transition probability for scattering into solid angle \( d\Omega \) is

\[ d\omega = |M_{aa}|^2 \Delta \omega \text{ (DENSIY OF FINAL STATES)} = |M_{aa}|^2 \frac{\Delta \omega}{2\pi} d\Omega \quad (\Delta \omega' = \Delta \omega) \]

Examining the denominators of the scattering amplitude, we see that in both the classical and quantum cases the denominators vanish at resonance, and hence these expressions become infinite. The inadequacy of these results to represent the scattering amplitude near resonance stems from the fact that they do not take into account the self-action of the scattering particle.

In the classical case, the equation of motion must be supplemented by the radiation reaction \[ \frac{2}{3} \frac{e^2}{c^3} \chi \] which has the effect of replacing the amplitude (1) by 

\[ \chi = \left( \frac{-\frac{1}{2} \frac{e}{m} \frac{E_0}{(\omega_0^2 - \omega^2)^2 + i \omega Y}}{\omega_0^2 - \omega^2 - i \omega Y} \right) \]

The emitted radiation field with polarization \( \epsilon' \) is

\[ \hat{\mathcal{E}}' \cdot \hat{\mathcal{E}}_{RAD} = \left( \frac{\frac{1}{2} \frac{e}{m} \frac{E_0}{(\omega_0^2 - \omega^2)^2 + i \omega Y}}{\omega_0^2 - \omega^2 - i \omega Y} \right) \frac{e^{iKR}}{R} \]

and the scattering cross section is

\[ \sigma_{sc} = \frac{8\pi \frac{e^2}{c^3} \omega^4}{3 \left[ (\omega_0^2 - \omega^2)^2 + \omega^2 Y^2 \right]} \sim \frac{3\pi x_0^2 Y^2}{2 \left[ (\omega - \omega_0)^2 + (\chi^2) \right]} \quad (\omega \approx \omega_0) \]

As long as \( |\omega^2 - \omega_0^2| \gg \frac{e^2}{c^3} \) the radiation reaction is negligible compared to the applied force and the previous expressions are valid.

For the emission from a free excited oscillator, \( \ddot{x} + \omega^2 \dot{x} + \omega_0^2 x = 0 \) with the well known results

\[ \chi = x_0 e^{-\frac{(x)^2}{2} - i\omega_0 t} \quad \text{for the amplitude} \]

\[ W = W_0 e^{-\frac{Yt}{2}} \quad \text{for the oscillator energy averaged per period} \]

\[ I(\omega) = I_0 \frac{Y}{[u - \omega_0)^2 + (x)^2]} \quad \text{for the spectral distributor of emitted intensity} \]
These relations show that $\gamma$ characterizes several things about the system. From equation (9) it is seen that $\gamma$ is the half width for the scattered radiation. From (10) it follows that $\left(\frac{1}{\gamma}\right)$ is the life time of a free system, and from (12) we see that $\gamma$ is the spectral width for emission.

Another important fact is seen from relation (9). Far from resonance the amplitude of the scattered wave is on the order of $e^2$, the coupling constant of the electron to the EM field, but at resonance the amplitude and is independent of $e^2$. Thus at resonance the amplitude must be a series of higher order approximations in $e^2$ which is summable in closed form in such a manner as to eliminate the $e^2$ dependence.

From the classical discussion we see several reasons why the quantum approximation (6) fails to give a resonance description. In the first place, approximation (6) is only of first order in $e^2$, but at resonance higher order terms must be considered. Also the Fermi transition rate is only valid for times during which the initial conditions are not appreciably altered\(^{(8)}\).

However, applying Heisenberg's principle to relation (8):

$$\frac{\hbar}{\mathcal{E}_a + \mathcal{E}_b - \mathcal{E}_n} \lesssim T$$

where $T$ is the time that the intermediate state can be expected to last. At resonance $T \to \infty$ which says that the intermediate state $|n\rangle$ will last an infinite time and hence the Fermi approximation is invalid. Physically we know that $|n\rangle$ will have a finite lifetime $\left(\frac{1}{\gamma}\right)$ and it is only for $|\langle \mathcal{E}_a + \mathcal{E}_b - \mathcal{E}_n \rangle| \gg \hbar \gamma$ that the Fermi approximation is valid.

A correct quantum mechanical treatment of damping, natural line breadth, and resonance fluorescence was first given by Wigner and Weisskopf\(^{(9)}\) and a more modern adaption of this method has been given by Heitler\(^{(10)}\). The approach used in both of these references is to develop a more accurate solution for the Schroedinger equation which is valid for all times. The methods are rather detailed mathematically and will not be outlined. Another very direct method of solving damping phenomena problems is obtained using Feynman techniques of quantum electrodynamics. This is the approach that we shall use.
II. RESONANT SCATTERING

A. Single Nucleus:

We shall develop our formalism by first treating the scattering from a single nucleus which has ground state Zeeman sublevels $a, a', \ldots$, and excited state Zeeman sublevels $n, n', \ldots$, all of which are in near resonance with the incident radiation. The multinuclear system will be treated in part (B) and phonon effects in part (C). The incident radiation is a monochromatic plane wave with wave vector $\vec{K}_o'$ and polarization $\vec{e}_o$ transfers to $\vec{K}_o$. The Feynman amplitude for the incident photon is

$$A_o(\vec{x}, \tau) = (4\pi)^{1/2} e_{\mu} e^{i \vec{K}_o \cdot \vec{x}}, \quad \kappa_o \cdot x = \vec{K}_o \cdot \vec{x} - \alpha_o \tau$$

We are primarily interested in the coherent elastic scattering process in which the initial and final states of the scatterer are the same. Only diagrams of the type 2(a) need be considered in resonant scattering.

---

Fig. 2. Feynman diagrams for elastic scattering from single nucleus. Time is in the upward direction.
In diagram (a) the nucleus propagates in its initial (Zeeman sublevel) ground state $|\alpha\rangle$ to time $t_1$. At $t_1$ a photon $|K_0\rangle$ is absorbed and the nucleus is excited to one of the states $|n\rangle$. The state $|n\rangle$ propagates from $t_1$ to $t_2$, where the nucleus deexcites to $|\alpha\rangle$ and emits a photon $|K\rangle$.

In diagram (b) the final photon is emitted at $t_1$ and the incident photon is absorbed at $t_2$. The contribution of diagrams of the type (b) to the scattering cross section are on the order of $|\gamma/\lambda K_0|^{2} \sim 10^{-2}$ (for Fe$^{57}$) with respect to (a), and therefore can be neglected. In non-resonant scattering however, diagrams of the form (b) must be considered, as will be done in section III.

Rather than calculate the scattering cross sections directly, we have found it more convenient to work with the excitation amplitudes $S_{n\alpha}(t)$—the amplitude that the nucleus, initially in ground state $|\alpha\rangle$, is in the excited sublevel $|n\rangle$ at time $t$. Under the influence of a monochromatic plane wave $|K_0\rangle$, $S_{n\alpha}(t)$ is a steady state amplitude

$$S_{n\alpha}(t) = e^{-i\omega_0 t} S_{n\alpha}$$

The amplitude of the scattering diagram 2(a) is related to $S_{n\alpha}$ by

$$S' = \int_{-\infty}^{\infty} dt \langle \alpha | \int \frac{dm}{m} e^{-iK \cdot \hat{\tau}} |n\rangle S_{n\alpha}(t)$$

$$= \langle \alpha | \int \frac{dm}{m} e^{-iK \cdot \hat{\tau}} |n\rangle S_{n\alpha} e^{i(\omega_\tau - \omega_0)}$$

The contributing diagrams for $S_{n\alpha}$ are given in figure (3).

$$S_{n\alpha}(t) = \prod_{1 \leftarrow 0}^{\varepsilon} + \sum_{\lambda'' < \lambda'} \prod_{1 \leftarrow 0}^{\varepsilon} + \sum_{\lambda'' < \lambda' < \lambda'''} \prod_{1 \leftarrow 0}^{\varepsilon} + \cdots$$

$$= \prod_{1 \leftarrow 0}^{\varepsilon} \sum_{\lambda'' < \lambda'} \prod_{1 \leftarrow 0}^{\varepsilon} \equiv \prod_{1 \leftarrow 0}^{\varepsilon}$$

*Fig. 3.* Feynman diagram for the excitation amplitude $S_{n\alpha}(t)$. The light
line represents the propagation of the ground state |\alpha\rangle, and the internal wavy line represents virtual photon emission and absorption. Finally the heavy shaded line in (b) represents the corrected propagator for the state |n\rangle (under the influence of the external field).

Inserting the potential amplitudes and propagators corresponding to diagram 3, we have

\[
(1) \quad S_{md}(\xi) = \left\{ \begin{array}{c}
\int_{-\infty}^{\xi} dt_0 \ e^{-iE_2(t-t_0)} \langle m(t)| \mathbf{A}_{\mu}(\mathbf{x},t) |\alpha\rangle \ e^{iE_0 t_0} \\
+ \sum_{n'\neq 0} \int_{-\infty}^{\xi} \int_{-\infty}^{\xi} dt_1 \ e^{iE_2(t-t_1)} \langle m(t)| \mathbf{A}_{\mu}(\mathbf{x},t) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p},t_1) \mathbf{A}_{\mu}(\mathbf{x},t_1) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p},t_1) |n\rangle \ e^{-iE_0 t_1} \ e^{i\mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p},t_1) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p},t_1) S_{md}(\xi)}
\end{array} \right.
\]

\[
= \left\{ \begin{array}{c}
(-i) \langle m| \mathbf{A}_{\mu}(p_0) |\alpha\rangle \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) \int_{-\infty}^{\xi} dt_0 \ e^{-i[K+\xi+i\xi]t_0} \\
- \sum_{n'\neq 0} \int_{-\infty}^{\xi} \int_{-\infty}^{\xi} dt_1 \ e^{i\mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p})} \langle m| \mathbf{A}_{\mu}(p_0) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) |n\rangle \ e^{-iE_0 t_1} \ e^{i\mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) S_{md}(\xi)}
\end{array} \right.
\]

\[
= \frac{-i[K+i\xi+i\xi]}{[K-(E_\mu-E_\alpha)]} \left\{ \int_{md}^{\mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p})} \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p})^{\mu}[K+(i\xi+i\xi)] \right. \\
\left. - \sum_{n'\neq 0} \int_{-\infty}^{\xi} \int_{-\infty}^{\xi} dt_1 \ e^{i\mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p})} \langle m| \mathbf{A}_{\mu}(p_0) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) |n\rangle \ e^{-iE_0 t_1} \ e^{i\mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) \mathbf{\mathbf{\hat{A}}}_{\mu}(\mathbf{p}) S_{md}(\xi)} \right\}
\]
where $\hat{R}_1$ is the nuclear center of mass, and

$$\mathcal{J}^{\mu}_{\text{nd}}(\vec{x}) = \langle \alpha' | \sum \sum \left[ \epsilon^{(n)}(\alpha')_{\nu} + \beta^{(n)}(\chi^{(n)}_{\nu} - \delta^{(n)}_{\nu \mu}) \right] e^{i \vec{x} \cdot \vec{R}_0} \chi^{(n)}_{\nu} | \alpha \rangle$$

is the matrix element of the nuclear interaction current operator (due to photon absorption $e^{i \vec{E} \cdot \vec{x}}$). The sum is carried out over the nucleus (n) comprising the nucleus. Similarly $\mathcal{J}^{\mu}_{\text{nd}}(\vec{x})$ is the matrix element corresponding to emission. More generally, $\mathcal{J}^{\mu}_{\text{nd}}(\vec{x}) = \int e^{i \vec{x} \cdot \vec{R}} \mathcal{J}^{\mu}_{\text{nd}}(\vec{R}) d\vec{R}$ is the Fourier transformation of the matrix element of the nuclear 4-current density operator. The repeated indexes $\mu$ in expression (1) are summed over all four components.

The propagator $\mathcal{K}(x; x') = \langle \alpha' | \chi_{x'}(\vec{x}, \vec{z}, t) \chi_{x'}(\vec{x}, \vec{z}, t') | \alpha \rangle$, and the internal photon propagator

$$\mathcal{S}_{n, \alpha}(\vec{x}, \vec{z}) = 4\pi \int \frac{d^3 \vec{p}}{(2\pi)^3(2\pi)} e^{i \vec{p} \cdot (\vec{x} - \vec{z})} e^{-i \mu \cdot (\vec{x} - \vec{z})}$$

for $t_2 > t_1$. The time dependence $\text{EXP}(\pm \epsilon t)$ inserted in $A_{\text{o}}(x, t)$ and $S_{n, \alpha}(t)$ cuts the interaction off in the distant past.

Due to selection rules, we have

$$\int \mathcal{J}^{\mu}_{\text{nd}}(\vec{x}) \mathcal{J}^{\mu}_{\text{nd}}(\vec{x}) = 0$$

unless $n' = n$. Assuming this condition we then have

$$\sum_{n, \alpha} \left[ \mathcal{K}(x; x') \mathcal{S}_{n, \alpha}(\vec{x}) \right] \mathcal{J}^{\mu}_{\text{nd}}(\vec{R}) = \left\{ \begin{array}{l} \mathcal{J}^{\mu}_{\text{nd}}(\vec{R}) \frac{A_{\text{o}}^{\mu}(\vec{R})}{\mathcal{K}_0 - (\Xi - \Xi_{\alpha})} \\
- \mathcal{J}^{\mu}_{\text{nd}}(\vec{R}) \frac{\mathcal{S}_{n, \alpha}(\vec{R})}{\mathcal{K}_0 - (\Xi - \Xi_{\alpha})} \end{array} \right.$$ 

The integral term in expression (2) gives the energy level shift and half width of the excited state $| n >$ (as a function of $K$)

$$\frac{\sum_{n, \alpha} (\Xi_{\alpha} - \Xi)^2 \int \frac{d^3 \vec{p}}{(2\pi)^3} \frac{\mathcal{J}^{(n)}_{\text{nd}}(\vec{p}) \mathcal{J}^{(n)}_{\text{nd}}(\vec{p})}{\mathcal{K}_0 - (\Xi - \Xi_{\alpha} - i\epsilon)} \mathcal{S}_{n, \alpha}(\vec{R})}{\mathcal{S}_{n, \alpha}(\vec{R})}$$

$$= \Delta E(K_0) + \frac{i}{\pi} \frac{\mathcal{F}(K_0)}{2}$$
Since \( \kappa_\nu = (E_e - E_\nu) \), we have \( \Delta \kappa = \gamma \), the radiative width of an isolated excited nucleus. Collecting terms, we finally obtain for the steady state excitation amplitude

\[
(4) \quad [\kappa_\nu - (E_m + \Delta E - E_e) + i \frac{1}{2} \gamma] S_{m\nu} = \hat{J}^\nu (\vec{R}_i) A_\mu (\vec{R}_e)
\]
or

\[
(4') \quad S_{m\nu} = \hat{J}^\nu (\vec{R}_i) A_\mu e^{i \frac{\vec{R}_i \cdot \vec{R}_e}{\kappa_\nu - (E_m + \Delta E - E_e) + i \frac{1}{2} \gamma}}
\]

What we are really interested in finding, however, are the coherent and total scattering cross sections, or equivalently, the scattered photon amplitude. It will be shown in the next section that the \( \mu \)-th component of the scattered photon amplitude at a point \((\vec{R} - \vec{R}_i)\) is

\[
(5) \quad A_\mu^m (\vec{R}, \zeta) = \sum_m J^\mu_m (-\vec{R}) S_{m\nu} e^{i \frac{\vec{R} \cdot \vec{R}_i + \omega_0 \zeta}{\kappa_\nu - (E_m + \Delta E - E_e) + i \frac{1}{2} \gamma}}
\]

where \( \vec{R} = -i \frac{\vec{R}_i}{\kappa_\nu} \), and the total photon amplitude at \( R \) is

\[
(5') \quad A_\mu^m (\vec{R}, \zeta) = A_\mu^m (\vec{R}, \zeta) + A_5^m (\vec{R}, \zeta)
\]

Expression (5) contains both scalar and longitudinal components, but at large distance this can be transformed to a purely transverse amplitude by a gauge transformation, as is shown in appendix (B).

From expressions (5'), (5), we see that the amplitude of the elastically scattered wave in the \( \vec{R} \) direction (for \( |\vec{R} - \vec{R}_i| \approx \lambda_0 \)) with polarization \( \hat{e}_m \), if a photon of energy \( K_0 \), polarization \( \hat{e}_m \), is incident in the \( \vec{K}_0 \) direction, is

\[
(6) \quad \langle \hat{e}_m, \vec{R}_i; \hat{e}_m, \vec{R}_e \rangle = \sum_m \left[ \frac{(\hat{e}_m \cdot \vec{R}_e)(\hat{e}_m \cdot \vec{R}_i)}{\kappa_\nu - (E_m - E_e) + i \frac{1}{2} \gamma} \right]
\]

For polarized \( \text{Fe}^{57} \), taking the \( z \)-axis in the direction of polarization, and calling the magnetic quantum number \( \alpha \) along the \( z \)-axis (1/2, \( m_0 \)), and \( n = (\frac{3}{2}, n_0 + u) \) for \( u = \pm 1, 0 \), then for magnetic dipole transitions the current amplitudes are

\[
\hat{J}_m (\vec{R}_i) = \kappa_\nu <\frac{3}{2}, m_0 + \mu | \hat{m} | \frac{1}{2}, m_0 > [\hat{e} \times \vec{R}_i]
\]

\[
\hat{J}_m (\vec{R}_i) = \kappa_\nu <\frac{3}{2}, m_0 | \hat{m} | \frac{1}{2}, m_0 + \mu > [\hat{e}_m \times \vec{R}_i]
\]
and the scattering amplitude is

\[
\langle m' | \mathbf{e}_m' \rangle = \sum_{\mu} \left( \frac{\mathbf{e}_{m'} \cdot [\mathbf{e}_m \times \mathbf{e}_{m'}]}{\mathbf{R}_{m-m} \cdot \mathbf{R}_{m-m}} \right) \frac{1}{\kappa_0 - (E_{(2,m_0+\mu)} - E_{(2,m_0)}) + i \Gamma/2}
\]

where in the last line we have used the relationship

\[
\kappa_0^2 | \mathbf{R}_{m_0\mu} |^2 = \left( \frac{3}{2} \kappa_0 \right) C^2 \langle \mathbf{R}_{0\mu} | \mathbf{R}_{m_0\mu} \rangle \frac{\Gamma}{\Gamma_2}
\]

which is derived in appendix A, and the notation for the Clebsch-Gordon coefficients (C) is that of Rose\(^{(1)}\). If the incident and scattered photons are taken as right- or left-hand circularly polarized about their corresponding wave vectors \(\mathbf{R}_0, \mathbf{R}'\) (then \(m, m' = \frac{+}{-} 1\)), then

\[
\langle \mathbf{e}_{m'} \cdot [\mathbf{e}_m \times \mathbf{e}_{m'}] \rangle \langle \mathbf{e}_{m} \cdot [\mathbf{e}_{m'} \times \mathbf{R}_0] \rangle = D_{m_0m}\left(\mathbf{R}_0, \mathbf{L}\right) D_{m_0m'}^{(1)}\left(\mathbf{R}_0, \mathbf{L}\right)
\]

when the notation for the rotation matrices (D) is again that of Rose. Substituting into (7), we then obtain Trammells\(^{(1)}\) result

\[
\langle m' | \mathbf{e}_m' \rangle = \sum_{\mu} \frac{1}{\kappa_0 - (E_{(2,m_0+\mu)} - E_{(2,m_0)}) + i \Gamma/2}
\]

Following Trammells development, to obtain the coherent scattering amplitude, we must average over the initial states \(m_0\) (\(= \frac{+}{-} 1/2\) for Fe\(^{57}\)). Since the splitting \(g\) of the ground state sublevels is extremely small, we have to a good approximation

\[
\langle m' | \mathbf{e}_m' \rangle = (g_0 + 1) \frac{1}{\kappa_0 - E_{(2,m_0)} + E_{(2,m_0)} + i \Gamma/2}
\]

for Fe\(^{57}\). For unsplit Fe\(^{57}\) in stainless steel, \(E_{(2,m_0+\mu)} = E_{\frac{3}{2}}, E_{(2,m_0)} = E_{\frac{1}{2}}\) for all \(m_0\), \(\mu\), and (8) reduces to

\[
\langle m' | \mathbf{e}_m' \rangle = \left( \frac{3}{2} \right)^{\frac{g_0}{3}(2g_0+1)} \frac{m_{m_0}(\mathbf{R}_0, \mathbf{L})}{\kappa_0 - E_{\frac{3}{2}} + E_{\frac{1}{2}} + i \Gamma/2}
\]

By the optical theorem, the total cross section is
\[ \sigma_T = \frac{4\pi}{k_0^2} \sum_{m} J \left[ \mathcal{C}_{\text{coh}}(m; \mathbf{r}_0; m; \mathbf{r}_0) \right] \]

\[ = \frac{2\pi}{3} \left( \frac{2J+1}{2J+1} \right) \frac{\Gamma^3}{4\pi^2} \left| \mathbf{r}_0 - (E_2 - E_2) + i \Gamma_2 \right|^2 \]

The coherent elastic scattering cross section is

\[ \sigma_{\text{coh}} = \sum_{m} \int d\Omega \left| \mathcal{C}_{\text{coh}}(m; \mathbf{r}_0; m; \mathbf{r}_0) \right|^2 \]

\[ = \frac{2\pi}{3} \left( \frac{2J+1}{2J+1} \right) \frac{(1)^2}{4\pi^2} \left| \mathbf{r}_0 - (E_2 - E_2) + i \Gamma_2 \right|^2 \]

In equations (8) - (8)' v, \( \Gamma \) is the internal width, and \( \Gamma \) is the total width including internal conversion as shown in section III. For Fe\(^{57} \) \( \langle \Gamma \rangle = \frac{1}{15} \) and we obtain \( \sigma_T = 1.1 \times 10^{-6} \), \( \sigma_{\text{coh}} = 3 \times 10^{-6} \) at resonance.

Before proceeding to the multinuclei case, it is useful to define the corrected propagator \( \tilde{K}_m(\mathbf{r}_0, \mathbf{r}_2) \) corresponding to diagram 3(b):

\[ S_{\text{mol}}(\mathbf{r}_2) = \int_{-\infty}^{\infty} dx \mathcal{K}_m(\mathbf{r}_0, \mathbf{r}_2) \langle m(\mathbf{r}_2) | \mathcal{P}_0(\delta_x, \mu_0) | n \rangle \left\{ \mathcal{A}_0(\mathbf{r}_0, \mathbf{r}_2) \right\} e^{-i \mathbf{r}_2 \cdot \mathbf{r}_0} \]

\[ = \int_{-\infty}^{\infty} \mathcal{K}_m(\mathbf{r}_0) \mathcal{A}_0(\mathbf{r}_2) e^{-i \mathbf{r}_2 \cdot \mathbf{r}_0} \]

Substituting \( \mathbf{r}_2 = \mathbf{r}_0 - \mathbf{r}_2 \), and denoting the Laplace transform by \( \tilde{\mathcal{A}} \),

\[ S_{\text{mol}}(\mathbf{r}_2) = \int_{-\infty}^{\infty} \mathcal{K}_m(\mathbf{r}_0) \left[ \mathcal{A}_0(\mathbf{r}_2) \right] e^{-i \mathbf{r}_2 \cdot \mathbf{r}_0} \]

Equating to expression (4), we obtain for the Laplace transform of \( \tilde{K}_m(\mathbf{r}_0, \mathbf{r}_2) \)

\[ \tilde{K}_m(-i [\mathbf{r}_0 + \mathbf{r}_2]) = -i \sqrt{\left[ \mathbf{r}_0 - (E_2 - E_2) + i \Gamma_2 \right]} \]

This quantity is useful for solving the multinuclei case.

**B. Multi Nuclei System:**

We now consider the elastic resonant scattering of the incident monochromatic plane wave \( | \mathbf{r}_0, \mathbf{e}_0 \rangle \) from a system of nuclei located at the positions \( \mathbf{r}_j \). Let \( \mathbf{r}_j \) be the initial ground state of the \( j \)th nucleus, and let \( n_j, n'_j, \ldots \) be the near resonant excited levels (for a
collection of identical nuclei, the sets \( \{ \alpha, \beta, \cdots \} \) and \( \{ \mu, \nu, \cdots \} \) will be the same for all nuclei). The excitation amplitude \( \langle \alpha' | \epsilon | \alpha \rangle \) is now the total amplitude that the \( i \)-th nucleus, initially in ground state \( \alpha_i \), is in the excited state \( \alpha_i' \) at time \( t \).

Summing up all singly connected diagrams of the form

\[
\langle \alpha' | \epsilon | \alpha \rangle = \sum_{i=1}^{n} \langle \alpha'_i | \epsilon | \alpha_i \rangle + \cdots + \langle \alpha'_{n-1} | \epsilon | \alpha_{n-2} \rangle + \langle \alpha'_{n-1} | \epsilon | \alpha_{n-2} \rangle
\]

\[
= \sum_{i=1}^{n} \sum_{j \neq i} \langle \alpha'_i | \epsilon | \alpha_j \rangle + \cdots + \langle \alpha'_{n-1} | \epsilon | \alpha_{n-2} \rangle + \langle \alpha'_{n-1} | \epsilon | \alpha_{n-2} \rangle
\]

\[
+ \sum_{i=1}^{n} \sum_{j} \left( \sum_{j} \langle \alpha'_i | \epsilon | \alpha_j \rangle + \cdots + \langle \alpha'_{n-1} | \epsilon | \alpha_{n-2} \rangle + \langle \alpha'_{n-1} | \epsilon | \alpha_{n-2} \rangle \right)
\]

**Fig. 4.** Diagram for the excitation amplitude of the \( i \)-th nucleus. The
light lines represent the propagators of the ground states of the various nuclei; the heavy shaded lines the corrected propagators of the excited nuclear state as derived in section (a); and the internal wavy lines represent internal photon exchanges.

The diagrams are all singly connected - that is, there is no multiple photon emission or absorption at a given nucleus -- and hence represents a single photon process. However, it should be noted that the diagrams contain contributions from multi-photon, multi-nuclear excitations simultaneously present, as $t_j$ is not restricted to be less than $t_1$. The major contributions are accounted for in a Tamm-Dancoff development by the single nuclear excitation or single photon amplitudes, but such a development introduces spurious $R^{-2}$ interactions among the nuclei which do not appear in our treatment.

Inserting the propagators and amplitudes corresponding to diagram (4), we have

\begin{equation}
\begin{split}
S_{\xi_1 \xi_2}^{(2)} &= \sum_{i=1}^{2} \langle \xi_i | \lambda(x_i)\langle \xi_i | e^{\frac{i}{\hbar} \int d^4x \bar{\lambda}(\xi_i)\lambda(x_i) e^{-iE_x} + \\
&+ \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \langle \xi_j | \lambda(x_j)\langle \xi_j | e^{\frac{i}{\hbar} \int d^4x \bar{\lambda}(\xi_j)\lambda(x_j) e^{-iE_x} + \\
&+ \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \langle \xi_l | \lambda(x_l)\langle \xi_l | e^{\frac{i}{\hbar} \int d^4x \bar{\lambda}(\xi_l)\lambda(x_l) e^{-iE_x} + \\
&+ \langle \xi_1 | \lambda(x_1)\langle \xi_1 | e^{\frac{i}{\hbar} \int d^4x \bar{\lambda}(\xi_1)\lambda(x_1) e^{-iE_x} + \\
&+ \langle \xi_2 | \lambda(x_2)\langle \xi_2 | e^{\frac{i}{\hbar} \int d^4x \bar{\lambda}(\xi_2)\lambda(x_2) e^{-iE_x} + \\
&+ (\xi) \\
\end{split}
\end{equation}

We now use the four dimensional integral representation of $\rho_4(\xi_{1,2})$ since this is valid for $\xi_1 < \xi_2$, as well as $\xi_1 < \xi_2$:

\begin{equation}
\rho_4(\xi_{1,2}) = -\frac{4\pi}{(2\pi)^4} \int \frac{d^4p}{\sqrt{-p^2}} \frac{\delta [\vec{p} \cdot (\vec{x}_2 - \vec{x}_1) - E_2 (\xi_2 - \xi_1)]}{p^2 - \vec{p}^2 - 2\varepsilon}
\end{equation}

The first term we have already calculated in section I(a) as:

\begin{equation}
\begin{split}
&- \frac{\delta}{\sqrt{g}} \rho_4(\vec{p}) \rho_4(\vec{q}) / \left[ \delta^2 (\vec{p} - \vec{q}) + i\pi \delta \right]
\end{split}
\end{equation}
For the second term we carry out the \( t_j \) integration first, which gives
\[
\int 2\pi \delta(\mathbf{x} - \mathbf{r})
\]. Carrying out the \( t_j \) and \( \mathbf{r} \) integrations, we then have for the second term:
\[
\left( 18 \right) \frac{e^{-i(\mathbf{k} \cdot \mathbf{r} - \mathbf{L} \cdot \mathbf{r})}}{\left[ \mathbf{k}_0 - \left( \frac{\mathbf{x}_0}{r} \right) + i\frac{\mathbf{L}}{r} \right]}
\]

The \( \mathcal{G}_0(\mathbf{r}) \) integral is simply the \( \mathcal{G}_0(r) \) Greens function:
\[
\left( 19 \right) \frac{1}{2\pi^2} \int \frac{d^2 \mathbf{q}}{\mathbf{k}_0^2 - \mathbf{q}^2 - i\varepsilon} = \frac{\delta(\mathbf{k} \cdot \mathbf{r} - \mathbf{L} \cdot \mathbf{r})}{|\mathbf{r} - \mathbf{r}^*|}
\]

To first approximation for \( |\mathbf{r} - \mathbf{r}^*| \gg \lambda_0 \),
\[
|\mathbf{r}_2 - \mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_1| = |\mathbf{r}_2 - \mathbf{r}_1| + |\mathbf{r}_2 - \mathbf{r}_1|
\]
and (19) can be replaced by
\[
\left( 20 \right) \frac{e^{i\mathbf{k}_0 \cdot \mathbf{r}} - e^{-i\mathbf{k}_0 \cdot \mathbf{r}}}{|\mathbf{r} - \mathbf{r}^*|}
\]

Where \( \mathbf{k} \) is the wave vector pointing from \( \mathbf{r} \) to \( \mathbf{r}_2 \). Even for the \( M^1 \) multipole expansion however, this approximation introduces an error. This situation is easily corrected by making the operator correspondence \( \mathbf{k} \leftrightarrow -i\mathbf{\nabla} \), for then
\[
\left( 21 \right) \frac{e^{i\mathbf{k}_0 \cdot (\mathbf{r}_2 - \mathbf{r})} - e^{-i\mathbf{k}_0 \cdot (\mathbf{r}_2 - \mathbf{r})}}{|\mathbf{r}_2 - \mathbf{r}_1|} = [\frac{1}{\mathbf{r}_2 - \mathbf{r}_1} + \frac{i}{2} (\mathbf{r}_2 - \mathbf{r}_1) \cdot \mathbf{\nabla}^2 + \cdots ] e^{i\mathbf{k}_0 \cdot \mathbf{r}_2}
\]

by the Taylor series expansion theorem. This operator identification is particularly convenient since then, when finding the coherent amplitudes,
the summation over \( j \) reduces to the summation 
\[
\sum_{j=2}^{\frac{e^{iK_{+z_j}}}{1 - K_{+z_j}}}
\]
Thus we have for the second term of equation (15)

\[
(22) \quad e^{-i[K_{+z_j}]z} \sum_{j=2}^{\frac{e^{iK_{+z_j}}}{1 - K_{+z_j}}} \frac{e^{iK_{+z_j} \cdot x_j}}{\left( \frac{e^{iK_{+z_j}}}{1 - K_{+z_j}} \right)} \cdot \frac{e^{-iK_{+z_j} \cdot (\mathbf{x}_j - \mathbf{y})}}{\left( \frac{e^{iK_{+z_j}}}{1 - K_{+z_j}} \right)} \cdot \frac{e^{iK_{+z_j} \cdot (\mathbf{y} - \mathbf{z})}}{\left( \frac{e^{iK_{+z_j}}}{1 - K_{+z_j}} \right)}
\]

\[
\equiv \quad e^{-i[K_{+z_j}]x} \sum_{j=2}^{\frac{e^{iK_{+z_j}}}{1 - K_{+z_j}}} \frac{e^{iK_{+z_j} \cdot x_j}}{\left( \frac{e^{iK_{+z_j}}}{1 - K_{+z_j}} \right)} \cdot \frac{e^{-iK_{+z_j} \cdot (\mathbf{x}_j - \mathbf{y})}}{\left( \frac{e^{iK_{+z_j}}}{1 - K_{+z_j}} \right)} \cdot \frac{e^{iK_{+z_j} \cdot (\mathbf{y} - \mathbf{z})}}{\left( \frac{e^{iK_{+z_j}}}{1 - K_{+z_j}} \right)}
\]

where \( \mathbf{z}_{+} = -i \mathbf{\nabla}_{+z_j} \)

Similarly, carrying out the integration for the third term of (15), we obtain

\[
(23) \quad e^{-i[K_{+z_j}]x} \sum_{j=2}^{\frac{e^{iK_{+z_j}}}{1 - K_{+z_j}}} \frac{e^{iK_{+z_j} \cdot x_j}}{\left( \frac{e^{iK_{+z_j}}}{1 - K_{+z_j}} \right)} \cdot \frac{e^{-iK_{+z_j} \cdot (\mathbf{x}_j - \mathbf{y})}}{\left( \frac{e^{iK_{+z_j}}}{1 - K_{+z_j}} \right)} \cdot \frac{e^{iK_{+z_j} \cdot (\mathbf{y} - \mathbf{z})}}{\left( \frac{e^{iK_{+z_j}}}{1 - K_{+z_j}} \right)}
\]

This term and the higher order term (d) give a density effect. Assuming the usual situation in which only the \( n_{+j} = n_{-j} \) term contributes, we can write (23) as
\[
\begin{align*}
\equiv \frac{-e}{[\kappa_0 - (\bar{E}_0 - \bar{E}_e) + i \frac{1}{2} \gamma_\mu \gamma_5]} \left[ \Delta \bar{E}_{\text{ad}}, + i \frac{1}{2} \gamma_\mu \gamma_5 \right] \mathcal{M}_0 \chi \\
\end{align*}
\]

Here \( \Delta \bar{E}_{\text{ad}}, \) and \( \gamma_\mu \) give small enhancements to the level shift \( \Delta \bar{E}_e \) and the level width \( \gamma_\mu \), respectively. If \( \gamma_\mu \) is the total width including internal conversion, then it can be shown from (14)'' that
\[
\Delta \bar{E}_{\text{ad}} \sim \frac{1}{2} \gamma_\mu \sim \sigma^2 \gamma_\mu 
\]
for Fe\(^{57}\). Similarly, it can be shown that the contribution from the neglected diagrams (d) gives width and shift enhancements \( \sim (\gamma_\mu)^3 \gamma_\mu \).

Noting that we can write \( \mathcal{M}_0 \chi \) as \( \mathcal{M}_0 \chi \equiv \mathcal{M}_0 \chi \), with \( \chi = -i \frac{1}{2} \bar{E}_e \), the final coupled expression for the nuclear excitation amplitudes is

\[
(24) \quad \left[ \kappa_0 - (\bar{E}_0 - \bar{E}_e) + i \frac{1}{2} \gamma_\mu \right] \mathcal{M}_0 \chi \equiv \mathcal{M}_0 \chi 
\]

\[
\equiv \mathcal{M}_0 \chi \left[ A_0^\mu (\vec{R}) + A_s^\mu (\vec{R}) \right] 
\]

where \( \vec{R} = -i \frac{1}{2} \bar{E}_e \), and \( \bar{E}_e, \gamma_\mu \) include the effects of diagrams 4(c) and 4(d), and where \( A_0^\mu (\vec{R}) \) is the Feynman amplitude at \( \vec{R} \) of the incident photon, and \( A_s^\mu (\vec{R}) \) is the scattered photon amplitude at \( \vec{R} \).

From (24) we see that if we put a test particle at a point \( \vec{R} \) outside of the system, which does not react back on the system, then the total photon amplitude at \( \vec{R} \) which acts on the particle is

\[
(25) \quad A^\mu (\vec{R}, \tau) = A_0^\mu (\vec{R}, \tau) + \sum \left[ \mathcal{M}_0 \chi \right] \left[ A_s^\mu (\vec{R}, \tau) \right] 
\]

\[
\equiv A_0^\mu (\vec{R}, \tau) + A_s^\mu (\vec{R}, \tau) 
\]

where now \( \vec{R} = -i \frac{1}{2} \bar{E}_e, A_0^\mu (\vec{R}) \) is the incident photon amplitude at \( \vec{R} \), and \( A_s^\mu (\vec{R}) \) is the scattered photon potential at \( \vec{R} \). The scattered photon amplitude contains both longitudinal and scalar components, but for \( \frac{1}{2} \bar{E}_e \gg \lambda_0 \), these can be removed by a gauge transformation as shown in appendix (B).
Equations (24) and (25) are our basic equations. The scheme of solutions is first to solve for the excitation amplitudes $S_{\alpha\alpha'}^{(2)}$ from the set of equations (24). Once these are known, the photon amplitude is given by (25), which in turn allows us to determine cross sections, or more appropriate for crystals, the reflection and transmission coefficients.

C. Phonon Effects:

Resonant Mössbauer scattering is a slow process with respect to the frequency of phonon vibration. For the 14.4 keV Fe$^{57}$ photon, the lifetime of the excited $3/2$ state is $\tau = 1.4 \times 10^{-7}$ sec. Photon energies are in the range $0.1 - 1$ eV, so that $\nu \sim (2 - 20) \times 10^{12}$ vibration/sec. Hence there are about $(2.8 - 28) \times 10^5$ phonon vibrations during the lifetime $\tau = 1.4 \times 10^{-7}$ sec. As shown by Trammell$^{(1)}$, such slow resonant elastic scattering leads to a phonon factor $e^{-\frac{1}{2} \langle [\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}]_r^2 \rangle}$ for absorption of a photon $\hat{\mathbf{r}}$ and a factor $e^{-\frac{1}{2} \langle [\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}]_r^2 \rangle}$ for reemission of a photon $\hat{\mathbf{r}}$.

The basic equations (24) and (25) of the last section should thus be modified by replacing $S_{\alpha\alpha'}^{(2)}$ by $S_{\alpha\alpha'}^{(2)} e^{-\frac{1}{2} \langle [\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}]_r^2 \rangle}$, and $\mathcal{J}(r, \omega) e^{-\frac{1}{2} \langle [\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}]_r^2 \rangle}$ respectively.
III. INTERFERENCE BETWEEN NUCLEAR AND ELECTRONIC SCATTERING

In addition to the interaction with the nuclei, there is considerable interaction of the Mössbauer gamma rays with the electrons. This gives rise to various types of nuclear-electronic interference.

The purely electronic processes give an electronic scattering amplitude \( \Phi_e \), which, as we will see later, interferes constructively or destructively with the nuclear scattering amplitude \( \Phi_n \) depending upon the frequency and the scattering angle.

The presence of the electrons also gives width and level-shift contributions to the excited nuclear states, primarily due to internal conversion. Also the Rayleigh and photo electric scattering will give a shielded total field at the nucleus, and the reverse process will give a phase shift to a photon emitted from the nucleus.

A. Electronic Scattering:

Before treating the interference effects in detail, it is instructive to derive the purely electronic scattering amplitude \( \Phi_e \). The major purely electronic processes are given in fig. (5).

![Diagram of five processes](image)

Fig. 5. Major photon-bound state electron interactions.

Where in fig. (5), processes (a) and (b) give the Rayleigh scattering and correspond to virtual transitions to negative energy states; (c) gives the photo electric effect when a photon is absorbed and an electron is ejected into a continuum state; (d) gives the Compton effect where both an electron and a frequency shifted photon are emitted; and (e) and (f) give the Raman Scattering in which the electronic transition is from the ground state \( |e_o\rangle \) to an unoccupied valence state \( |e_n\rangle \) to find state \( |e'_o\rangle \), not necessarily equal to \( |e_o\rangle \), so that generally the emitted photon is
frequency shifted. Only the Rayleigh scattering is an elastic scattering process, and the remainder are inelastic on absorptive, but all processes give a contribution to the elastic scattering amplitude as shown in fig. (6).

\[ \text{Fig. 6. Electronic contributions to elastic scattering amplitude.} \]

Process (a), (ω) give both the Rayleigh and photo-elastic contributions to Fe, the Rayleigh contribution coming from the virtual transitions to the negative energy states, the photoelectric contribution coming from the virtual transitions to continuum states. Processes (d) give the Compton contribution to Fe, and (e), (f) give the Raman contribution. The real part of Fe will be determined primarily from the Rayleigh scattering, while the imaginary part of Fe will come from the photoelectric, Compton, and Raman processes.

For most Mössbauer photons, we only need to consider the Rayleigh and photoelectric effects. The Compton effect is only significant for high photon energies; and for metals we do not need to consider the Raman contribution since there are no unoccupied optical states. (The valence levels are spread into electronic energy bands for the entire metal which are filled up to the Fermi surface.) For this reason we will only calculate diagrams (a) and (b), but if the contribution (d) - (f) are needed, they can also be calculated easily in the Feynman manner.

In addition to the diagrams shown in fig. (6), there are also higher order diagrams such as shown in fig. (7). These diagrams give the effect of scattering within the electronic cloud - these effects give a shielded field at any electron, which is the superposition of the incident field and the radiation scattered by the remainder of the electron cloud. However, these effects can be neglected. (But we will see later that the shielding of the nucleus can be important.) For process (a), the matrix element is given by
From expression (1) and similar expressions for diagrams (b) - (d), we find that the contribution of (a) - (d) is of the order of magnitude

$$\sum \left( \frac{f_{1}}{g_{1}^{2}} \right) f_{2}^{(0)}$$

where $f_{1}^{(1)}$ is the scattering length for the scattering process from electron (1) ($\sum f_{1}^{(0)} f_{2}^{(0)} \sim 10^{-12}$ cm for Rayleigh scattering, $\sim 10^{-13}$ cm for photoelectric scattering), and $d_{12}$ is the average separation of the two electrons ($\sim \frac{d_{12}}{2} \approx 2 \times 10^{-2}$ cm). Thus for Rayleigh screening

$$\sum \sum \left( \frac{f_{1}^{(0)}}{g_{1}^{2}} \right) f_{2}^{(0)} \sim 10^{-2} f_{2}$$

and for photoelectric screening $\sim 10^{-3} f_{e}$. Similarly the $N^{th}$ order processes are of the order $\frac{f_{N}}{m=1} \left( \frac{f_{1}}{g_{1}^{2}} \right) f_{2}$, so the contribution of all higher order diagrams is of the order

$$\left[ \frac{f_{2}}{1 - f_{2}} \right] f_{2} \ll f_{2}$$

and can be neglected in comparison to $f_{e}$.
Returning to the Rayleigh and photoelectric contributions, diagrams (a), (b) of fig. (6), and carrying out the integrations as in section (II), we have immediately for the electronically scattered photon Greens function

\[
\langle \mathcal{A} \rangle \left( \mathbf{r}, \mathbf{r}' \right) = \frac{\Sigma_e \Sigma_e \langle \mathbf{r}_e | \mathbf{r}_e \rangle - \Sigma_e \Sigma_e \left( \mathbf{r}_e \times \mathbf{r}_e \right) \cdot \mathbf{r}_e}{\left( \mathbf{K}_e - \mathbf{K}_e \right) + i\epsilon \left| \mathbf{r}_e \right|} \cdot \mathbf{r}_e \cdot \mathbf{r}_e
\]

where \( \mathbf{R} = -i \nabla \mathbf{r} \), \( \mathbf{r}_e = \mathbf{r} \left( 1, \mathbf{R} \right) \), and contractions are taken in the four vector fashion \( \mathcal{A}^\nu \mathcal{A}^\mu = \mathcal{A}_e \mathcal{A}_e - \mathcal{A}_e \mathcal{A}_e \). Expression (2) contains both longitudinal and scalar parts, but as shown in appendix (B), we can make a gauge transformation in the wave region \( \mathbf{K}_e \mathbf{r}_e \gg \) to obtain a purely transverse photon. The sum over negative energy transitions in (2) gives the Rayleigh scattering, which the sum over unoccupied continuum states gives the photoelectric contribution.\(^\ast\) From expression (2) we easily obtain the electronic scattering amplitude \( f_e \).

As stated above, the Rayleigh contribution comes from the virtual transitions to negative energy states \( \langle \mathcal{E}_- \rangle \). For these states, we

\(\ast\) The transitions to the negative energy states can be calculated in the Feynman manner without regard to the Pauli exclusion principle. This procedure can be shown to be equivalent to a more sophisticated treatment of photon refraction in a medium, where the diagrams \( \mathcal{A}_n \mathcal{E}_n \), \( \mathcal{E}_n \) an electronic bound state energy, are subtracted from the vacuum photon propagator

\[
\mathcal{A} = \mathcal{A} + \mathcal{A} \mathcal{E} + \cdots = \mathcal{A} + \mathcal{A} \mathcal{E}.
\]
have to good approximation

\[
\left[ \kappa_0 (\xi_m - \xi_e) \right] \approx - \left[ \kappa_0 + (\xi_m - \xi_e) \right] \approx 2mc^2
\]

Following Feynman(12), we can then extend the sum over positive energy states, \( \sum_+ \xi_n x_\xi_n - \xi_e \), which only introduces errors of order \( (v/c)^2 \).

Also, as shown in appendix (B), we only need to consider the transverse part of the scattered photon Green's function. Noting that

\[
\frac{\hat{\mathbf{X}}_e}{\kappa_e} \cdot e^{-i \hat{\mathbf{X}}_e \cdot \hat{\mathbf{X}}_e} \bigg|_{\kappa_e} = \frac{1}{\kappa_e} \hat{\mathbf{X}}_e \times [\hat{\mathbf{X}}_e \times \hat{\mathbf{X}}_e] e^{-i \hat{\mathbf{X}}_e \cdot \hat{\mathbf{X}}_e}
\]

then the Rayleigh scattering amplitude is given by

\[
(3) \quad \mathcal{F}(\hat{\mathbf{X}}_o, \hat{\mathbf{X}}_e; \hat{\mathbf{X}}_e, \xi_e) = \left< \xi_e \bigg| \sum_{\xi'_e} \frac{\hat{\mathbf{X}}_e}{\kappa_e} \cdot \hat{\mathbf{X}}_e \times \left[ \hat{\mathbf{X}}_e \times \hat{\mathbf{X}}_e \right] \hat{\mathbf{X}}_e \cdot \xi_e e^{i (\hat{\mathbf{X}}_e - \hat{\mathbf{X}}_o) \cdot \hat{\mathbf{X}}_e} \right|_{\xi_e} >
\]

Noting also that \( \hat{\mathbf{X}}_e \cdot \hat{\mathbf{X}}_e \times [\hat{\mathbf{X}}_e \times \hat{\mathbf{X}}_e] = \hat{\mathbf{X}}_e \cdot \hat{\mathbf{X}}_e \) (since \( \hat{\mathbf{X}}_e \cdot \hat{\mathbf{X}}_e = \sigma \))

and that \( (\hat{\mathbf{X}}_e \cdot \hat{\mathbf{X}}_e)(\hat{\mathbf{X}}_e \cdot \hat{\mathbf{X}}_e) + (\hat{\mathbf{X}}_e \cdot \hat{\mathbf{X}}_e)(\hat{\mathbf{X}}_e \cdot \hat{\mathbf{X}}_e) = 2 \hat{\mathbf{X}}_e \cdot \hat{\mathbf{X}}_e \)

then

\[
(4) \quad \mathcal{F}(\hat{\mathbf{X}}_o, \hat{\mathbf{X}}_e; \hat{\mathbf{X}}_e, \xi_e) = \frac{a^2}{mc^2} \left< \xi_e \bigg| \sum_{+} \frac{\hat{\mathbf{X}}_e}{\kappa_e} \cdot \hat{\mathbf{X}}_e e^{i (\hat{\mathbf{X}}_e - \hat{\mathbf{X}}_o) \cdot \hat{\mathbf{X}}_e} \right|_{\xi_e} > \hat{\mathbf{X}}_e \cdot \hat{\mathbf{X}}_e
\]

where \( a = \frac{e^2}{mc^2} = 2.8 \times 10^{-13} \text{ cm} \), and \( \mathcal{F}(\hat{\mathbf{X}}_o, \hat{\mathbf{X}}_e) = \left< \xi_e \bigg| e^{i (\hat{\mathbf{X}}_e - \hat{\mathbf{X}}_o) \cdot \hat{\mathbf{X}}_e} \right|_{\xi_e} > \)

is the electronic form factor. Expression (4) is the usual Rayleigh scattering amplitude. ***) The phonon modifications are given at the end of this section.

***) Actually this expression differs by a minus sign from the usual expression. This occurs because in taking fourvector contractions, the space part enters with a minus sign — \( \mathcal{A}^{\alpha^*} = A^\alpha - \hat{\mathbf{A}} \cdot \hat{\mathbf{B}} \). The incident field
To obtain the photoelectric contribution, we replace the sum over continuum states \( \sum_{\xi} \) by the integral \( \int \rho(\xi) d\xi \), and if we approximate the continuum states by plane wave states \( e^{i\xi \cdot \mathbf{x}} \), then we must also integrate over angles. In the integration we can replace \( [\xi_+ (E_+ - E_0) + i \varepsilon]^{-1} \) by \(-i \pi \delta \left[ \xi_+ - (E_0 + \xi_0) \right] - \theta \nu \left[ \xi_+ - (E_0 + \xi_0) \right]^{-1} \). \( [\xi_+ (E_+ - E_0)]^{-1} \) has no singularities in the region of integration. In the region away from the electronic absorption edge, the real part of the integral can be neglected in comparison to the Rayleigh scattering, and we only need to consider the imaginary part of the photoelectric contribution. Defining \( E_+ = (E_0 + \xi_0) \), the imaginary part of the photoelectric scattering amplitude is given by

\[
\frac{\mathcal{J}(\mathbf{\hat{r}}, \mathbf{\hat{s}}; \mathbf{\hat{r}_0}, \mathbf{\hat{s}}_0)}{-i \pi \rho_0} = \int d\Omega d\xi \sum_{\xi} \left( \mathbf{\hat{s}}_+ \cdot \mathbf{\hat{r}}_0 \right) \rho(\xi) \left( \mathbf{\hat{s}}_+ \mathbf{\hat{r}}_0 \right) \mathbf{\hat{r}}_0 \mathbf{\hat{s}}_0
\]

As discussed by Heitler, the primary contribution to (5) comes from the K-shell electrons. Using the wave functions

\[ |\xi_+\rangle = \frac{1}{\sqrt{4\pi}} e^{-\frac{a_0}{r}} \], \[ |\xi_{+}\rangle = \frac{1}{\sqrt{2\pi}} e^{-\frac{a_0}{r}} \]

and following Heitler's development of the photoelectric cross section, we obtain

\[
\mathcal{J}(\mathbf{\hat{r}}, \mathbf{\hat{s}}_0; \mathbf{\hat{r}_0}, \mathbf{\hat{s}}_0) = -i \frac{\varepsilon_0}{4\pi} \sigma_{\text{ph}} I(\mathbf{\hat{s}}_0, \mathbf{\hat{s}}_0) / I'
\]

where \( \sigma_{\text{ph}} \) is the photoelectric cross section, and

\[
I(\mathbf{\hat{s}}, \mathbf{\hat{s}}_0) = \int d\Omega \frac{(a \sin \theta \sin \phi + b \sin \theta \cos \phi + c \cos \theta) \sin \theta \cos \theta}{|1 - \frac{1}{\varepsilon} (a' \sin \theta \sin \phi + b' \sin \theta \cos \phi + c' \cos \theta)|^2}
\]

\[
I' = \int d\Omega \frac{\sin^2 \theta \cos^2 \theta}{|1 - \frac{1}{\varepsilon} \cos \theta|^2}
\]

was defined with a +1 phase factor \( A_0 = a_0 \mathbf{\hat{s}}_0 \) so that a contraction of this field enters with a minus sign \( A_0^* A_0 = -a_0^2 \).

To obtain the more usual expressions for the scattering amplitudes, we should choose the incident phase factor as \((-1\). In this thesis however, we will simply multiply the scattering amplitudes by \((-1\) to obtain the more customary forms.
\[ \alpha = \hat{e}_x^+ (\vec{r}_x) \cdot \vec{R}_0 \times \hat{e}_0 (\vec{r}_0) \]

\[ \alpha' = \vec{r}_x \cdot \vec{R}_0 \times \hat{e}_0 (\vec{r}_0) \]

\[ \hat{c} = \hat{e}_x^+ (\vec{r}_x) \cdot \hat{e}_0 (\vec{r}_0) \]

\[ c' = \vec{r}_x \cdot \hat{e}_0 (\vec{r}_0) \]

Expanding the denominator of \( I \) in powers of \( \frac{\nu}{c} \), and integrating, we obtain

\[ I (\hat{e}_x (\vec{r}_x), \hat{e}_0 (\vec{r}_0)) / I = \hat{e}_x^+ (\vec{r}_x) \cdot \hat{e}_0 (\vec{r}_0) + O (\nu^2) \]

to order \( \left( \frac{\nu}{c} \right)^2 \). For \( \text{Fe}^{57} \) and incident 14.4 FeV radiation, \( (\nu^*) = \sqrt{\frac{m(c^2)}{mc^2}} \)

\[ = 1.14, \quad (\nu^*)^2 = 2 \times 10^{-2} \]

Thus to the same order of accuracy as in the Rayleigh case, the photoelectric scattering amplitude is

\[ f_{\nu} (\vec{r}_x, \hat{e}_x, \vec{r}_0, \hat{e}_0) = -i \frac{e^0}{4\pi} \epsilon_{\vec{r}_x} \hat{e}_x^+ (\vec{r}_x) \cdot \hat{e}_0 (\vec{r}_0) \]

We note that the polarization factor \( \hat{e}_x^+ (\vec{r}_x) \cdot \hat{e}_0 (\vec{r}_0) \) is the same as for Rayleigh scattering.

Expressions (2) - (8) must now be modified by the appropriate phonon factors. Following Trammells development, we see that Rayleigh scattering is a non-resonant process with large energy denominator \( 2mC^2 \) and we can neglect the phonon energies \( \epsilon_{\nu} \approx 0.1 \text{ eV} \) in comparison to \( 2mC^2 \). The phonon dependent terms of the Rayleigh scattering amplitude are then

\[ \bar{f}_{\nu} \text{ photon Greens function are then} \]

\[ \sum_{\chi_m} \langle \chi_0 | -e^{i (\vec{r}_x \cdot n - \vec{r}_0 \cdot n)} | \chi_m \rangle \langle \chi_m | -e^{i (\vec{r}_x - \vec{r}_0) \cdot n} | \chi_0 \rangle / 2mC^2 \]

\[ = e^{-i [c (\vec{r}_x - \vec{r}_0) \cdot n]^2} / 2mC^2 \]

\[ = f_D (\vec{r}_x - \vec{r}_0) / 2mC^2 \]

where \( f_D \) is the usual Debye phonon factor.

The primary contribution to the photoelectric scattering comes from the resonant continuum state transitions. However, these transitions are very fast with respect to the frequency of phonon vibrations, and we will see that the correct phonon factor for this process is again the Debye factor \( f_D (\vec{r}_x - \vec{r}_0) \).
To see that the photoelectric scattering is a fast process, we can use the following qualitative argument. The photoelectric effect primarily concerns the K-shell electron, and any emission-absorption process will take place within the immediate vicinity of the K-shell, as dictated by the $e^{-\alpha r}$ part of the transition integral.

If $v^* = \sqrt{2(\epsilon - \epsilon_0) / m_e}$ is the velocity of the excited electron, and $a = \frac{2a_0}{\lambda} = \frac{4a_0^2}{\lambda} \times 10^{-8}$ cm is the diameter of the K-shell, then the length of time during which such an emission-reabsorption process can take place is

\[ \tau_{pe} \sim \frac{\lambda}{v^*} = \frac{2a_0}{\sqrt{2(\epsilon - \epsilon_0)}} = 9 \times 10^{-19} \text{ sec.} \]

The phonon frequencies are on the order of $v \sim (2-20) \times 10^{12}$ vib/sec. Hence $v \sim (2-20) \times 10^7$ vib/\(\tau_{pe}\), so that photoelectric emission-absorption is a very fast process. Using Trammell's time dependent form of the phonon factor,

\[ \langle \hat{X}_0 | e^{-\frac{i \hat{X}_0 \cdot \hat{\eta}}{\hbar}} e^{i \hat{\eta} \cdot \hat{X}_0} | \hat{X}_0 \rangle \]

we can set $\xi_{pe} = 0$ and we again obtain the Debye phonon factor $f_D$.

Thus, expression (2) for the Greens function should be modified to

\[ A^<(\vec{r},t) = \sum \sum \int \frac{d^3 \vec{K}}{2\pi^3} \frac{\langle \phi_{\vec{K}} | e^{-\frac{i \vec{K} \cdot \vec{r}}{\hbar}} | \phi_{\vec{K}} \rangle \langle \phi_{\vec{K}} | e^{i \vec{K} \cdot \vec{r}} | \phi_{\vec{K}} \rangle}{[\omega_{\vec{K}} - (\epsilon - \epsilon_0) + i\epsilon]} \right( \frac{\phi_{\vec{K}}}{|\vec{K}|} \right) \]

\[ \left( -\frac{e^{i \vec{K} \cdot \vec{r}}}{\hbar} \right) \]

and for the scattering amplitude, expressions (4), (8) are modified to

\[ \mathcal{F}(\vec{r},\vec{r}_0;\vec{K}_0,\vec{E}_0) = \left\{ \frac{-e^{i \vec{K}_0 \cdot \vec{r}}}{\hbar c} \mathcal{F}(\vec{K}_0,\vec{E}_0) \right\} \mathcal{F}(\vec{K}_0,\vec{E}_0)^* \cdot \vec{E}_0(\vec{r}) \]

\[ + i \frac{e^{i \vec{K}_0 \cdot \vec{r}}}{\tau_{pe}} \]

In expression (11) we have multiplied by (-1) to put our results in the standard form (See footnote (**)) if this section.)
B. Interference Between Nuclear And Electronic Scattering

We now consider the interference effects between the nuclear and electronic scattering. For a single atom we have the following processes contributing to the scattered photon Greens function:

\[
\begin{align*}
\left(\alpha\right) & + \left(\alpha'\right) \\
\left(\beta\right) & + \left(\beta'\right) \\
\left(\gamma\right) & + \left(\gamma'\right) \\
\left(\delta\right) & + \left(\delta'\right) \\
\left(\epsilon\right) & + \left(\epsilon'\right)
\end{align*}
\]

Fig. 8. Nuclear electronic interference.

In figure (8), we have represented Rayleigh scattering by and photoelectric scattering by . That is we have replaced

This is done only to keep in mind the different nature of these processes, but the calculations are still made as in section (A).
Diagrams (a), (b), (c) of fig. (8) give respectively the pure nuclear, Rayleigh, and photoelectric contributions. (d) and (e) give the shielding of the nucleus due to Rayleigh and photoelectric scattering. (f) and (g) give phase change effects to a photon emitted from the nucleus due to the electron cloud. Diagrams (h) - (k) give higher order effects which are included automatically in our formulation. Finally the nuclear propagator (a') includes width and level contributions due to radiative processes (c'), internal conversion (d'), and Rayleigh effects (e').

Neglecting phonon effects for the moment, the nuclear excitation amplitude is given by

\[ S_{\gamma \gamma} \equiv \begin{array}{c}
\begin{array}{c}
\includegraphics{diagram12a} \\
\begin{array}{c}
\includegraphics{diagram12b} \\
\begin{array}{c}
\includegraphics{diagram12c} \\
\begin{array}{c}
\includegraphics{diagram12d} \\
\begin{array}{c}
\includegraphics{diagram12e} \\
\begin{array}{c}
\includegraphics{diagram12f} \\
\end{array}
\end{array}
\end{array}
\end{array}
\end{array}
\end{array} \]

Carrying out the integrations as in section (II), and including the radiative self energy and level shift (f) on the left hand side, we have explicitly

\[ \left[ \kappa_0 - \left( \frac{E_\gamma - E_0}{\omega} \right) + \frac{\mathcal{R}_0}{\Delta_0} \right] S_{\gamma \gamma} = \begin{array}{c}
\begin{array}{c}
\includegraphics{diagram13a} \\
\begin{array}{c}
\includegraphics{diagram13b} \\
\begin{array}{c}
\includegraphics{diagram13c} \\
\begin{array}{c}
\includegraphics{diagram13d} \\
\begin{array}{c}
\includegraphics{diagram13e} \\
\begin{array}{c}
\includegraphics{diagram13f} \\
\end{array}
\end{array}
\end{array}
\end{array}
\end{array}
\end{array} \]
In expression (13), \( \varepsilon \) includes the sum over negative energy states as well as continuum states (but not occupied positive energy states). \( \mid \omega_0 \rangle \) is the initial state of the electron \( e \), with corresponding energy \( \varepsilon_e \). It can be the ground state of the entire electronic system and \( \varepsilon_e \) is the total electronic ground state energy. Similarly \( \mid \varepsilon \rangle \) is an excited state of the electron \( e \), with corresponding energy \( \varepsilon_e \). It is a state of the entire electronic system with one electron in an excited state and the remaining electrons in the ground state, and \( \varepsilon_e \) is the total electronic energy of such a state. Also all repeated indices are to be contracted in a four vector fashion (\( A^n B^n = A^a B^a - \beta(\alpha) \beta(\alpha) \)).

The first factor in each of the two brackets on the right hand side of (13) correspond to absorption preceding emission \( \beta(\alpha) \) while the second terms correspond to emission preceding absorption \( \beta(\alpha) \). The sum over the negative energies gives the Rayleigh effects, and the sum over the continuum states gives the photoelectric, internal conversion effects.

One thing that should be noted in the terms (d) + (e) of (13), which give the width and level shift contribution, is that all matrix elements involve outgoing waves \( \xi_k^R, \xi_k^L \) and are thus not complex conjugate matrix elements - that is, we have

\[
\langle \xi_k^R | \xi_k^L \rangle \neq \langle \xi_k^L | \xi_k^R \rangle
\]

rather than

\[
\langle \xi_k^R | \xi_k^L \rangle \times \langle \xi_k^L | \xi_k^R \rangle
\]

and this gives rise to unexpected width and level contributions. However, the outgoing wave \( \xi_k^L \) gives us precisely the type of terms we would expect for both the emission \( \Theta \), reabsorption \( \Theta \) processes. We see this as follows: since \( |x_k| \ll |x_e| \) over most of the region of integration, we have to very good approximation \( \xi_k^L \approx \xi_k^R \). For process \( \Theta \), the photon is emitted from

\( x_k \rightarrow x_e \) so the wave vector is \( \vec{K} = k (x_e / x_k) \).

Noting also that \( e^{ix_k x_e} = e^{ix_e (x_k / x_e)} = e^{ix_e K} \), we have

\[
\xi_k^L \xi_k^R \mid x_k - x_e \rangle = e^{ix_e K} \xi_k^L \xi_k^R \mid x_k - x_e \rangle
\]

which is precisely the form we would expect for emission of a photon \( \vec{K} \) by the nucleus, and absorption of \( \vec{K} \) by the electron. Similarly for
process (2), we see that 
\[ \tilde{r}' = \kappa_0 (\tilde{r} / \kappa_0) \]
and we have
\[ e^{i \theta / \kappa_0} \tilde{r}' = e^{i \theta / \kappa_0} \tilde{r} / \kappa_0 \]
which is again of the form we would expect.

We see from (13) that the nuclear electronic interaction term is
\[ \mathcal{L} = \int dx^i \frac{2 \kappa_0}{|x^i - x^i_0|} e^{i \kappa_0 (x^i - x^i_0)} \]

We can make a multipole expansion of this interaction, and for the simplified nuclear current operator \( \mathcal{J}_n = \frac{e}{2 \pi} \hat{\kappa} \sigma \), Akheizer and Berestetskzy (14) obtain the matrix elements \( \langle x_0 | x_0' \rangle \)

\( (14) \) \( \langle x_0 | x_0' \rangle = \int dx^i \frac{e^{i \kappa_0 (x^i - x^i_0)}}{1 - \frac{x^i - x^i_0}{x^i_0 - x^i_0}} \)

where the \( \hat{A}_m, \hat{B}_m \) are spherical vectors. The matrix elements with \( \lambda = 1 \) give the electric \( 2^j \)-pole transition elements, and \( \lambda = 0 \) gives the magnetic \( 2^j \)-pole transitions. We note from expression (14) that nuclear E-2\( j \) transitions couple only to electronic E-2\( j \) transitions, and similarly nuclear M-2\( j \) transitions couple only to electronic M-2\( j \) transitions.

Actually the multipole expansion should be carried out with the nuclear current
\[ \mathcal{J}_n = \sum \left[ \alpha_\lambda \hat{A}_\lambda + \beta_\lambda \hat{B}_\lambda \right] (\hat{e}^{\lambda \mu} \kappa^\mu - \hat{e}^{\mu \nu} \kappa^\nu) \]
The additional terms give the contribution of the neutron magnetic moments. For M-1 nuclear transitions such as considered below, the additional terms will not change the form of the results, but will simply add the neutron magnetic moments \( \sum \hat{A}_\lambda \) to the proton magnetic moment
\[ \hat{H}_n = \sum \hat{A}_\lambda / (2m_r c) (\hat{L} + 2 \hat{S}) = \sum (\hat{A}_\lambda / (2m_r c) \hat{L} + \hat{S}) \]
Thus the correct M-1 results are given below if we interpret \( \hat{H}_n \) as the total magnetic moment operator of the nucleus.

Restricting our attention to nuclear M-1 transitions such as occur in Fe\( ^{57} \), then the nuclear-electronic interaction term from (14) is

\[ (15) \mathcal{H}^{(m-1)}_e = -4 \pi i / \kappa_0 \sum_{\lambda = -1}^1 e^{i \theta / \kappa_0} \hat{A}_\lambda (\hat{A}_\lambda^* \hat{A}_\lambda^0 - \hat{A}_\lambda^0 \hat{A}_\lambda^*) \]
where

\[
\hat{A}^{(\omega)}_{\lambda \lambda} = J_1(\kappa r) \tilde{Y}_{1 \lambda}^{(\omega)}(\hat{r}/r) \hat{r}/r \]

\[
\hat{B}^{(\omega)}_{\lambda \lambda} = J_1'(\kappa r) \tilde{Y}_{1 \lambda}^{(\omega)}(\hat{r}/r) \]

The radial functions \( \hat{J}_1 \), \( h_1^{(1)} \) are the spherical Bessel and Hankel functions given explicitly by

\[
J_1(x) = \frac{\sin x}{x} - \frac{\cos x}{x} = \frac{\pi}{2} + O(x^2)
\]

\[
J_1'(x) = \left( -\frac{1}{x^2} - \frac{1}{x} \right) e^{ix} = -\frac{i}{2x} - \frac{i}{x} + \frac{3}{x^2} + O(x^2)
\]

The vector spherical harmonics \( \tilde{Y}_{1 \lambda}^{(\omega)} \) are given by

\[
\tilde{Y}_{1 \lambda}^{(\omega)}(\hat{r}) = \frac{i}{\sqrt{2}} \hat{r} \times (\nabla Y_{1 \lambda}^{(\omega)}) = -\frac{1}{\sqrt{2}} \hat{r} Y_{1 \lambda}^{(\omega)}
\]

and for reference, we have explicitly

\[
\frac{1}{\sqrt{2}} \hat{r} Y_{1 \lambda}^{(\omega)} = -\frac{1}{\sqrt{2}} Y_{1 \lambda}^{(\omega)} \hat{e}_0 + \frac{1}{\sqrt{2}} Y_{1 \lambda}^{(\omega)} \hat{e}_1
\]

\[
\frac{1}{\sqrt{2}} \hat{r} Y_{1 \lambda}^{(\omega)} = -\frac{1}{\sqrt{2}} Y_{1 \lambda}^{(\omega)} \hat{e}_0 + \frac{1}{\sqrt{2}} Y_{1 \lambda}^{(\omega)} \hat{e}_1
\]

\[
\frac{1}{\sqrt{2}} \hat{r} Y_{1 \lambda}^{(\omega)} = -\frac{1}{\sqrt{2}} Y_{1 \lambda}^{(\omega)} \hat{e}_0 + \frac{1}{\sqrt{2}} Y_{1 \lambda}^{(\omega)} \hat{e}_1
\]

where the quantization basis is \( \hat{e}_0 = -\frac{1}{\sqrt{2}} (\hat{\mathbf{e}}_x + i \hat{\mathbf{e}}_y) \),

\( \hat{e}_1 = \frac{1}{\sqrt{2}} (\hat{\mathbf{e}}_x - i \hat{\mathbf{e}}_y) \),

\( \hat{e}_0 = \hat{\mathbf{e}}_z \),

and \( \mathbf{e}_{(0)} \) is in the direction of the magnetic field at the nucleus. A very useful expression for the \( \tilde{Y}_{1 \lambda}^{(\omega)} \) vectors which can be verified by direct calculation is

\[
\tilde{Y}_{1 \lambda}^{(\omega)}(\hat{r}/K) = -i \sqrt{\frac{3}{2\pi}} \hat{e}_{(0)} \times \hat{r}/K
\]

where \( \hat{K} \) is an arbitrary vector.

When the transitions are between positive energy states, as is the case for the nuclear transitions and the internal conversion, photoelectric electronic transitions, a non-relativistic approximation is sufficient
for most Mössbauer processes. To obtain the non-relativistic approximation, we make the replacement

\[\mathcal{J}_1 \rightarrow \frac{\hbar}{2m} \left[ (\delta(n-r_0) \vec{e} + \delta(n-r_0) \vec{e}) \right] \]

\[\hat{e} (\delta(n-r_0) (\vec{s} \times \vec{s}) - (\vec{s} \times \vec{s}) \delta(n-r_0)) \]

\[= \mathcal{J}_1 + \mathcal{J}_2 \]

We then have for the nuclear part

\[\mathcal{J}_2 \rightarrow \frac{\hbar}{\beta_m} \left[ (\vec{e} + \vec{e}) \right] \left[ (\delta(n-r_0) \vec{e} \times \vec{r}) \right] \left[ \alpha \mathcal{J}_1 \right) \]

\[= \frac{\hbar}{\beta_m} \vec{e} \cdot \left[ \frac{\hbar}{\beta_m} (\vec{e} + \vec{e}) \right] \left( \frac{\hbar}{\beta_m} \vec{e} \times \vec{r} \right) \mathcal{J}_1 \]

\[= 2i \frac{\hbar}{\beta_m} \left( \frac{\hbar}{\beta_m} \vec{e} \right) \left( \frac{\hbar}{\beta_m} \vec{e} \times \vec{r} \right) \mathcal{J}_1 \]

\[= i \frac{2 \hbar^2}{\beta_m^3} \vec{e} \times \vec{r} \mathcal{J}_1 \]

where in the last line we have used the first term in the expansion of \(\mathcal{J}_1(r_0) = \kappa_0 r_0 / 3\), which is sufficient since \(\kappa_0 r_0 \approx 10^{-3}\).

Similarly for the electronic contribution

\[\mathcal{J}_2 \rightarrow \frac{\hbar}{\beta_e} \left[ (\vec{e} + \vec{e}) \right] \left[ (\delta(n-r_0) \vec{e} \times \vec{r}) \right] \left[ \alpha \mathcal{J}_1 \right) \]

\[= -2i \frac{\hbar}{\beta_e} \left( \frac{\hbar}{\beta_e} \vec{e} \right) \left( \frac{\hbar}{\beta_e} \vec{e} \times \vec{r} \right) \mathcal{J}_1 \]

\[= -2i \frac{\hbar^2}{\beta_e^3} \vec{e} \times \vec{r} \mathcal{J}_1 \]

And we finally have for the nuclear-electronic interaction term
(23) $\mathbf{H}_{x}^{(m)} = -4\pi \hbar \kappa \left( i \frac{2\gamma}{\hbar} \sqrt{\frac{3}{4\pi}} \left( \frac{\vec{\tau} \cdot \vec{m}_x \kappa (\lambda) \vec{r}_x \cdot \vec{m}_z} \right) \right) $

$= -2\kappa \vec{M}_n \cdot \vec{M}_x \left( \frac{1}{\kappa \tau_2^3} - \frac{i}{\tau_2^2} \right) e^{i \kappa \tau_2}$

Since most internal conversion, photoelectric processes only involve K or L shell electrons, and since for most Mössbauer processes $\kappa_0 \tau_2^{(l,m)} \ll 1 \ (\tau_1 \cdots \tau_3)$, we can replace

$\left( \frac{1}{\kappa \tau_2^3} - \frac{i}{\tau_2^2} \right) e^{i \kappa \tau_2}$

by

$\left( \frac{1}{\kappa \tau_2^3} + \frac{\kappa}{\tau_2^2} + \frac{i}{\kappa \tau_2^3} \right) \equiv \frac{1}{\kappa \tau_2^3}$

and we have

(24) $\mathbf{H}_{x}^{(n)} = -2\kappa \vec{M}_n \cdot \vec{M}_x \left( \frac{1}{\kappa \tau_2^3} \right)$

Another procedure for obtaining the non-relativistic interaction is the following. First we note in the relativistic expression (14) that the longitudinal and scalar contributions have canceled leaving us with essentially transverse interaction terms. Further we note that we can write

$\frac{e^{i \kappa_0 \vec{r}_x \cdot \vec{m}_n}}{1 - e^{i \vec{r}_x \cdot \vec{m}_n}} = e^{-i \vec{r}_x \cdot \vec{r}'} \frac{e^{i \kappa \vec{r}'}}{\vec{r}'}$

where $\vec{r}' = -\vec{v}_2 \tau_2$

We then have for the transverse nuclear magnetic dipole current

$\mathbf{J}_n \cdot e^{-i \vec{r}_x \cdot \vec{r}'} = -i \vec{M}_n \times \vec{r}'$

or

(25) $\mathbf{J}_n \cdot \frac{e^{i \kappa_0 \vec{r}_x \cdot \vec{m}_n}}{1 - e^{i \vec{r}_x \cdot \vec{m}_n}} = -i \vec{M}_n \times (-i \vec{v}_2 \tau_2) \frac{e^{i \kappa \vec{r}_2}}{\vec{r}_2}$

$= \kappa_0 \vec{M}_n \times \vec{r}_2 \left[ \frac{e^{i \kappa \vec{r}_2}}{\vec{r}_2} + \frac{1}{\kappa \vec{r}_2^3} \right] e^{i \kappa \tau_2}$

and for the interaction term we again have

(26) $\mathbf{J}_n \cdot \frac{e^{i \kappa_0 \vec{r}_x \cdot \vec{m}_n}}{1 - e^{i \vec{r}_x \cdot \vec{m}_n}} - \kappa_0 \vec{M}_n \times \vec{r}_2 \left[ \frac{1}{\kappa \tau_2^3} - \frac{i}{\tau_2^2} \right] e^{i \kappa \tau_2} \left( \mathbf{J}_n + \mathbf{J}_2 \right)$

$= -2 \kappa \vec{M}_n \cdot \vec{M}_x \left( \frac{1}{\kappa \tau_2^3} - \frac{i}{\tau_2^2} \right) e^{i \kappa \tau_2}$
For the negative energy transitions Rayleigh contributions we make the non-relativistic approximation as in section (A) by extending the sum \( \Sigma_{E_n} \) to include positive energy states. These contributions are worked out explicitly below.

We shall first calculate the internal conversion and photoelectric screening terms - that is, we shall consider the effects of the continuum states \( |E_x \rangle \) in expression (13). The sum \( \Sigma_{E_x} \) is replaced by the integral \( \int \int \int \rho(\xi) \xi d\xi d\xi' \), where \( \rho(\xi) \) is the density of continuum state, and \( E_x \) varies from \( \frac{m^2 c^4}{e^2} \) (or \( m_c^2 + \epsilon_F^2 \)) to infinity. The factor \( \left[ \kappa_x - (E_x - E_{\omega}) \right]^{-1} \)

is replaced by \( \left[ -\frac{2\nu}{E_x - (E_\omega + \kappa_x)} - \delta \pi \delta (E_x - E_{\omega} - \kappa_x) \right] \),

while the factor \( \left[ \kappa_x + (E_x - E_\omega) \right]^{-1} \)

has no singularities.

For the internal conversion contribution (d) of equation (13) we now have

\[
(27) \quad \langle \delta \rangle = \sum_{E_x} \sum_{\omega} \left( m_{\omega} \right)^2 \int \int \rho(\xi) \xi d\xi d\xi' \langle E_x | \hat{\lambda} \left( \frac{\omega}{\omega_0} \right) | E_x \rangle \langle E_x | \hat{\lambda} \left( \frac{\omega}{\omega_0} \right) | E_x \rangle
\]

\[\times \left[ -\frac{2\nu (E_x - E_\omega)}{(E_x - E_\omega + \kappa_x)} - \delta \pi \delta (E_x - E_\omega + \kappa_x) \right]
\]

\[= \sum_{E_x} \sum_{\omega} \left( m_{\omega} \right)^2 \left[ \Delta \omega \hat{\omega} \right] \]

where we have used the notation \( \langle \omega \rangle \hat{m} | \omega \rangle = m_{\omega} \hat{\lambda} \left( \frac{\omega}{\omega_0} \right) \)

and \( \hat{\lambda} \left( \frac{\omega}{\omega_0} \right) \hat{m} \)

(with \( \hat{m} \) in the direction of the magnetic field at the nucleus) depending upon which transition is involved. Also in the principal value term we have combined \( \left[ \kappa_x - (E_x - E_\omega) \right]^{-1} + \left[ \kappa_x + (E_x - E_\omega) \right]^{-1} \) making use of the fact that for any transition \( \langle E_x | \hat{\lambda} \left( \frac{\omega}{\omega_0} \right) | E_x \rangle \)

is another continuum state \( \langle E_x \rangle \) of the same energy such that
\[ \langle \xi | \hat{\mathcal{E}}_{\mu}^{+} \hat{\mathcal{E}}_{\nu} \mathcal{N}(\lambda) | \xi \rangle \]
gives the same matrix element, (and we neglect Zeeman energy differences as the \( \mathcal{E}_{\mu} \rightarrow \mathcal{E}_{\nu} \) transition may involve a spin down ground state rather than a spin up state, or vice versa). The principal value part gives a small level shift \( \Delta \mathcal{E} \), and the delta function gives the internal conversion width \( \frac{\gamma}{\gamma_{2}} = \frac{\alpha}{\gamma_{2}} \). Recalling that
\[ \kappa_{\lambda}^{2} | M_{\lambda_{\mu}}^{\lambda_{\nu}} |^{2} = \left( \frac{3}{2\alpha_{\lambda}} \right) c^{2} (\lambda_{\mu}^{\prime} \nu_{\mu}^{\prime}) \frac{\gamma_{2}}{\gamma} \]
where \( c (\lambda_{\mu}^{\prime} \nu_{\mu}^{\prime}) \) is the Clebsch-Gordon coefficient for the transition \( (\lambda_{\mu}^{\prime} \nu_{\mu}^{\prime}) \), and letting \( \mathcal{E}_{\mu}^{\ast} = (\mathcal{E}_{\mu} + \kappa_{\lambda}) \), we have the following expression for the internal conversion coefficient
\[
(28) \quad \alpha = \sum_{\lambda_{\mu}^{\prime}} \sum_{\nu_{\mu}^{\prime}} \left| \mathcal{E}_{\mu}^{\ast} \hat{\mathcal{E}}_{\lambda_{\mu}^{\prime}} \right|^{2} \frac{\gamma_{2}}{\gamma} c^{2} (\lambda_{\mu}^{\prime} \nu_{\mu}^{\prime}) \left| \langle \xi | \hat{\mathcal{E}}_{\mu}^{+} \hat{\mathcal{E}}_{\nu} \mathcal{N}(\lambda) | \xi \rangle \right|^{2} \rho (\mathcal{E}_{\mu}^{\ast})
\]
\[
= \sum_{\lambda_{\mu}^{\prime}} \sum_{\nu_{\mu}^{\prime}} \left| \mathcal{E}_{\mu}^{\ast} \hat{\mathcal{E}}_{\lambda_{\mu}^{\prime}} \right|^{2} \frac{\gamma_{2}}{\gamma} c^{2} (\lambda_{\mu}^{\prime} \nu_{\mu}^{\prime}) \sum_{m_{\mu}^{\prime} m_{\mu}} \left| \langle \xi | m_{\mu}^{\prime} \lambda_{\mu}^{\prime} \nu_{\mu}^{\prime} | m_{\mu} \rangle \right|^{2} \left| \langle \xi | m_{\mu} \rangle \right|^{2}
\]
\[
= \sum_{\lambda_{\mu}^{\prime}} \sum_{\nu_{\mu}^{\prime}} \left| \mathcal{E}_{\mu}^{\ast} \hat{\mathcal{E}}_{\lambda_{\mu}^{\prime}} \right|^{2} \frac{\gamma_{2}}{\gamma} c^{2} (\lambda_{\mu}^{\prime} \nu_{\mu}^{\prime}) \kappa^{2} (\mathcal{E}_{\mu}^{\ast} | \mathcal{E}_{\mu} ) \left| \langle \xi | m_{\mu}^{\prime} \lambda_{\mu}^{\prime} \nu_{\mu}^{\prime} | m_{\mu} \rangle \right|^{2} \left| \langle \xi | m_{\mu} \rangle \right|^{2}
\]
\[
= \frac{\gamma_{2}}{\gamma} \sum_{\lambda_{\mu}^{\prime}} \sum_{\nu_{\mu}^{\prime}} \kappa^{2} (\mathcal{E}_{\mu}^{\ast} | \mathcal{E}_{\mu} ) \left| \langle \xi | m_{\mu}^{\prime} \lambda_{\mu}^{\prime} \nu_{\mu}^{\prime} | m_{\mu} \rangle \right|^{2} \left| \langle \xi | m_{\mu} \rangle \right|^{2}
\]
where \( \kappa^{2} (\mathcal{E}_{\mu}^{\ast} | \mathcal{E}_{\mu} ) = \sum_{m_{\mu}^{\prime} m_{\mu}} \left| \langle \xi | m_{\mu}^{\prime} \lambda_{\mu}^{\prime} \nu_{\mu}^{\prime} | m_{\mu} \rangle \right|^{2} \left| \langle \xi | m_{\mu} \rangle \right|^{2} \)
and we have used the relation \( \sum_{\lambda_{\mu}^{\prime}} c^{2} (\lambda_{\mu}^{\prime} \nu_{\mu}^{\prime}) = 1 \).

Because of the \( \kappa^{3} \) dependence, the integrals can only be carried out using correct continuum wave functions, which involve hypergeometric functions. We will not attempt to carry out these integrations, but will simply use the measured value of \( d = 9.7 \).

The total effect of the contribution (d) combines with the left hand side of equation (13) to give
\[
\left[ \kappa_{\lambda} - (\mathcal{E}_{\mu} - \mathcal{E}_{\nu}) + i \frac{\gamma}{2} (\gamma_{2} + \gamma_{1}) \right] S_{\mu \lambda}
\]

Returning to the photoelectric screening, contribution (c) of equation (13), we have for the delta function part
We will see that this gives a very small screening effect, the principal value contribution is much smaller for transitions away from the absorption edge, and can be neglected in comparison to the $S$-function contribution. In expression (29), the first matrix element only couples even parity, M-1 transitions, and therefore we only need to keep the M-1 part of

$$
\sum_{\alpha} e^{i \mathbf{K} \cdot \mathbf{R}_{\alpha}} \epsilon_{\alpha} \mathbb{P} = - \left[ \frac{e^2}{m} + i \frac{e \hbar}{2m^2 \epsilon_{\alpha}} (\mathbf{K}^2 + 2 \mathbf{K} \cdot \mathbf{R}_{\alpha} + ...) \right] \cdot \mathbb{P} \tag{29}
$$

and we have

$$
(\mathbb{P}) = -i M \sum_{\alpha} \sum_{\chi_{\alpha}} \frac{e^2}{\hbar \epsilon_{\alpha}} \mathbf{K} \cdot \mathbf{R}_{\alpha} \epsilon_{\alpha} \mathbb{P} = -i \frac{e^2}{\hbar \epsilon_{\alpha}} \mathbf{K} \cdot \mathbf{R}_{\alpha} \epsilon_{\alpha} \mathbb{P} \tag{30}
$$

where the photoelectric screening factor $\mathbb{P}$ is given by

$$
\mathbb{P} = \sum_{\alpha} \sum_{\chi_{\alpha}} \frac{e^2}{\hbar \epsilon_{\alpha}} \mathbf{K} \cdot \mathbf{R}_{\alpha} \epsilon_{\alpha} \mathbb{P} \tag{31}
$$

*) Actually we should also keep the E-2 part of the electronic current, and this will cause some modification to the results obtained below. Calculation of the E-2 modifications will be given in a forthcoming paper.
Without carrying out the integrations, we can obtain an order of magnitude estimate by comparing expression (31) with the internal conversion coefficient expression (28). From these two expressions we see that
\[ S_{\text{res}} \approx \left( \varepsilon_l \right) (\kappa \chi_{\text{e}})^2 \approx \left( \varepsilon_l \right) 10^{-6} \approx 1 \times 10^{-2} \quad \text{for } \frac{1}{\chi_{\text{e}}}. \]

Although \( S_{\text{res}} \) is quite small, it still gives a scattering amplitude contribution comparable to the electronic scattering amplitude. The electronic scattering amplitude \( S_{\text{e}} \approx (-7 \times 10^{-12} + \varepsilon 5 \times 10^{-13}) \) cm, while at resonance \( S_{\text{res}} \approx 10^{-10} \) cm, so that the photoelectric screening amplitude \( S_{\text{res}} \approx 10^{-12} \) cm.

For the Rayleigh screening contribution (b), we extend the sum to include positive energy states as was done in section (A) to obtain the Rayleigh scattering amplitude, and we have approximately

\[
(32) \quad \langle \hat{\epsilon} \rangle = \langle \nu \rangle \langle \epsilon \rangle \langle \sum_{\lambda} e_{\lambda}^* \frac{e^{i \kappa_{\lambda} l_{\lambda}}}{|l_{\lambda}|} \epsilon_{\lambda} \frac{1}{2m \epsilon_{\lambda}^2} \sum_{\gamma} \epsilon_{\gamma} \epsilon_{\gamma}^* \frac{e^{i \kappa_{\gamma} l_{\gamma}}}{|l_{\gamma}|} \epsilon_{\gamma} \frac{1}{2m \epsilon_{\gamma}^2} \epsilon_{\gamma}^* \rangle \epsilon_{\lambda} \epsilon_{\lambda}^* \epsilon_{\gamma} \epsilon_{\gamma}^*
\]

\[
= \langle \nu \rangle \langle \epsilon \rangle \langle \sum_{\lambda} \frac{1}{\sqrt{m}} \kappa_{\lambda} \hat{\epsilon}_{\lambda} \hat{\epsilon}_{\lambda}^* \hat{\epsilon}_{\lambda} \hat{\epsilon}_{\lambda}^* \epsilon_{\lambda} \frac{1}{2m \epsilon_{\lambda}^2} \sum_{\gamma} \epsilon_{\gamma} \epsilon_{\gamma}^* \frac{1}{2m \epsilon_{\gamma}^2} \epsilon_{\gamma} \epsilon_{\gamma}^* \rangle \epsilon_{\lambda} \epsilon_{\lambda}^* \epsilon_{\gamma} \epsilon_{\gamma}^*
\]

where in the last line we have used the identity
\[
(\hat{\epsilon}_{\lambda} \cdot \hat{\epsilon}_{\lambda}^*) \langle \hat{\epsilon}_{\lambda} \cdot \hat{\epsilon}_{\lambda} \rangle = (\hat{\epsilon}_{\lambda}^* \cdot \hat{\epsilon}_{\lambda}) = \epsilon_{\lambda} \hat{\epsilon}_{\lambda} \cdot \hat{\epsilon}_{\lambda}^*.
\]

Using the explicit expression for
\[ \hat{\epsilon}_{\lambda} = -i \sqrt{\frac{e}{2m}} \hat{\epsilon}_{\lambda} \times \hat{\epsilon}_{\lambda} \lambda \langle \kappa_{\lambda} l_{\lambda} \rangle \]

and noting that
\[ \langle \nu \rangle \sum_{\lambda} \hat{\epsilon}_{\lambda}^* \hat{\epsilon}_{\lambda} \langle \hat{\epsilon}_{\lambda} \rangle = M_{\nu \lambda} \hat{\epsilon}_{\lambda}^* (\nu \hat{\epsilon}_{\lambda}) \]
we obtain

\[ (33) \quad \mathcal{I} = -i \kappa_0 \mathbf{M}_{\nu_0} \times \mathbf{\hat{J}}_{\nu_0} \cdot \hat{R}_0 \mathbf{e}_0 \mathbf{e}^{2 \mathbf{R}_0 \cdot \mathbf{e}} \]

where

\[ (34) \quad \mathcal{I}(\mathbf{R}_0) = \langle \mathbf{e}_0 | \frac{\mathbf{e}_0}{2} \left[ \frac{\mathbf{e}_0}{\mu_0 \mathbf{e}_0} + \frac{1}{\mu_0^2} \right] e^{i \mathbf{R}_0 \cdot \mathbf{R}_0} e^{2 \mathbf{R}_0 \cdot \mathbf{e}} | \mathbf{e}_0 \rangle \]

We note that if it were not for the factor \( e^{2 \mathbf{R}_0 \cdot \mathbf{e}} \), \( \mathcal{I}(\mathbf{R}_0) \) would be zero, since

\[ \mathcal{I} | \mathbf{Q}_0(\mathbf{e}) |^2 = -(-1) | \mathbf{Q}_0(-\mathbf{e}) |^2 \]

This is what we would expect, since for electric dipoles driven in phase, the magnetic fields at any point of symmetry vanish. Thus it is only due to the slight phase differences \( e^{2 \mathbf{R}_0 \cdot \mathbf{e}} \) at various points of the electron cloud that prevent a vanishing (magnetic) field at the nucleus due to Rayleigh scattering.

If we assume electronic wave functions of the form \( \mathbf{Q}(\mathbf{r}) = \mathcal{R}(\mathbf{r}) Y_{\ell m}(\theta, \phi) \), then we obtain

\[ (35) \quad \mathcal{I}(\mathbf{R}_0) = \sum_{m, \ell, \lambda, \mu} \sum_{\ell, \lambda} \beta_{\mu} \left( \frac{2\ell+1}{2\ell-1} \right) \left( \frac{\mathbf{R}_0}{\mathbf{R}_0} \right) \]

\[ \left( \text{COMPLETE SHELLS} \right) + \left( \text{INCOMPLETE S-SHELLS} \right) \]

\[ \left( \text{INCOMPLETE SHELLS} \neq S \right) \]

\[ \sum_{m, \ell, \lambda} \beta_{\mu} \left( \frac{2\ell+1}{2\ell-1} \right) \sum_{\lambda=1}^{2\ell+1} Y_{\ell 1}^* Y_{\ell 1} \delta_{\lambda 0} \]

\[ \approx \mathcal{I}(\mathbf{R}_0) + \mathcal{I}(\mathbf{R}_0) \]

where
\[ \beta_{\alpha} = \frac{e^2}{m c^2} \sum_{l} \left[ \int \frac{1}{r} \left( \frac{d}{dr} \chi_{l}(r) \right) \left( \bar{L} \chi_{l}(r) + \frac{1}{r} \chi_{l}(r) \right) \right] (r_{0}\chi_{l}(r)) \right|_{r_{0}}^{|R_{l}(r)|^2 n^2 d\mu} \]

Defining the Rayleigh screening factors \( \mathcal{F}_{l}^{(0)}, \mathcal{F}_{l}^{(6)} \) by

\[ \mathcal{F}_{l}^{(0)} = \sum_{m_{l}, \lambda, \ell} \frac{(2\ell+1)}{3} \beta_{\alpha} \]

\[ \mathcal{F}_{l}^{(6)} = (\text{COMPLETE}) + (\text{INCOMPLETE}) \]

\[ \mathcal{F}_{l}^{(0)}(k_{0}, \lambda_{\ell}(n_{\ell} \ell)) = \frac{(\mathcal{E}^{+}_{\lambda_{\ell}(n_{\ell} \ell)} \chi_{0}) \cdot \mathcal{E}_{0}}{(\mathcal{E}^{+}_{\lambda_{\ell}(n_{\ell} \ell)} \chi_{0}) \cdot \mathcal{E}_{0}} \]

then the effect of the Rayleigh screening is given by

\[ \sum_{l} \mathcal{F}_{l}^{(0)}(k_{0}, \lambda_{\ell}(n_{\ell} \ell)) = \sum_{l} \mathcal{F}_{l}^{(0)}(k_{0}, \lambda_{\ell}(n_{\ell} \ell)) \cdot \mathcal{E}_{0} \cdot \mathcal{E}_{0} \cdot \mathcal{E}_{l} \cdot \mathcal{E}_{l} \]

For an Fe\(^{57}\) K-shell electron \( \beta_{\alpha} = -0.5 \times 10^{-3} \) so that as an upper bound \( \mathcal{F}_{l}(K_{0}) = 1.3 \times 10^{-2} \) for the entire electronic cloud (plus some smaller imaginary factors) which is about the same order of magnitude as the photoelectric screening, but real. Although we have used a rather simple form for the electronic wave function (with good \( j \)), one would also expect wave functions of good \( j \) to give the same general result - closed shells and \( s \)-shells give a vector function \( \chi_{0}(k) \) proportional to \( k_{0} \lambda \), while the incomplete (\( \not\equiv s \)) shells give an \( \chi_{0}(k) \) which is not generally proportional to \( k_{0} \). Since Mössbauer elements have large values of \( z \) (\( z = 26 \) for Fe\(^{57}\) is the smallest), most electrons are in completed shells (in particular the inner electrons, which give the largest effect) and \( \mathcal{F}_{l}(K_{0}) \) is much larger than \( \mathcal{F}_{l}(K) \).

Finally we compute the Rayleigh contribution to the width and energy level shifts, process (e). Again extending the sum \( \sum_{\ell} \mathcal{F}_{l}(K) \) over positive energy states, and using expansion (19) for \( \mathcal{F}_{l}(K) \) and

\[ \kappa_{\alpha}^2 |M_{\mu, \alpha}|^2 = \left( \frac{\gamma}{\kappa} \right) \frac{3C_{2}(\kappa \alpha)}{2 \kappa_{0}} \]

we obtain
\[(39) \quad \langle \psi \rangle = \sum_{l=1}^{\infty} \left( \frac{n}{2} \right) \frac{2C_{l}^{2}(\nu_{l}^{2})}{m_{c}^{2}} \frac{C_{l}^{2}}{m_{c}^{2}} \psi_{l}^{2} \left( \frac{\hbar}{2} \right) \frac{1}{2} \left( \frac{1}{n_{l}^{2} + \frac{1}{4}} \right) \psi_{l}^{2} \left( \frac{1}{n_{l}^{2} + \frac{1}{4}} \right) \frac{1}{2} \langle \psi \rangle \]

We note that there is an obvious difficulty with this expression - the leading term is \( \left( \frac{\hbar}{n} \right)^{4} \) which gives a \( \left( \frac{\hbar}{n} \right)^{2} \) divergence for s electrons (for \( \ell = 0 \)), there is no divergence since the radial wave functions are of the form

\[
\langle \psi \rangle \left( r^{2}, \ell \right) \left( \frac{n}{2} \right) \frac{2C_{l}^{2}(\nu_{l}^{2})}{m_{c}^{2}} \frac{C_{l}^{2}}{m_{c}^{2}} \psi_{l}^{2} \left( \frac{\hbar}{2} \right) \frac{1}{2} \left( \frac{1}{n_{l}^{2} + \frac{1}{4}} \right) \psi_{l}^{2} \left( \frac{1}{n_{l}^{2} + \frac{1}{4}} \right) \frac{1}{2} \langle \psi \rangle \]

giving a radial integral of the form

\[
\int r^{2} \frac{2\ell + 1}{2n_{l}^{2} + 1} \frac{1}{2} \left( \frac{1}{n_{l}^{2} + \frac{1}{4}} \right) \psi_{l}^{2} \left( \frac{\hbar}{2} \right) \frac{1}{2} \langle \psi \rangle \]

The origin of the \( \left( \frac{\hbar}{n} \right)^{4} \) singularity comes from extending the sum \( \sum_{n} \) over positive energy states - the interaction connecting the positive energy state \( \left\langle \ell \psi \right\rangle \) to the negative energy state \( n_{l} \left\langle \ell \psi \right\rangle \) only contains a \( \left( \frac{\hbar}{n} \right)^{2} \) singularity, which can be integrated, but by completing the sum we square this singularity. Clearly accurate results can only be obtained by staying in the relativistic framework. However even for the non-relativistic expression the divergence can be removed if we take into account two things. First the expansions used in obtaining (14) are only valid for \( \nu_{l} \geq n_{l} \).

Secondly, for \( \nu_{l} < n_{l} \), the electronic wave functions are no longer coulombic. Akhuzer(14) states that a good approximation is to use purely coulombic wave functions, but to restrict \( \nu_{l} > n_{l} \), where \( n_{l} \) is the effective nuclear radius \( (R_{N} = 5.6 \times 10^{-13} \text{cm} \text{ for } \text{Fe}) \).

Using this approximation, and assuming electronic wave functions of the form \( \psi_{l}^{m} n_{l} \), we finally obtain

\[(40) \quad \langle \psi \rangle = \sum_{l=1}^{\infty} \left( \frac{n}{2} \right) \frac{2C_{l}^{2}(\nu_{l}^{2})}{m_{c}^{2}} \sum_{m, l, \ell, b} \left[ (2\ell + 1) \left( \psi_{l}^{m} - \psi_{l}^{m*} \right) \right] \]

\[
\left[ \text{COMPLETE SHELLS} \right] + \left[ \text{INCOMPLETE SHELLS} \right]
\]

\[
\left( \frac{n}{2} \right) \frac{2C_{l}^{2}(\nu_{l}^{2})}{m_{c}^{2}} \sum_{l=1}^{\infty} \left[ \frac{(2\ell + 1)}{2(2\ell + 1)(2\ell + 3)} \delta_{\ell, 0} \right] \left[ \psi_{l}^{m} - \psi_{l}^{m*} \right]
\]

\[
\equiv \sum_{l=1}^{\infty} \left[ \Delta E_{l}^{(1)} - \frac{1}{2} \Delta E_{l}^{(2)} + \Delta E_{l}^{(3)} \right]
\]
where

\begin{align}
\beta^0_{n\ell} &= \int \rho^2 d\rho \left( -\mathcal{N}_0(\ell, n) + j_0(\ell, n) \right) | R_{n\ell}(\gamma)|^2 \\
\beta^0_{n\ell} &= \int \rho^2 d\rho \left[ 2(\mathcal{N}_0(\ell, n) - j_0(\ell, n)) \right] | R_{n\ell}(\gamma)|^2
\end{align}

In the last expressions, $-\mathcal{N}_0(\ell, n)$ is a spherical Neumann function, and $j_0(\ell, n)$ is a spherical Bessel function. The width, energy level shift $\Delta E_{RS}^{0\ell} - \frac{i}{2} R_{n\ell}^{0\ell}$ is independent of the excited level $N_e$, while $\Delta E_{RS}^{0\ell} - \frac{i}{2} R_{n\ell}^{0\ell}$ is dependent on $N_e$. However, the latter quantity is completely negligible. For a wave function of the form $(\ell \ell) C_{\ell}^{n\ell} e^{-i\beta_{n\ell}}$, we have

$$\Delta E_{RS}^{0\ell}(\gamma) \sim -\left( \frac{\alpha^2}{mc^2} \right) \left( \frac{1}{\kappa e_{\gamma, \ell = 1}} \right)^3 \left( \frac{n_\gamma}{\gamma} \right)^2 \sim -3 \times 10^{-5} \left( \frac{n_\gamma}{\gamma} \right)^2$$

and

$$\frac{1}{2} R_{n\ell}^{0\ell}(\gamma) \sim \left( \frac{\alpha^2}{mc^2} \right) \left( \frac{1}{\kappa e_{\gamma, \ell = 1}} \right)^3 \sim 3 \times 10^{-5} \left( \frac{n_\gamma}{\gamma} \right)^2$$

for Fe$^{57}$ (we have taken $e_{\gamma, \ell = 1} \sim 10^{-6}$ cm). The width $R_{n\ell}^{0\ell}$, although much larger than $R_{n\ell}^{0\ell}$, still makes only a negligible contribution to the total width. For the K-shell, $R_{n\ell}^{0\ell} \sim 8 \times 10^{-3} (\gamma)$ for Fe$^{57}$, and for the total filled shells, $R_{n\ell}^{0\ell} \sim 10^{-1} (\gamma)$, which gives a negligible contribution to $\gamma$. However, the level shift $\Delta E_{RS}^{0\ell}$ is quite large in comparison to $\gamma$ and the Zeeman splitting. For the K-shell

$$\Delta E_{RS}^{0\ell} = -\frac{1}{2} \left( \frac{\alpha^2}{mc^2} \right) \left( \frac{1}{\kappa e_{\gamma} \gamma} \right)^3 \sim -10^3 \left( \frac{\gamma}{\gamma} \right)^2$$

for Fe$^{57}$.

This is not a measureable effect, however, since $\Delta E_{RS}^{0\ell}$ is independent of $N_e$, and hence all excited levels are shifted by the same amount.

Collecting all the contributions (a) - (f) we finally have for expression (13),

\begin{align}
\left[ \gamma - (\mathcal{E}_e - \mathcal{E}_{\ell \ell}) + \frac{1}{2} \gamma \right] S_{\gamma, \ell \ell}^{(1)} = \mathcal{S}_F^{(1)} \mathcal{L}_a^{\ell \ell} \left[ 1 + \mathcal{S}_F^{(0)} + \mathcal{S}_F^{(1)} \right] e^{i \mathcal{K}_{\ell \ell} \cdot \mathcal{K}_{\ell \ell}}
\end{align}
In this form we see that the effect of the electron cloud is to shift the excited levels $E_n$, to broaden the width from $\Gamma_Y$ to $\Gamma_T$, and to give a screened incident field at the nucleus.

Finally we calculate the scattered photon Greens function for the system, and the scattering amplitude. Diagrammatically, the total contribution is now given by

$$\begin{align*}
\begin{array}{c}
\text{(a)} \\
\text{(b)} \\
\text{(c)} \\
\text{(d)} \\
\text{(e)}
\end{array}
\end{align*}$$

**Fig. 9.** Diagrams for photon Greens function.

For process (a) of fig. (9), the photon Greens function is given as in section (II) by

$$A(\vec{r}, \epsilon) = A(\vec{r}, \epsilon) \sum_{\alpha, \alpha'} \frac{\epsilon (\kappa |\vec{r} - \vec{r}_e| - \kappa \epsilon)}{1 - \kappa \epsilon}$$

but with $\Sigma_{\alpha, \alpha'}$ now given by expression (42).

For processes (b) + (c),

$$A^\alpha(\vec{r}, \epsilon) = \sum_{\alpha, \alpha'} \left( \frac{\epsilon (\kappa |\vec{r} - \vec{r}_e| - \kappa \epsilon)}{1 - \kappa \epsilon} \right)$$

Carrying out the non-relativistic approximation as before we obtain for the photoelectric contribution (neglecting the E-2 contribution in comparison to the M-1 contribution.)
\[ A_0^*(\vec{r}, \vec{r}) = -i \frac{\lambda}{\kappa_0^2 \kappa_2^*} \hat{\kappa}_\lambda(\lambda, \kappa_0^2) \cdot \vec{r} \cdot \vec{S}(\vec{r}) \cdot S(\vec{r}) \cdot e^{i(x^2 - \vec{r} \cdot \vec{r} - \kappa_0^2)} \]

\[ = \frac{\vec{f}(\vec{r}) \cdot \vec{S}(\vec{r}) \cdot S(\vec{r}) \cdot e^{i(x^2 - \vec{r} \cdot \vec{r} - \kappa_0^2)}}{1 \cdot \vec{r} \cdot \vec{r}} \]

where

\[ f_0^0 = \sum \lim_{x \to \kappa} \kappa^2 \langle \vec{E}_x | \vec{E}_x \rangle \langle \vec{S}(\vec{r}) | \vec{S}(\vec{r}) \rangle \cdot \langle \vec{E}^* \rangle \cdot \langle \vec{E}^* \rangle \cdot \langle \vec{E}_x | \vec{E}_x \rangle \cdot \langle \vec{E}_x | \vec{E}_x \rangle \]

Comparing with expansion (31) we see that \[ f_0^0 = f_0^0 \]

Similarly for the Rayleigh contribution

\[ \tilde{A}_0(\vec{r}, \vec{r}) = -i \frac{\lambda}{\kappa_0^2 \kappa_2^*} \hat{\kappa}_\lambda(\lambda, \kappa_0^2) \times \vec{r} \cdot \vec{r} \cdot \vec{S}(\vec{r}) \cdot S(\vec{r}) \cdot e^{i(x^2 - \vec{r} \cdot \vec{r} - \kappa_0^2)} \]

where

\[ \vec{f}(\vec{r}) = -\langle \vec{E}_0 | \sum \lim_{x \to \kappa} \frac{x^2}{\kappa_0^2} \cdot \hat{\kappa}_\lambda(\lambda, \kappa_0^2) \cdot \hat{\kappa} \rangle \cdot \langle \vec{E}_0 | \vec{E}_0 \rangle \cdot e^{-\vec{r} \cdot \vec{r} - \kappa_0^2} \]

The additional minus sign come from the relation

\[ \langle \vec{E}_0 | \sum \lim_{x \to \kappa} \frac{x^2}{\kappa_0^2} \cdot \hat{\kappa}_\lambda(\lambda, \kappa_0^2) \cdot \hat{\kappa} \rangle \cdot \langle \vec{E}_0 | \vec{E}_0 \rangle = -\lambda \lambda \hat{\kappa}_\lambda(\lambda, \kappa_0^2) \]

Again electronic wave functions of the form \[ \mathcal{R}(\lambda, \kappa_0^2 \varphi \rho \sigma) \], and neglecting the small contribution from the incomplete shells ( s ), then
\[
\mathcal{G}(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') = \sum_{n} \mathcal{G}_n(\vec{r}) \mathcal{G}_n(\vec{r}') \sum_{\mu} \frac{e^{i \mathcal{K}(\vec{r} - \vec{r}')} \mathcal{A}_{\mu}(\vec{r}, \vec{r}')}{\mathcal{K} - \mathcal{K}_n}
\]

where

\[
\mathcal{F}(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') = \left\{ \mathcal{F}_n(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') \left(1 + \mathcal{F}_n(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') \right) \right\}^{-1/2}
\]

Comparing with expression (37) we see that \( \mathcal{F}(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') \)

Thus we see that the scattered photon Greens function is given by

\[
\mathcal{A}_{\mu}(\vec{r}, \vec{r}') = \mathcal{G}(\vec{r}, \vec{r}') \mathcal{G}(\vec{r}, \vec{r}')
\]

where the purely electronic contribution is given by (10). Substituting from equation (42) for \( S_{\mu}e^{-\frac{\mathcal{K}}{\mathcal{K} - \mathcal{K}_n}} \), we finally have

\[
\mathcal{A}_{\mu}(\vec{r}, \vec{r}') = \left\{ \mathcal{F}_n(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') \mathcal{F}_n(\vec{r}, \vec{r}') \left(1 + \mathcal{F}_n(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') \right) \right\}^{-1/2}
\]

\[
\mathcal{F}(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') = \left\{ \mathcal{F}_n(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') \left(1 + \mathcal{F}_n(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') \right) \right\}^{-1/2}
\]

From expressions (II-6), and (11), we immediately obtain the scattering amplitude for the Mössbauer atom

\[
\mathcal{F}(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') = \left\{ \mathcal{F}_n(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') \left(1 + \mathcal{F}_n(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0') \right) \right\}^{-1/2}
\]

\[
+ \mathcal{F}_n(\vec{r}, \vec{r}' ; \epsilon_0, \epsilon_0')
\]

where \( f_e \) is given by
(54) \[ \mathcal{S}(\hat{r}, \hat{r}; \hat{r}_0, \hat{r}_0) = \left\{ \frac{-\mathcal{K}^2}{\mathcal{K}^2 + 1} \mathcal{F}(\hat{r}_0 - \hat{r}) \mathcal{S}(\hat{r}_0 - \hat{r}) \cdot \mathcal{S}(\hat{r}) \right\} + \frac{\mathcal{K}^2}{\mathcal{K}^2 + 1} \mathcal{S}_{\text{SE}} \]

and \( f_N \) is given by

(55) \[ f_N(\hat{r}, \hat{r}; \hat{r}_0, \hat{r}_0) = \]

If we analyze the incident and scattered radiation in terms of right and left hand circularly polarized bases, then \( \alpha_{\lambda} = \pm 1 \), AND

\( (\mathcal{S}_{\lambda}(\hat{r}) \cdot [\mathcal{S}_{\lambda}(\hat{r}_0) \times \hat{r}_0]) \cdot [\mathcal{S}_{\lambda}(\hat{r}) \times \hat{r}) = \mathcal{D}_{\lambda}(\hat{r}, \lambda) \mathcal{D}_{\lambda}(\hat{r}_0, \lambda) \)

We see from (53) that the effect of the electronic screening processes is to modify \( f_N \) by the factor \( (1 + \mathcal{S}_{\text{PE}}^0 + \mathcal{S}_{\text{RS}}^0)^2 \). This factor is polarization independent, so the polarization of the nuclear scattered radiation is determined entirely by the nuclear transitions. (This is not true, when the uncompleted shells (\( \neq s \) make a significant contribution to \( \mathcal{S}_{\text{RS}} \), or when there is a significant E-2 contribution to \( \mathcal{S}_{\text{PE}} \)). Thus the nature of the polarization dependent nuclear-electronic interference is determined entirely by the polarization dependence of \( f_N \) and \( f_e \).

Examining the screening factor \( (1 + \mathcal{S}_{\text{PE}}^0 + \mathcal{S}_{\text{RS}}^0)^2 \) in more detail, since \( |\mathcal{S}_{\text{PE}} + \mathcal{S}_{\text{RS}}|^2 \ll 1 \), we have

\[ (1 + \mathcal{S}_{\text{PE}}^0 + \mathcal{S}_{\text{RS}}^0)^2 \approx 1 + 2 (\mathcal{S}_{\text{PE}}^0 + \mathcal{S}_{\text{RS}}^0) \]

Moreover, unless the real parts of the screening factors are greater than \( 10^{-1} \), we can also neglect these parts. The most important contribution comes from the imaginary parts of the screening factors. For the Fe\(^{57} \) case, we have seen that \( \mathcal{S}_{\text{PE}}^0 \approx i \cdot 10^{-2} \), and \( \mathcal{S}_{\text{RS}}^0 \approx -i \cdot 10^{-2} \), so that \( (1 + \mathcal{S}_{\text{PE}}^0 + \mathcal{S}_{\text{RS}}^0)^2 \approx 1 + 2i \cdot 10^{-2} \). The nuclear scattering amplitude \( f_N \) has of the form \( f_N = \alpha \frac{\alpha}{\chi^2 + 1} \) where \( \chi = \frac{\mathcal{K} - \mathcal{A} \mathcal{E}}{\mathcal{K}^2} \).}

Thus the screened scattering amplitude has the form
\[ \alpha \frac{F}{r^2} \left( e^{-0.02 \frac{r}{x}} + i \left[ -0.02 x \right] \right) \] 

At resonance the screened nuclear scattering amplitude is not purely imaginary, as \( f_N \) is, but contains the real part \(-0.02 \alpha f / r_1 \sim -10^{-12} \text{ cm} \), which interferes constructively with the electronic scattering amplitude

\[ \left( z_e \sim \left[ -7 \times 10^{-12} + i 5 \times 10^{-13} \right] \text{ cm} \right) \]

It is clear, however, that in order for the screening effects to be significant, the imaginary parts of the screening factors must be at least of the order \(| I - 2 (F_{pe} + F_{rs}) | \sim 1\) or for the real parts,

\[ | R - 2 (F_{pe} + F_{rs}) | \sim 0.1 \]

The correct phonon factors for the screening processes have not been worked out yet. However, we believe that, following Trammells development, the elastic scattering phonon factor for a screening process such as fig. (10) can be put in the time dependent form

\[ \langle x_0 | e^{-i \vec{r} \cdot \vec{r}(t) / \hbar} e^{i \vec{r} \cdot \vec{r}(t) / \hbar} e^{i \vec{r} \cdot \vec{r}(t) / \hbar} e^{i \vec{r} \cdot \vec{r}(t) / \hbar} \mid x_0 \rangle \]

where \( \vec{r} \) is the center of mass displacement of the nucleus. As we have already seen in section (A),

\[ (t_1 - t_0) \lesssim 10^{-19} \text{ sec.} \]

This is a very fast process with respect to the phonon frequencies \((\nu_x \approx 2 \times 10^{12} \text{ v/\sec})\)

so we can set \( t_1 = t_0 \). Also \((t_2 - t_1) \sim \frac{\hbar}{2 \pi} \frac{\hbar}{E_C} = \frac{1.6 \times 10^{-19}}{2 \pi} \text{ sec.} \), and we can set \( t_2 = t_1 \). The nuclear excited state lifetime \( \tau \sim 10^{-7} \) (for \( E \ll 57 \)) so \((t_2 - t_2) \sim 10^{-7} \text{ sec.} \)

This is very long compared to the phonon frequencies and we can set \( t_3 = \infty \).

The phonon factor then reduces to

\[ \langle x_0 | e^{-i \vec{r} \cdot \vec{r}(t) / \hbar} e^{i \vec{r} \cdot \vec{r}(t) / \hbar} \mid x_0 \rangle = e^{-\frac{\eta}{2} \left( \vec{r} \cdot \vec{r} \right)^2 + \left( \vec{r}_0 \cdot \vec{r} \right)^2} \]

which is just the usual Mössbauer factor. The results given above in expressions (53) - (55) are then correct, since we have already included this factor in \( f_N \) (55).

If however this picture is not correct, then phonon effects could seriously alter the previous results. As an example we consider the case where each scattering process occurs elastically, so that the electronic processes are governed by the Dybye factor, and the nuclear processes by the Mössbauer factor. This will introduce a strong asymmetry in the scattering from the electron cloud to the nucleus since the momentum...
change for elastic scattering from the "front side" of the electron cloud (side toward the incident radiation) to the nucleus is much less than from the "back side". Naively, the phonon factor for the electronic process is

\[ \langle \chi_0 | e^{i(\vec{K}_0 - \vec{K}_r) \cdot \vec{r}} | \chi_0 \rangle = e^{-\frac{2\pi i x^2(\vec{K}_0 \cdot \vec{r})}{\lambda_0}} \]

\[ = e^{-\left(\frac{\lambda_0}{\lambda_0}\right)\left(1 + \frac{\vec{K}_0 \cdot \vec{r}}{\lambda_0 \gamma}\right)} \]

Where for Fe\(^{57}\), 14.4 KeV radiation, \( M = 0.35 \), \( \lambda_0 = \frac{\lambda_0}{\lambda_0} = 0.86 \). Inserting this into expressions for the Rayleigh screening, we again obtain expression ( ) for \( \tilde{F}_{\gamma_{5\gamma}}^{(1)} \) and \( \tilde{F}_{\gamma_{5\gamma}}^{(0)} \)' but with \( \tilde{\alpha}_{\lambda_0} \) now given by

\[ \tilde{\alpha}_{\lambda_0} = \frac{2\pi}{mc^2} \int_{0}^{\infty} \Phi_G(K, \kappa r + i\frac{\alpha_0}{\kappa}) \langle \frac{\alpha_0}{\kappa} + \frac{\alpha_0}{\kappa} \rangle \langle e^{i \kappa r} \rangle |R_{\alpha_0}|^2 \mathrm{d}K \mathrm{d}r \mathrm{d}\kappa \]

\( \tilde{F}_{\gamma_{5\gamma}}^{(0)} \) would then contain a large imaginary part in addition to the small real part. For the K shell, this contribution is \( \sim -2.1 \times 10^{-2} \), or for the entire electron cloud \( 2 \tilde{F}_{\gamma_{5\gamma}} \sim -1 i \), which is larger than, and of opposite sign to the previous \( \tilde{F}_{\gamma_{5\gamma}}^{(0)} \) term. The real part of the screened nuclear scattering amplitude would then interfere destructively with the electronic amplitude \( f_e \) at resonance.

The effect of such a phonon term on the photoelectric screening is much more complicated. We define

\[ F(\vec{r}) = e^{-\frac{\lambda_0}{\lambda_0} \frac{\alpha_0}{\kappa} \vec{r} \cdot \frac{\alpha_0}{\kappa} R_{\alpha_0} / \kappa} \]

\[ = e^{-\left(\frac{\lambda_0}{\lambda_0}\right)\left(1 + \frac{\alpha_0}{\kappa} \frac{\alpha_0}{\kappa} \right) \kappa r + i \frac{\alpha_0}{\kappa} \frac{\alpha_0}{\kappa} \kappa r + \frac{\alpha_0}{\kappa} \frac{\alpha_0}{\kappa} \kappa r} \]

Then returning to expression (22) and combining

\[ F(\vec{r}) \quad \text{with} \quad (-i \sqrt{\frac{\alpha_0}{\kappa}} \hat{\beta}_l / \alpha_r \left( \lambda_0 \gamma \right), \]

and using the symmetrized electronic current \( \left( \hat{J}_e^{(S)} + \hat{J}_e^{(P)} \right) \), we obtain instead of expression (29),

\[ \langle \vec{e}_1 \vec{e}_2 \rangle = i \alpha_0(\hat{x}_1^{(S)} + \hat{x}_1^{(P)}) \frac{\lambda_0}{\lambda_0} \sum_{m_1 m_2} \sum_{m_0} \langle \vec{e}_1 (\lambda_0, \vec{e}_1, m_1, \vec{e}_2, (\lambda_0, \vec{e}_2, m_2) \rangle \left[ F(\vec{r}) \hat{J}_e^{(S)} + \hat{J}_e^{(P)} \hat{J}_e^{(S)} \right] \frac{\lambda_0}{\lambda_0} \]
We will not carry out the calculations, but this expression would apparently lead to direction, polarization dependent screening factors
\[ \tilde{\xi}_{\alpha}(\hat{K}, \hat{q}), \tilde{\xi}'_{\alpha}(\hat{K}, \hat{q}) \]

A thorough analysis of the phonon modifications will be given in a following article.
IV. DYNAMICAL THEORY OF MÖSSBAUER DIFFRACTION

We will now consider the dynamical theory of Mössbauer diffraction. Our approach will be somewhat similar to the Darwin-Prin approach\(^{(16)}\). We will first treat the scattering from a single plane layer, and will then consider an M-layer crystal.

A. Scattering From a Plane Layer:

It is instructive to solve the scattering problem first for a single plane layer. As we will see, there are a number of interesting features of such scattering. To bring out these features, it is sufficient to consider purely resonant nuclear scattering, and to take as a concrete example the scattering of 14.4 KeV radiation from a plane of Fe\(^{57}\) nuclei imbedded in stainless steel.

For magnetic dipole transitions the nonrelativistic current operator is given by

\[
\mathbf{J}(\mathbf{r}) = -ie\mathbf{A}\times\mathbf{L} - ie\mathbf{R}
\]

where \(\mathbf{M} = \sum \mathbf{M}_n = \sum (\mathbf{L}_n \cdot \mathbf{I}_n)\) is the total magnetic moment operator of the nucleus. For the Zeeman split case it is convenient to express \(\mathbf{M}\) in terms of the circular basis \((\hat{e}_0, \hat{e}_+1, \hat{e}_0)\) with \(\hat{e}_0\) in the direction of magnetic polarization \((-\mathbf{B})\), since the transitions select this basis - i.e.,

\[
\langle \hat{e}_0, \mathbf{k}_0 | \mathbf{M} | \mathbf{k}_0, \mathbf{e} \rangle
\]

etc. Denoting the six M1 transitions by the subscript \((\chi; \lambda)\); \(\chi = +, -, 0\); \(\lambda = 1, 2\), we have six coupled equations from (II-18)

\[
(1) \quad Q_{\chi}(\chi; \lambda) \sum_{\chi} = \alpha_{\chi, \lambda} e^{-\frac{i}{2} \langle \hat{L} \cdot \mathbf{r} \rangle} +
\]

\[
+ \sum_{\chi} \sum_{\chi} \alpha_{\chi, \lambda} e^{-\frac{i}{2} \langle \hat{L} \cdot \mathbf{r} \rangle} \sum_{\chi} (\chi; \lambda) G_{\chi, \lambda} e^{-\frac{i}{2} \langle \hat{L} \cdot \mathbf{r} \rangle} \frac{2}{|\hat{L} - \mathbf{r}|}
\]

where \(\hat{L} = -ie\mathbf{L}\), and \(Q_{\chi}(\chi; \lambda) = -[\lambda - \Delta E(\chi; \lambda) + i \frac{\tau}{2}]\)

\(\Delta E(\chi; \lambda)\) is the energy of the \((\chi; \lambda)\) transition. The scattered photon Greens function is again given by (II-18) \((\Pi-19)\).
For the unsplit case however, the states are degenerate and we can express \( \hat{M} \) in any convenient orthogonal basis. If the incident field is \( | \vec{E}_0, \vec{E}_0 \rangle \) we can select the bases \( \hat{\vec{E}}_{(1)}, \hat{\vec{E}}_{(2)}, \hat{\vec{E}}_{(3)} \) such that \( \hat{\vec{E}}_{(1)} \) is in the direction of \( \hat{\vec{k}}_0 \), \( \hat{\vec{E}}_{(2)} \times \hat{\vec{k}}_0 \cdot \vec{E}_0 = 1 \), and \( \hat{\vec{E}}_{(3)} \times \hat{\vec{k}}_0 \cdot \vec{E}_0 = 0 \) and we have the currents \( \hat{J}_{(1)}(\vec{x}) = \hat{m} \hat{\vec{E}}_{(1)} \times \hat{\vec{k}}_0 \), etc. We then have the three coupled equations (for \( x = 1, 2, 3 \))

\[
\begin{align*}
\mathcal{Q}_\nu \sum_{\nu(x)} c^{(x)}_\nu &= \mathcal{J}_{\nu(1)} \mathcal{S}_{\nu(1)}(\vec{x}) \mathcal{S}_{\nu(1)}(\vec{r}) \mathcal{S}_{\nu(1)}(\vec{r}) \mathcal{S}_{\nu(1)}(\vec{r}) \\
&\quad+ \sum_{\nu(1)} \mathcal{J}_{\nu(1)}(\vec{x}) \mathcal{S}_{\nu(1)}(\vec{r}) \mathcal{S}_{\nu(1)}(\vec{r}) \mathcal{S}_{\nu(1)}(\vec{r}) \mathcal{S}_{\nu(1)}(\vec{r}) \\
&\quad+ \sum_{\nu(1,2,3)} \mathcal{J}_{\nu(1,2,3)}(\vec{x}) \mathcal{S}_{\nu(1,2,3)}(\vec{r}) \mathcal{S}_{\nu(1,2,3)}(\vec{r}) \mathcal{S}_{\nu(1,2,3)}(\vec{r}) \mathcal{S}_{\nu(1,2,3)}(\vec{r})
\end{align*}
\]

where \( \hat{\vec{k}}, \hat{\mathcal{Q}}_\nu \) are defined in equation (1). By the choice of bases only the \( \hat{\vec{E}}_{(1)} \) transition couples to the external field - i.e. only \( \hat{J}_{\nu(1)}(\vec{x}) \cdot \vec{E}_0 = 0 \), and the other two transitions \( \hat{\vec{E}}_{(2)}, \hat{\vec{E}}_{(3)} \) are excited only by the scattered photon field.

We now assume that the nuclei form a plane lattice which we take as the \((x, y)\) plane. The positive \( z \)-axis is taken in the direction of \( \vec{K}_z \). For simplicity we shall assume the lattice is a square lattice specified by the lattice vectors \( a \hat{\vec{a}}_x, a \hat{\vec{a}}_y \), but the method of solution carries through for any plane lattice. Due to translational invariance by a lattice vector, \( \hat{\mathcal{S}}_{\nu(x)} = \hat{e}^{i \vec{k}_y \cdot \vec{r}} \hat{\mathcal{S}}_{\nu(x)} \). Substituting into (2) and (II-19), and transforming the sum

\[
\sum_{\nu(x)} \hat{\mathcal{S}}_{\nu(x)} = \hat{e}^{i \vec{K}_y \cdot \vec{r}} \sum_{\nu(x)} \hat{\mathcal{S}}_{\nu(x)} \exp\left(i \vec{k}_y \cdot (\vec{r} - \vec{r})\right)
\]

into a sum over the \((x, y)\)-reciprocal lattice vectors \( \vec{\eta}_{x'y'} \) as shown in appendix (C), we obtain the coherent photon Greens function

\[
\hat{A}(\vec{r}) = \hat{e}_0 \hat{\mathcal{S}}_{\nu(x)} \hat{e}^{i \vec{k}_y \cdot \vec{r}} + \sum_{\eta_{x'y'}} \hat{\mathcal{J}}_{\nu(x)} \hat{\mathcal{S}}_{\nu(x)} \left\{ \hat{\mathcal{S}}_{\nu(x)} \hat{\mathcal{S}}_{\nu(x)} \right\} \exp\left(i \vec{k}_y \cdot (\vec{r} + \vec{\eta}_{x'y'})\right)
\]

\[
= \hat{e}_0 \hat{\mathcal{S}}_{\nu(x)} \hat{e}^{i \vec{k}_y \cdot \vec{r}} + \sum_{\eta_{x'y'}} \hat{\mathcal{J}}_{\nu(x)} \hat{\mathcal{S}}_{\nu(x)} \left\{ \hat{\mathcal{S}}_{\nu(x)} \hat{\mathcal{S}}_{\nu(x)} \right\} \exp\left(i \vec{k}_y \cdot (\vec{r} + \vec{\eta}_{x'y'})\right)
\]
where

\( i \mathcal{G}_g = \sqrt{\kappa_0^2 - (\mathbf{r}^2 + \mathbf{r}^2)^2} \)

\[ \mathbf{r}^2 = (\pm \mathcal{G}_g, \mathbf{r}^{(0)}_x + \mathbf{r}^{(0)}_y) \] (PLUS SIGN FOR Z>0, MINUS FOR Z<0)

\( s_{\nu(1)} = (\mathbf{r}^{(0)}_x \cdot \mathbf{a}_z \mathbf{a}_z)/[c_0 - i \pm (\gamma(1;1_i) + \gamma(1;2) x_2 + \gamma(1;3) x_3)] \)

\( s_{\nu(2)} = x_2 s_{\nu(1)} \; ; \; s_{\nu(3)} = x_3 s_{\nu(1)} \)

\[ x_2 = \frac{2i c_0 \gamma(2;1) + \gamma(2;1) \gamma(3;3) - \gamma(2;3) \gamma(3;1)}{4 c_0^2 - [2i c_0 (\gamma(3;3) + \gamma(2;2)) + \gamma(2;2) \gamma(3;3) - \gamma(2;3) \gamma(3;2)]} \]

\( x_3 = x_2 \leftrightarrow 3 \)

\[ i \gamma(x;x) = i \sum_{\mathcal{G}_g} \frac{\mathbf{F}_{\mathcal{G}_g} \mathbf{F}_{\mathcal{G}_g}^\dagger}{(2\pi \alpha^2)} \gamma(x) \gamma(x) \left( \mathbf{J}_{\mathcal{G}_g} \mathbf{J}_{\mathcal{G}_g} - \frac{1}{2} \mathbf{J}_{\mathcal{G}_g} \mathbf{J}_{\mathcal{G}_g}^\dagger + \mathbf{J}_{\mathcal{G}_g}^\dagger \mathbf{J}_{\mathcal{G}_g} \right) \]

\[ i \gamma(x;y) = i \sum_{\mathcal{G}_g} \frac{\mathbf{F}_{\mathcal{G}_g} \mathbf{F}_{\mathcal{G}_g}^\dagger}{(2\pi \alpha^2)} \gamma(x) \gamma(y) \left( \mathbf{J}_{\mathcal{G}_g} \mathbf{J}_{\mathcal{G}_g} - \frac{1}{2} \mathbf{J}_{\mathcal{G}_g} \mathbf{J}_{\mathcal{G}_g}^\dagger + \mathbf{J}_{\mathcal{G}_g}^\dagger \mathbf{J}_{\mathcal{G}_g} \right) \]

There are a number of interesting features of the solution (3). First we note that the scattered photon amplitude is a superposition of plane wave channels having wave vectors \( \mathbf{r}^{(0)}_x = \{ \pm \mathcal{G}_g, \mathbf{r}^{(0)}_x + \mathbf{r}^{(0)}_y \} \). These channels are symmetric about the scattering plane. For each forward scattered wave in the direction, there is a reflected wave in the direction. We see from (4i) that there are only a finite number of vectors \( \mathbf{r}^{(0)}_y \) for which the corresponding \( \mathcal{G}_g \) is real. For \( K_0 = 14.4 \text{ KeV} \), and the BCC lattice constant \( a = 2.9 \times 10^{-8} \text{ cm} \), there are a maximum of
about 13 \( \bar{\gamma}_g^{(l)} \) for which the corresponding \( \bar{\epsilon} \) are real. The \( \bar{\epsilon}_g \) corresponding to the remaining \( \bar{\gamma}_g^{(l)} \) are imaginary and give exponentially damped waves \( \left( e^{-\mu_{g,l} |z|} / \mu_{g,l} |z| \right) \). The sum over all the imaginary \( \bar{\epsilon}_g \) gives a contribution to (3) on the order of \( \left( e^{-\mu_{g,l} |z|} / \mu_{g,l} |z| \right) \) which is only appreciable within a wavelength of the plane and can be neglected.

The "excitation amplitudes" \( \bar{\epsilon}_g^{(l)} \) correspond to the classical vibrational amplitudes \( \bar{\delta}_g^{(l)} \) of three orthogonal oscillators. By the choice of basis, only the \( \bar{\delta}_g^{(l)} \) transition is excited directly by the external field, as given by (4iii). The \( \bar{\delta}_g^{(l)} \), \( \bar{\delta}_g^{(l)} \) transitions can only be excited by the scattered photon potential, and are coupled to the excitation of the \( \bar{\delta}_g^{(l)} \) transition by (4iv) - (4vi). Unless the coupling constants \( X_2 = X_3 = 0 \), the response of the layer is not in the direction of the polarization of the external field. Classically, the isotropic oscillators will vibrate along a direction determined by the superposition of the incident field and the self field of the plane at a lattice site. As we will show below, unless a channel is just open, \( \bar{\epsilon}^{(l)} \), \( \bar{\epsilon}^{(l)} \) are small with respect to the total width \( \Gamma_l \), and to good approximation the coupling constants \( X_{1,2} \equiv \bar{\epsilon}^{(l)} \equiv \left( 1 / \Gamma_l \right) \). For Fe\( ^{57} \), \( \bar{\epsilon}^{(l)} \approx 10^{-3} \) and the radiation scattered by the \( \bar{\delta}_g^{(l)} \), \( \bar{\delta}_g^{(l)} \) transitions are thus down by three orders of magnitude from that of the \( \bar{\delta}_g^{(l)} \) transition. This is because the radiation from the \( \bar{\delta}_g^{(l)} \), \( \bar{\delta}_g^{(l)} \) transition must first be scattered from an \( \bar{\delta}_g^{(l)} \) transition, and the amplitude for each scattering process is small.

The quantity \( \bar{\epsilon}^{(l)} \) of expression (4iv) gives a width-energy level shift due to the virtual emission-absorption of a photon by the \( \bar{\delta}_g^{(l)} \) transition into any of the \( \bar{\delta}_g^{(l)} \) channels. Similarly \( \bar{\epsilon}^{(l)} \) gives the width-energy level shift due to the virtual photon emission by the \( \bar{\delta}_g^{(l)} \) transition \( \left( \bar{\delta}_g^{(l)} \rightarrow \gamma \right) \) and absorption of the photon by the \( \bar{\delta}_g^{(l)} \) transition \( \left( \gamma \rightarrow \bar{\delta}_g^{(l)} \right) \). If \( X_2 = X_3 = 0 \) such that we are selectively exciting the \( \bar{\delta}_g^{(l)} \) transition, then \( \bar{\epsilon}^{(l)} \) gives the coherent width (and energy level shift) for scattering from a nucleus in the plane. As we shall see, this is generally quite different from the isolated nucleus elastic scattering width \( \Gamma_g \). The contribution from the open channels \( \bar{\epsilon}_g^{(l)} \) (real) gives the coherent scattering width:
\( \frac{\Pi(x;x)}{x} = \frac{2 \pi}{(2\beta a)^2} \left( \frac{E - \beta a x \cdot x}{2\beta + 1} \right) \left( \sum_{\beta(\beta)} \frac{i}{2\sin \phi_{(\beta)}} \left[ \sin^2(\phi_{(\beta)} \theta_{(\beta)}) + \sin^2(\phi_{(\beta)} \theta_{(\beta)}) \right] \right) \left( \frac{\gamma}{x} \right) \)

where \( \sin \phi_{(\beta)} = \left( \frac{\beta a}{\kappa_0} \right) \), \( F \) is the fraction of resonant nuclei, and \( \sin^2(\phi_{(\beta)} \theta_{(\beta)}) = \frac{1}{2} \). Unless one of the channels is just opened \( (\sin \phi_{(\beta)} \sim 0) \), as we will discuss below, then \( \Pi(x;x) \) is generally much smaller than the isolated nucleus elastic scattering width \( \Gamma \). For 14.4 KeV radiation incident on a plane containing Fe\(^{57}\), with \( a = 2.9 \text{ A} \), and assuming about 12 channels open with \( \sin \phi_{(\beta)} \sim \frac{1}{2} \), \( \sin^2(\phi_{(\beta)} \theta_{(\beta)}) \sim \frac{1}{2} \), then \( \Pi(x;x) \sim 2F \times 10^{-2} \Gamma \sim 2F \times 10^{-2} \Gamma \sim F \times 10^{-2} \text{ eV} \).

The contribution from the closed channels (\( \phi_{(\beta)} \text{ imag.} \)) gives the energy level shift. As given by (4vi), this term is divergent. This is because the sum \( \sum_{\beta(\beta)} \left\{ \frac{E - \beta a x \cdot x}{2\beta + 1} \right\} \left( \frac{\gamma}{x} \right) \) included the singular \( \beta = \frac{1}{2} \) term, or equivalently, because we have included the infinite self energy of a single nucleus. Renormalizing by subtracting out the singular term from the sum, we have

\( \Delta E(x;x) = \mathcal{R}(\frac{x}{2}) \frac{E - \beta a x \cdot x}{2\beta + 1} \left( \frac{\gamma}{x} \right) \)

Unless a channel is just closed \( (\phi_{(\beta)} \sim 0) \), this gives a very small shift. For a plane containing Fe\(^{57}\) scattering 14.4 KeV radiation,

\( \Delta E(x;x) \sim -\left( \frac{1}{\kappa_0} \right) \left( \frac{E - \beta a x \cdot x}{2\beta + 1} \right) \left( \frac{\gamma}{x} \right) \sim -10^{-2} \Gamma \sim 5 \times 10^{-2} \text{ eV} \).
Although the width-energy level shift for a single layer is usually small, if a channel \( S' \) is just opened \( (\gamma_{S'} = 0) \) the width \( \gamma_{(S' \lambda)} \) becomes infinite; while just before the channel is opened, the energy level shift is infinite. As we shall see in the example considered below, when the width becomes infinite the layer becomes perfectly transparent to the incident radiation. However, this effect is confined to extremely well defined directions of the incoming radiation. For a newly opened channel, \( \sin \theta_{(S)} = a(S) \) and

\[
\gamma_{(S' \lambda)} = \frac{2\pi}{\hbar^2} \left( \frac{E_x - k_x^2}{E_0} \right) \left( \frac{1}{\epsilon(S)} \right) \gamma_T = \left( \frac{2\pi}{\hbar^2} \right) \gamma_T
\]

for \( \text{Fe}^{57}, 14.4 \text{ KeV incident radiation. Thus } \epsilon(S) \text{ must be less than about } 10^{-4} \text{ radians to doubt the total width, or equivalently, the incident radia-}

To bring out some of the physics more clearly, it is useful to consider a particularly simple case of the general solution (3). We define the basis \( (\hat{e}_c, \hat{e}_\alpha, \hat{e}_\lambda) \) such that \( \hat{e}_c \) is in the direction of the incident photon \( (= \hat{e}_x/k_x) \). \( \hat{e}_\alpha \) is perpendicular to \( \hat{e}_c \) and parallel to the \( \{xy\} \) plane, and \( \hat{e}_\lambda = \hat{e}_c \times \hat{e}_c \), as shown in figure (11). The simplest possible case for scattering from a plane of isotropic magnetic dipole currents occurs when the incident photon is \( |\hat{e}_c, \hat{e}_\alpha \rangle \), and for which the sums over the allowed \( \hat{e}_{x}^{(\prime)} \) only include \( \hat{e}_x \) and vectors \( \hat{e}_y \) parallel to \( \hat{e}_{x}^{(\prime)} \). This is because for incident \( \hat{e}_\alpha \), the magnetic vector is in the \( \hat{e}_c \) direction, and if only the \( \hat{e}_{x}^{(\prime)}, \hat{e}_{y}^{(\prime)} \parallel \hat{e}_{x}^{(\prime)} \) channels are open, the magnetic dipoles oscillate in the \( \hat{e}_c \) direction, which lies in the plane of the dipoles, perpendicular to all transmitted and reflected channels. Quantum mechanically, this corresponds to only exciting the \( \hat{e}_{y}^{(\prime)} \) transition. The basis for the magnetic moment operator is \( (\hat{e}_c, \hat{e}_\alpha, \hat{e}_\lambda) = \hat{e}_c, \hat{e}_\alpha, \hat{e}_\lambda \). If only \( \hat{e}_{x}^{(\prime)}, \hat{e}_{y}^{(\prime)} \parallel \hat{e}_{x}^{(\prime)} \) terms appear in the sum, it is easily shown that \( \gamma_{(S' \lambda)} = 0, \lambda = 2, 3 \), and hence that \( X_2 = X_3 = \)
\( S_{N(2)} = S_{N(3)} = 0 \). The photon Greens function at \( \vec{r} \) is then given by

\[
\vec{A}(\vec{r}) = \alpha_0 \hat{e}_\alpha \cdot e^{i \vec{k}_0 \cdot \vec{r}} + \alpha_0 \hat{e}_\alpha \times \left( \frac{\vec{k}_0}{\kappa_0} \right) \frac{\gamma_0^2 (\vec{k}_0 \cdot \vec{r})}{\kappa_0 - (\vec{\kappa}_y - \vec{\kappa}_y^0) \cdot \vec{r} + i \frac{\gamma_0}{2} + \frac{i}{\gamma_0} \sum \gamma_i} \\
\equiv \alpha_0 \hat{e}_\alpha \cdot e^{i \vec{k}_0 \cdot \vec{r}} + \alpha_0 \hat{e}_\alpha \times \left( \frac{\vec{k}_0}{\kappa_0} \right) \frac{\gamma_0^2 (\vec{k}_0 \cdot \vec{r})}{1 - i \frac{\gamma_0}{\kappa_0} \gamma_i}
\]

where

\[
\gamma_i = \frac{\sin \theta_i}{\gamma_0} \gamma \left( \gamma \vec{r}_i \right) = \frac{2\pi F_y \gamma_i \vec{\vec{K}}_y}{(\gamma_0 \kappa_0 \sin \theta_j)^2 + (\gamma_0 \kappa_0)^2 + 1} \gamma_j
\]

\[
f_{(s)} = \left( \frac{\gamma_j}{\gamma_0} \right) e^{-\kappa_i \vec{r}_i}
\]

The more explicit have \( \gamma_i \) is the internal conversion width, \( \gamma_j \) the single nucleus elastic scattering width. The sum \( \sum_i = \sum \gamma_i \) over \( \vec{\vec{K}}_y \) gives the coherent scattering width for the system, which for most incident \( \vec{r}_i \) is less than \( \gamma_j \) - as we have already seen (eq. (5)).

As shown by equation (8) below, \( f_{(s)} \) can be interpreted as the scattering amplitude of the plane into the channel. \( f_{(s)} \) is a dimensionless quantity and is related to the single particle scattering length (amplitude) \( f_{nucl.} \) by

\[
f_{(s)} = \frac{2\pi \alpha_0 \gamma_j}{\gamma_0} \left( \frac{\gamma_0^2 \vec{r}_i}{\gamma_0 + 1} \right) f_{nucl.} \left( \vec{e}_\alpha', \vec{r}_i; \vec{e}_\alpha, \vec{r}_i \right)
\]

\[
= \frac{2\pi \alpha_0 \gamma_j}{\gamma_0} \left( \frac{\gamma_0^2 \vec{r}_i}{\gamma_0 + 1} \right) f_{nucl.}
\]
where in the second line \( d \) is an interplanar distance for a three dimensional crystal and \( N = \frac{(2\pi)^{3}}{3} \) is the number of atoms per unit volume for such a crystal. For Fe\(^{57} \), 14.4 KeV incident radiation, \( \alpha = 2.9 \times 10^{-6} \text{ cm} \), the scattering amplitude into the (0) channel (reflected and forward scattered waves) is

\[
\frac{\mathcal{F}(0)}{\langle \mathcal{F}(0) \rangle} = \left( \frac{\sigma_{s}}{2\pi} \right) \times 10^{-4} \left[ \frac{\xi + \delta}{\xi^{2} + 1} \right] \]

where \( \chi = \frac{\alpha_{s} - \delta}{\rho_{s} / 2} \)

From (8), (9) we see that the scattering amplitude of the plane into the various channels are quite small. It is clear that in order to get appreciable scattering we must have more than \( 10^{3} \) layers which scatter with constructive interference.

From (6) we see that the reflected wave \( \left( \mathbf{R}_{6-7} \right) \) amplitude into the \( s \) channel is

\[
\tilde{\mathbf{A}}_{s}(\mathbf{r}) = \alpha_{s} \hat{\mathbf{e}}(\mathbf{R}_{6-7}) \frac{\hat{\mathbf{R}}_{6-7} \cdot \mathbf{R}}{(\alpha_{s} - \delta) - \frac{1}{2} (\alpha_{s} + \delta)} = \frac{\alpha_{s} \hat{\mathbf{e}}(\mathbf{R}_{6-7}) \hat{\mathbf{R}}_{6-7} \cdot \mathbf{R}}{1 - \frac{1}{2} \frac{\alpha_{s} + \delta}{\rho_{s}}} \]

where \( \hat{\mathbf{e}}(\mathbf{R}_{6-7}) = \hat{\mathbf{e}} \times \mathbf{R}_{6-7} / \rho_{s} \)

Similarly for the forward scattered wave

\[
\tilde{\mathbf{A}}_{s}(\mathbf{r}) = \alpha_{s} \hat{\mathbf{e}}(\mathbf{R}_{6+7}) \left[ \delta_{0s} + \frac{\hat{\mathbf{e}}(\mathbf{R}_{6+7}) \cdot \mathbf{r}}{1 - \frac{1}{2} \frac{\alpha_{s} + \delta}{\rho_{s}}} \right] \]

where \( \delta_{0s} = 1, \delta_{s = 0} \)

For the (0) channel the reflection and transmission coefficients are

\[
(i) \quad \mathcal{R} = \left| \frac{\hat{\mathbf{e}}(\mathbf{R}_{0})}{1 - \frac{1}{2} \frac{\alpha_{s} + \delta}{\rho_{s}}} \right|^{2}
\]

\[
(ii) \quad \mathcal{T} = \left| \frac{1 - \frac{1}{2} \frac{\alpha_{s} + \delta}{\rho_{s}}}{1 - \frac{1}{2} \frac{\alpha_{s} + \delta}{\rho_{s}}} \right|
\]
An interesting feature of the plane layer is that total transmission can occur. For well defined directions of \( \vec{k}_0 \) such that a channel \( (s') \) is just opened, \( J(s') = 0 \) and \( R(s') = R(s) = \infty \). The coherent width is infinite and the nuclear excitation amplitudes \( S_{\mu_k l} \) are identically zero. From (10) and (11) we see that the forward scattered wave is 
\[
\hat{A}_{(s')} = \hat{A}_s \hat{e}_a e^{i \vec{k}_0 \cdot \vec{R}}
\]
which is equal to the incident wave. Furthermore, the wave amplitudes scattered into all other channels are zero except for the \( (s') \) channel, 
\[
\hat{A}_{(s', s)} = -\hat{A}_s \hat{e}_a (\vec{k}_s \cdot \vec{R}) e^{i (\vec{k}_s \cdot \vec{R} + \vec{k}_s \cdot \vec{R}')}.
\]
The \( (s') \) wave is parallel to the surface with intensity equal to the incident wave. However, the ratio of the total energy of this wave to the total incident energy is zero. Geometrically this is because the energy incident in an area \( A^2 \) is reflected into an area \( A^2 (\sin \phi_0 / \sin \phi) \) in the \( (s) \) channel, and the energy ratio is thus proportional to \( \sin \phi_0 \) which goes to zero as a channel is just opened. From (12-i) we see that the transmission coefficient is unity, and the layer is perfectly transparent to the incident radiation.

Another way of viewing this situation is as a type of Bormann effect (17), (18) - the wave radiated by the plane in the \( (s') \) channel is equal in magnitude and 180° out of phase with the incident field at the lattice sites, and hence the excitation amplitudes \( S_{\mu_k l} \) are zero, and total transmission occurs. Actually it is the magnetic vectors which are equal and out of phase for M1 scattering -
\[
\hat{e}_a \times \vec{R} \cdot \left[ \hat{e}_a e^{i \vec{k}_0 \cdot \vec{R}} - \hat{e}_a (\vec{k}_s \cdot \vec{R}) e^{i (\vec{k}_s \cdot \vec{R} + \vec{k}_s \cdot \vec{R}')} \right] = 0
\]
where \( \vec{k}_s = -\hat{z} / k \)

If we consider a plane of finite extent, the degeneracies associated with this anomalous transmission are removed. As we have seen, an infinite plane lattice interacting with a monochromatic plane wave will produce well defined plane waves \( \vec{R}_{(s')} = \{ \pm \vec{R}_{(s)}, \vec{R}_{(s')} + \vec{R}_{(s')} \} \)
However, for a finite plane lattice containing \( N^2 \) nuclei, the vectors are only defined to within an area \( (\frac{2\pi}{a})^2 \) of reciprocal lattice space, and the waves scattered by a finite plane are correspondingly spread. If \( \vec{R}_{(s')} \) corresponds to a just opened channel for incident radiation \( (\vec{k}_s, \vec{k}_{s'}) \) (for an infinite plane), then letting 
\[
\vec{R}_{(s')} = \vec{R}_{(s')} + \vec{R}_a (\cos \gamma \cos \theta - \sin \gamma \sin \alpha \cos \phi) + \vec{R}_a (\cos \gamma \sin \theta - \sin \gamma \sin \alpha \cos \phi)
\]
we have 
\[
J(s') = \sqrt{2} [\vec{R}_{(s')} \cdot \vec{k}_s - (\vec{k}_s \cdot \vec{k}_{s'})^2] = \sqrt{2} \left[ \vec{R}_{(s')} \cdot \vec{k}_s + \vec{R}_{(s')} \cdot \vec{k}_s \right] \cos \phi
\]
Averaging 
\[
\bar{J}(s') = \frac{2\pi e^{-k_0^2 x^2 / (k_0)} n_{\text{con}}(x, \psi) \cos \phi\overline{(\xi)} \overline{(\xi)}
\]
over \( (x, \psi) \) we obtain
\begin{equation}
\langle \xi_{\mu} \rangle = \sqrt{\frac{2\pi}{\alpha_c}} e^{-\frac{k_{\mu}^2}{2\alpha_c^2}} \xi_{\mu} \quad \text{for } (N)^2 = (\alpha_c^2)^2
\end{equation}

The surface wave \( \vec{\mathbf{K}}_{(s)} = \{ \alpha_c, \vec{\mathbf{K}}_{x} \} \) is no longer strictly parallel to the surface, but is spread with a z-component varying between

\( \alpha_c \propto \sqrt{\frac{2\pi}{\alpha_c^2} \frac{\alpha_c}{\nu}} \), or for an angular spread \( \phi_{(s)} \propto \sqrt{\frac{2\pi}{\alpha_c^2}} \). This spreading of a surface wave for a finite plane can also be obtained using the uncertainty principle \( \langle \delta \alpha_c \rangle (\delta \alpha_c) \propto \frac{\alpha_c}{\nu} \). For an open channel \( \delta \alpha_c = \alpha_c \delta \alpha_c \), \( \delta \alpha_c = \frac{\alpha_c}{\nu} \sin \alpha_c \) and hence \( \delta \alpha_c \propto \frac{\alpha_c}{\nu} \alpha_c \sin \alpha_c \), while for a just opened channel, \( \delta \alpha_c = \frac{\alpha_c}{\nu} \alpha_c \) and hence \( \delta \alpha_c \propto \frac{\alpha_c}{\nu} \alpha_c \) as before. It is interesting to note that the spread, or uncertainty of the wave in a just opened channel, such as at grazing incidence, is much greater than the spread of an open channel wave \( \alpha_c \propto \sqrt{\alpha_c} \).

The ratio of the energy carried off in the surface wave to the energy incident on the surface is

\begin{equation}
\langle s' \rangle = \langle \left| \frac{\hat{E}_{(s)}}{1 - \frac{\hat{E}_{(s)}}{\hat{E}_{(s)}}} \right|^2 \rangle \left[ \frac{\nu \alpha_c \alpha_c}{(\nu \alpha_c^2)^2} \right] \frac{\nu \alpha_c \alpha_c}{(\nu \alpha_c^2)^2}
\end{equation}

while the transmission coefficient is

\begin{equation}
\langle T \rangle = \langle \left| \frac{\hat{E}_{(s)}}{1 - \frac{\hat{E}_{(s)}}{\hat{E}_{(s)}}} \right|^2 \rangle
\end{equation}

in the limit \( N \rightarrow \infty \), then \( \langle T \rangle \rightarrow 1 \) and \( \langle s \rangle \rightarrow 0 \) as we obtained before.

B. Multilayer Crystal-Dynamical Theory of Mössbauer Scattering:

We now consider the nuclei to be in a lattice consisting of \( M \) plane layers, each of infinite extent in the direction. We will again make use of the plane layer solutions and the break up into channels. The analysis is similar to that of Laue\(^{(13)}\). Any wave of appreciable magnitude within the crystal is built up by the constructive interference of the
radiation scattered into one of the \( \mathcal{E}_{x_{\rho_y}} \) channels by the crystalline planes. We will then say that the \( \langle s \rangle \) channel is open in the crystal. There are usually only one or two channels open. Off Bragg, or for Bragg scattering from the \( \langle x, y \rangle \) planes, only the \( \langle 0 \rangle \) channel is open. The forward scattered branch of the \( \langle 0 \rangle \) channel is always open, corresponding to direct penetration. For Bragg scattering from any other set of planes, one additional channel is open.

For simplicity we shall only consider the cubic type crystals which can be described by the lattice vectors \( a_{\bar{x}}, a_{\bar{y}}, \) and \( a_{\bar{z}} = \alpha \bar{x} + \beta \bar{y} + \gamma \bar{z} \). Here the interplanar distance \( \alpha \) equals \( \alpha \) for s.c., \( \mathcal{E} \) for B.C.C., F.C.C., and \( \alpha, \beta, \gamma \) are the appropriate \( \langle x, y \rangle \) components for the three lattices.

From equations (II-18), (II-19), (III-10), and (III-52), we see that the photon Greens function is given by

\[
\mathcal{A}^{\mu}(\mathbf{r}, \mathbf{r}) = \mathcal{A}_0^{\mu}(\mathbf{r}, \mathbf{r}) + \mathcal{A}_w^{\mu}(\mathbf{r}, \mathbf{r}) + \mathcal{A}_e^{\mu}(\mathbf{r}, \mathbf{r})
\]

\[
= \mathcal{A}_0^{\mu}(\mathbf{r}, \mathbf{r}) + \sum \sum \mathcal{J}^{\mu}(\mathbf{r}) \mathcal{S}_{x_{\rho_y}}(\mathbf{r}, \mathbf{r}) \mathcal{F}(\mathbf{r} - \mathbf{r}) \frac{e^{i(\mathbf{k} \cdot \mathbf{r} - \mathbf{E} \cdot \mathbf{r})}}{\mathbf{r} - \mathbf{r}}
\]

where the sum over \( x \) is a sum over nuclear and electronic portions —

\[
\sum_{x_{\nu}} = \sum_{x_{\rho_y}} \quad \sum_{x_{\mu}} = \sum_{x_{\rho_y}}
\]

and

\[
\mathcal{J}^{\mu}(\mathbf{r}) \mathcal{F}(\mathbf{r} - \mathbf{r}) \mathcal{S}_{x_{\mu}}(\mathbf{r}) = \left( \frac{\nu + 1}{\nu + 1} \right) \mathcal{S}_{x_{\mu}}(\mathbf{r}) \left( \mathcal{J}^{\mu}(\mathbf{r}) \mathcal{F}(\mathbf{r} - \mathbf{r}) \mathcal{S}_{x_{\mu}}(\mathbf{r}) \right)
\]

\[
\mathcal{J}^{\mu}(\mathbf{r}) \mathcal{F}(\mathbf{r} - \mathbf{r}) \mathcal{S}_{x_{\mu}}(\mathbf{r}) = \mathcal{J}^{\mu}(\mathbf{r}) \mathcal{F}(\mathbf{r} - \mathbf{r}) \mathcal{S}_{x_{\mu}}(\mathbf{r}) - \mathcal{J}^{\mu}(\mathbf{r}) \mathcal{F}(\mathbf{r} - \mathbf{r}) \mathcal{S}_{x_{\mu}}(\mathbf{r})
\]

\[
= \text{NEXT PAGE}
\]
\[
\begin{align*}
\mathcal{F}_{\mathbf{R}}^r (\mathbf{R} - \mathbf{R}') &= \mathcal{F}_{\mathbf{R}}^r (\mathbf{R} - \mathbf{R}') \mathcal{F}_{\mathbf{R}}^r (\mathbf{R}') \mathcal{A}_{\mathbf{R}} (\mathbf{R}, t) / Q_{\mathbf{R} \mathbf{R}'} \\
&= \left\{ \begin{aligned}
\mathcal{F}_{\mathbf{R}}^r (\mathbf{R} - \mathbf{R}') \mathcal{F}_{\mathbf{R}}^r (\mathbf{R}') \mathcal{A}_{\mathbf{R}} (\mathbf{R}, t) / Q_{\mathbf{R} \mathbf{R}'} \\
- \mathcal{F}_{\mathbf{R}}^r (\mathbf{R} - \mathbf{R}') \mathcal{F}_{\mathbf{R}}^r (\mathbf{R}') \mathcal{A}_{\mathbf{R}} (\mathbf{R}, t) / Q_{\mathbf{R} \mathbf{R}'}
\end{aligned} \right. \\
\end{align*}
\]

(iii) 
\[
Q_{\mathbf{R} \mathbf{R}'} = [\kappa - (E_{\mathbf{R}'} - E_{\mathbf{R}}) + i \varepsilon / 2]
\]

\[
Q_{\mathbf{R} \mathbf{R}'} = [\kappa - (E_{\mathbf{R}'} - E_{\mathbf{R}}) + i \varepsilon]
\]

\[
Q_{\mathbf{R} \mathbf{R}'} = [\kappa + (E_{\mathbf{R}'} - E_{\mathbf{R}}) + i \varepsilon]
\]

In equations (16) and (17), \( \hat{K} \) and \( \hat{K}' \) are again gradient operators, given by

\[
\begin{align*}
(18) \quad & (i) \quad \hat{K} = -i \hat{\nabla}_{\mathbf{R}} \\
& \text{operating only on } e^{i (\kappa |\mathbf{R} - \mathbf{R}'| - \kappa t)} \\
(ii) \quad & \hat{K}' = -i \hat{\nabla}_{\mathbf{R}'} \\
& \text{operating only on } \mathcal{A}_{\mathbf{R}'} (\mathbf{R}, t)
\end{align*}
\]

and finally, \( \mathcal{F}_X (\hat{K}' - \hat{K}) \) is the appropriate phonon factor for the transition involved,

\[
\begin{align*}
(19) \quad & (i) \quad \mathcal{F}_X (\hat{K}' - \hat{K}) = e^{-\frac{1}{2} \left[ (\hat{K}', \mathbf{n}) \right]^2 + (\hat{K}, \mathbf{n})^2} \\
& (ii) \quad \mathcal{F}_X (\hat{K}' - \hat{K}) = e^{-\frac{1}{2} \left[ (\hat{K}', \mathbf{n}) \cdot \mathbf{n} \right]^2}
\end{align*}
\]

In equations (16) and (17) we are dealing with an infinite number of electronic transitions \( \chi_e \), and generally a large number of nuclear transitions \( \chi_n \), and it is not convenient to solve for the excitation amplitudes \( S_X \) as was done in section (A). Instead we solve directly for the photon Greens function by means of coupled equations analogous to the Darwin-Prin equations \( ^{(13)} \). Again we make the substitution

\[
S_X^{(m)} = \mathcal{F}_X e^{i K_{\mathbf{R}} \cdot \mathbf{R}_m}
\]

where \( m \) refers to the \( m \) atom of the \( n \)th layer, and carry out the sum

\[
\sum_{m} e^{i K_{\mathbf{R}} \cdot \mathbf{R}_m} \exp \left( \kappa |\mathbf{R} - \mathbf{R}'| / \left| \mathbf{R} - \mathbf{R}' \right| \right)
\]
as shown in appendix (B). We then find that the wave incident on the \(m^{th}\) layer form above is

\[
\mathbf{A}_{m+}^{(\lambda)} = \sum_{m=0}^{m-1} \frac{2\pi i}{\mathbf{f}_{m}^{(s)} \mathbf{z}_{m+}} \mathbf{f}_{m+}^{(s)} \mathbf{z}_{m+} \mathbf{A}_{m+}^{(\lambda)} + \mathbf{i} \mathbf{S}_{\mathbf{x}}^{(m)} \mathbf{x}_{\mathbf{x}}^{(m)} \mathbf{A}_{m-}^{(\lambda)}
\]

\[
+ \delta_{m,0} \mathbf{A}_{0}^{(\lambda)} e^{i\mathbf{G}_{0} \mathbf{m} a}
\]

and similarly the total reflected wave incident on the \(m^{th}\) layer form below is

\[
\mathbf{A}_{m+}^{(\lambda)} = \sum_{m=0}^{m-1} \frac{2\pi i}{\mathbf{f}_{m}^{(s)} \mathbf{z}_{m+}} \mathbf{f}_{m+}^{(s)} \mathbf{z}_{m+} \mathbf{A}_{m+}^{(\lambda)} + \mathbf{i} \mathbf{S}_{\mathbf{x}}^{(m)} \mathbf{x}_{\mathbf{x}}^{(m)} \mathbf{A}_{m-}^{(\lambda)}
\]

where \(\mathbf{S}_{\mathbf{x}}^{(m)} = \mathbf{f}_{\mathbf{x}}^{(s)} + \mathbf{z}_{\mathbf{x}}^{(s)} \mathbf{A}_{3}\), the \(\mathbf{z}_{\mathbf{x}}^{(s)}\) are again the \((s,y)\)-plane reciprocal vectors, and \(\mathbf{f}_{\mathbf{x}}^{(s)} = \sqrt{k_{x}^{2} - (k_{y}^{(s)} + \mathbf{z}_{\mathbf{x}}^{(s)})^{2}}\)

Let \(\mathcal{E}_{\lambda}^{(s)}(\mathbf{r}_{+})\), \(\lambda = 1, 2\), be any convenient orthogonal basis vectors perpendicular to \(\mathbf{K}_{y}^{(s)}\), and similarly \(\mathcal{E}_{\lambda}^{(s)}(\mathbf{r}_{-})\) is a basis perpendicular to \(\mathbf{K}_{y}^{(s)}\). Then the amplitude that a photon \(\mathcal{E}_{\lambda}^{(s)}(\mathbf{r}_{+})\) is incident on the \(m^{th}\) layer (from above, in the \((s)\) channel), is *

\[
\mathbf{T}_{m}^{(\lambda; s)} = \mathcal{E}_{\lambda}^{(s)}(\mathbf{r}_{+}) \cdot \mathbf{A}_{m}^{(s)}(\mathbf{r}_{+})
\]

*) Here, and in the following development, we are making implicit use of the fact that the longitudinal and scalar parts of the photon Greens function can be eliminated in the wave region \(\langle k_{y}^{(s)} \rho_{y}^{(s)} \rangle \approx 1\), as shown in appendix (B).
Similarly the amplitude that a photon \( \hat{E}_{\lambda}^{(n)}(K_{c_s-1}) \) is incident from below is

\[
(23) \quad \mathcal{R}_{m}^{(n)} = \hat{E}_{\lambda}^{(n)}(K_{c_{s-1}}) \cdot \hat{A}_{m}(K_{c_{s-2}})
\]

Making use of the general expression \( S_{X}^{(n)} = \mathcal{S}_{X}^{(n)}(K) A_{m}^{(n)} / \mathcal{Q}_{X} \)
where \( \hat{K}_{c_{s-2}} \) and \( \mathcal{R}_{m} \) is the total photon amplitude at the \( n \)th layer including the self field of the \( n \)th layer and the upper and lower incident waves (20) and (21), we have

\[
(24) \quad \mathcal{S}_{X}^{(n)} = \mathcal{S}_{X}^{(n)}(K) A_{m}^{(n)} / \mathcal{Q}_{X}
\]

\[
= \sum_{k} \left[ \mathcal{S}_{X}^{(n)}(K_{c_{s-2}}) A_{m}^{(n)} + \mathcal{S}_{X}^{(n)}(K_{c_{s-1}}) A_{m}^{(n)} \right] \mathcal{R}_{m}^{(n)}
\]

\[
= \frac{1}{\mathcal{Q}_{X}} \sum_{k} \left[ \mathcal{S}_{X}^{(n)}(K_{c_{s-2}}) A_{m}^{(n)} + \mathcal{S}_{X}^{(n)}(K_{c_{s-1}}) A_{m}^{(n)} \right] \mathcal{R}_{m}^{(n)}
\]

where \( \mathcal{S}_{X}^{(n)}(K) \) includes the shielding factor \( (1 + \mathcal{S}_{X}^{(n)} + \mathcal{S}_{X}^{(n)}) \) and the fraction of resonant nuclei \( \sqrt{F} \). In the second line we have used the fact that for a multilayer system, the self field of a layer can be neglected in comparison to the scattered fields of the other layers. This is certainly valid if there are no newly opened channels, because then the planar scattering amplitudes are extremely small as we saw in (A ), and hence each layer gives a very small contribution to an open channel of the crystal. (Even if a channel is just opened, (24) is still a good approximation if there are greater than about \( 10^{2} \) layers. That is, the singular effects of one layer can be neglected in comparison to the singular effect of many layers.) The neglect of the self field does lead to slightly altered dispersion equations, but to find order in the planar scattering amplitudes, the same values of \( K' \) are obtained.
From (20), (22) and (24) we now have

\[
\mathcal{T}_m(1; s) = \sum_{\lambda=1}^{\infty} \sum_{m=0}^{\infty} e^{i \delta_0 (m-s)} \left( \sum_{s'} \frac{e^{i \delta_0 (s-s')}}{(s')} \left[ \sum_{\chi} \frac{e^{i \delta_0 (\chi)}}{2\pi (s+1) Q_\chi} \times \right. \right.
\]
\[
\left. \left. \left( \frac{1}{(s')} \left( \hat{\mathcal{T}}_{m, s'}^{(m,s)} \cdot \hat{\mathcal{E}}_\chi^{(s',s)} \right) / Q_\chi \right) \mathcal{T}_{m-1}(1; s') \right) \right]
\]
\[
+ \sum_{\lambda=1}^{\infty} \sum_{m=0}^{\infty} e^{i \delta_0 (m-s)} \left( \sum_{s'} \frac{e^{i \delta_0 (\lambda,s')}}{(s')} \left[ \sum_{\chi} \frac{e^{i \delta_0 (\chi)}}{2\pi (s+1) Q_\chi} \times \right. \right.
\]
\[
\left. \left. \left( \frac{1}{(s')} \left( \hat{\mathcal{T}}_{m-1, s'}^{(\lambda,s')} \cdot \hat{\mathcal{E}}_\chi^{(s',s)} \right) / Q_\chi \right) \mathcal{T}_{m-1}(1; s') \right) \right]
\]
\[
+ \hat{\mathcal{E}}_0^{+}(\vec{\mathcal{R}}_{(s+1)}) \cdot \hat{\mathcal{E}}_0 \delta_{(s+1), (s+1)} e^{i \delta_0}
\]

By carrying out the sums in (25) to \((m-2)\) and collecting terms, we finally obtain the difference equation

\[
\mathcal{T}_m(1; s) = e^{i \delta_0} \sum_{\lambda=1}^{\infty} \sum_{s'} \left( \mathcal{T}_{m-1}(1; s') \mathcal{T}_{\lambda, s'} \right)
\]
\[
+ \sum_{\lambda=1}^{\infty} \sum_{s'} \left( \mathcal{T}_{m-1}(1; s') \mathcal{T}_{\lambda, s'} \right) \mathcal{T}_{m-1}(1; s')
\]
\[
+ \delta_{(s+1), (s+1)} e^{i \delta_0}
\]

where

\[
\mathcal{T}_{\lambda, s'} = \frac{-2IF}{(s+1) Q_\chi} \sum_{\chi} \hat{\mathcal{T}}_{\lambda, s'}^{(\lambda,s')} \hat{\mathcal{E}}_\chi^{(s',s)} \hat{\mathcal{E}}_\chi^{(s',s)} / Q_\chi
\]

Equation (26) has an obvious interpretation. The amplitude \( \mathcal{T}_{m,(1; s)} \) that a wave \( \hat{\mathcal{E}}_{(1; s)} \) is incident on the \( m \)th layer is equal to the amplitude \( \mathcal{T}_{m-1,(1; s)} \) that such a wave is incident on the \((m-1)\) layer, plus the forward scattering \( \mathcal{T}_{(1; s')} \mathcal{T}_{m-1,(1; s')} \) of this wave by the \((m-1)\) layer, plus the amplitudes \( \mathcal{T}_{m-1,(1; s')} \) \( \mathcal{T}_{\lambda,(1; s')} \) of all other waves incident on the \((s+1)\) channel by this layer. These effects are then propagated to the \( m \)th layer by the phase factor \( e^{i \delta_0} \).
The planar scattering amplitudes (27) are dimensionless quantities and are related to the single particle scattering lengths (amplitudes) by

\[ f_{\text{atom}}(\lambda, s) = \frac{2\pi \hbar\omega N}{\sin \alpha_{(s)}} \int \frac{\hat{c}(\hat{R}_{(s)})}{\hat{c}(\hat{R}_{(s')})} d \]

where \( N = (a^2d)^{-1} = \text{number of atoms}/\text{cm}^3 \) and \( d \) is the interplanar distance. For M-1 nuclear transitions, the scattering lengths \( f_{\text{atom}} \) are given by expressions (53) - (55). The matrix elements

\[ \langle \hat{c}_{(s)}(\hat{R}_{(s)}) \cdot \hat{c}_{(s')}(\hat{R}_{(s')}) \rangle \]

for arbitrary multipole transitions have been worked out in detail by FRAUENFELDER, VISSCHER, etc. (20).

To generalize (26), (27) to include several atoms per unit cell, it is only necessary to replace (27) by

\[ f_{(s)}(\lambda, s') = \sum_{s'} f_{(s)}(\lambda, s') \cdot e^{-i(\hat{R}_{(s)} - \hat{R}_{(s')})} \]

There are two reasons that the substitution is a good approximation. Because the scattering from a single plane is very small, the field amplitudes \( T, R \) are essentially unchanged in magnitude in the neighborhood of a given layer (in fact it takes about \( 10^3 \) layers to cause an appreciable change), and also, as we shall see later, the smallness of the scattering amplitudes means that the internal wave vectors lie very close to \( \hat{R}_{(s)} \), \( \hat{R}_{(s')} \).

Equations similar to (21) can be obtained for \( T_{nm}^{(2,s)}, R_{nm}^{(1,s)}, R_{nm}^{(2,s)} \) and we can express all \( 4 \times n_s \) equations (where \( n_s \) = number of channels open) as \( 2 \times n_s \) coupled matrix equations.

\[ (30) \quad \Pi_{(m)}^{(s)} = \sum_{s'} \Gamma_{(s')}^{(s)} \Pi_{(m-1)}^{(s)} + i \sum_{s''} \Gamma_{(s'')}^{(s')} \Pi_{(m-1)}^{(s'')} + i \sum_{s'''} \Gamma_{(s''')}^{(s')} \Pi_{(m-1)}^{(s''')} \]

\[ + \sum_{s''''} \Gamma_{(s'''')}^{(s')} \Pi_{(m-1)}^{(s'''')} \]
\[ R_{(m)}^{(s)} = e^{i\xi R_{kl}^{(s)}} R_{(m+1)}^{(s')} + \delta \sum_{(s')} \langle s' L' | T_{mn}^{(s')} | s'' L'' \rangle R_{(m+1)}^{(s')} + \delta \sum_{(s')} \langle s' L' | T_{mn}^{(s')} | s'' L'' \rangle R_{(m+1)}^{(s')}. \]

where \[ P_{(m)}^{(s)} = \begin{pmatrix} T_{mn}^{(1,s)} \\ T_{mn}^{(2,s)} \end{pmatrix}, \quad R_{(m)}^{(s)} = \begin{pmatrix} R_{mn}^{(1,s)} \\ R_{mn}^{(2,s)} \end{pmatrix}, \quad \text{and} \]

\[ F_{(s')}^{(s \pm)} = \begin{pmatrix} F_{(1,s)}^{(1,s)} & F_{(1,s)}^{(2,s')} \\ F_{(2,s')}^{(1,s)} & F_{(2,s')}^{(2,s')} \end{pmatrix}. \]

In addition we have the boundary conditions

\[ \sum_{\lambda=1}^{2} \lambda T_{\lambda}^{(s)} \hat{\mathsf{e}}_{\lambda}(\mathcal{R}_{(s)}) = \alpha_0 \hat{\mathsf{e}}_{0} \delta(s,0+) = \hat{\mathsf{e}}_{0} \delta(s,0+) \quad \text{(normalized in units of \( \epsilon_0 = \sqrt{\frac{2m}{A}} \))} \]

\[ R_{n}^{(1,s)} = R_{n}^{(2,s)} = 0. \]

Equations (30) (i), (ii) are analogous to the Darwin equations (19), but have \( 4 \times 4 \) amplitudes to be determined rather than two. For certain cases, such as isotropic scattering, it is possible to select a basis such that all non diagonal elements of the scattering matrices (30-(iii) (30-iii) are zero, and, if only the \( (0\pm) \) channels are open, the equations decouple into two sets of Darwin type equations - one coupling \( \hat{\mathsf{e}}_{0}(\mathcal{R}_{(0+)}) \) to \( \hat{\mathsf{e}}_{0}(\mathcal{R}_{(0-)}) \) and the other coupling \( \hat{\mathsf{e}}_{2}(\mathcal{R}_{(0+)}) \) to \( \hat{\mathsf{e}}_{2}(\mathcal{R}_{(0-)}) \).

Under these conditions the Darwin-Prin solutions carry through essentially unchanged. Generally, however, it is not possible to make such a separation.

We will discuss the cases of off-Bragg, Bragg, Bormann transmission, and grazing incidence below. We note here though that off-Bragg only the \( (0+) \) channel is open; while for Bragg and grazing incidence,
the (0+) and (0-) channels are open; and for Bormann transmission, the (0+) and a (1+) channel are open. Thus for the most important optical cases, we only need to deal with one or two channels.

The general method of solving equations (30) is to make the substitutions.

\[
\begin{align*}
\mathcal{I}_m(\lambda, s) &= \sum_{\lambda'} \mathcal{I}_m(\lambda, s) e^{i\lambda' m d} \\
\mathcal{R}_m(\lambda, s) &= \sum_{\lambda'} \mathcal{R}_m(\lambda, s) e^{i\lambda' m d}
\end{align*}
\]

We will restrict our attention to the most useful case in which only two channels are open. To be definite, we will assume the (0+) and (0-) channels are open, but the same form of the equations is obtained in the Bormann case as we will show in section (??). Substituting the expressions (31) into equations (30), we obtain

\[
\begin{bmatrix}
\mathcal{I}_0(\lambda') \\
\mathcal{I}_1(\lambda') \\
\mathcal{R}_0(\lambda') \\
\mathcal{R}_1(\lambda')
\end{bmatrix}
= \begin{bmatrix}
\mathcal{I}_0(\lambda') \\
\mathcal{I}_1(\lambda') \\
\mathcal{R}_0(\lambda') \\
\mathcal{R}_1(\lambda')
\end{bmatrix}
\]

where \(\tilde{I}\) is the 4x4 unit matrix,

\[
\begin{bmatrix}
1 & 0 \\
0 & 1 \\
0 & 0 \\
0 & 0
\end{bmatrix}
\]

and the dispersion equation to determine the allowed \(K'\) is then

\[
\text{Det} \begin{bmatrix}
\mathcal{I}_0(\lambda') \\
\mathcal{I}_1(\lambda') \\
\mathcal{R}_0(\lambda') \\
\mathcal{R}_1(\lambda')
\end{bmatrix} = 0
\]

Equation (71) gives four values of \(K'\) (independent of the basis of representation), two with positive imaginary parts, and two with negative imaginary parts. If the magnetic polarization is symmetric with respect
to the scattering planes, the values are $\pm K'_1, \pm K'_2$. With the four values of $K'$ determined from (33), equations (32) give twelve independent relationships, and the remaining four relationships are given by the boundary conditions (30 iii, iv). For any particular polarization, these sixteen linear equations can be solved for the $R_{\lambda K'}^{(\lambda)}$, $T_{\lambda K'}^{(\lambda)}$ to give the reflection and transmission coefficients,

$$R_{\lambda}^{(\lambda)} = \sum_{K'} R_{\lambda K'}^{(\lambda)}, \quad T_{\lambda}^{(\lambda)} = \sum_{K'} T_{\lambda K'}^{(\lambda)} e^{i\delta K'}$$

(i) Off Bragg:

Off Bragg the problem greatly simplifies because to good approximation we can neglect the reflected wave amplitudes $R_{\lambda}^{(\lambda)}$, and we have the Fermi eigenvalue problem for the $T_{\lambda}^{(\lambda)}$:

$$\begin{bmatrix} \tilde{\omega} + i \tilde{f}_{(0)}^{(c)} \end{bmatrix} \begin{bmatrix} T_{\lambda}^{(1)} \\ T_{\lambda}^{(2)} \end{bmatrix} = e^{-ix_1} \begin{bmatrix} T_{\lambda}^{(1)} \\ T_{\lambda}^{(2)} \end{bmatrix} = e^{ix_1 - i\delta} \begin{bmatrix} T_{\lambda}^{(1)} \\ T_{\lambda}^{(2)} \end{bmatrix}$$

This gives two values of $K'$, which correspond to the two approximate eigenwaves (neglecting back scattering) which can propagate through the crystal in the forward direction

$$K'_{1,2} = \omega + \frac{d}{c} \left( \frac{f_{(1)}^{(1,0)}}{f_{(2)}^{(1,0)}} \pm \sqrt{\left( \frac{f_{(1)}^{(1,0)}}{f_{(2)}^{(1,0)}} \right)^2 - f_{(2)}^{(1,0)} f_{(1)}^{(1,0)}} \right)$$

$$= \omega + \frac{d}{c} \begin{pmatrix} f_{(1)}^{(1,0)} \\ f_{(2)}^{(1,0)} \end{pmatrix}$$

in terms of the eigen basis $\hat{E}_{(1')}$, $\hat{E}_{(2')}$.

The indexes of refraction for the two eigenwaves $\hat{E}_{(1')}$, $\hat{E}_{(2')}$ are given by

$$(35)' \quad n_{\lambda}^{(\lambda)} = \frac{K_{\lambda}^{(\lambda)}}{\lambda c} = 1 + \frac{\sin \phi f_{(\lambda,0)}}{2K_{\lambda}^{(\lambda)}}$$

for $\lambda = 1', 2'$. We note that $\sin \phi$ cancels the $(1/\sin \phi)$ term of $f_{(\lambda,0)}^{(\lambda)}$.,
so \( R_0 \) is not dependent upon the angle of incidence as it might appear.

For transmission we have the usual result

\[
(35)' \quad T_0 = e^{-2 \ell \left( C_{\lambda}^{(\alpha, o)} \right)^2} = e^{-\left[ \frac{N}{\sin \phi} \sigma_T^{(\lambda)} \right] \ell}
\]

where \( \ell = M d \) is the film thickness, and \( \sigma_T^{(\lambda)} \) is the total cross section for incident \( E_{\omega}^{(\lambda)} \) on an atom. For the nuclear contribution,

\[
NF \delta_{m} \sim \left[ \frac{C_F x_{10}^2}{(x+1)^n} \right] \mbox{cm}^{-1} \quad (Fe^{57})
\]

and hence for an incident Fe\(^{57} \) crystal, a resonant wave is damped out after about \( 10^4 \) layers.

Since the two \( K' \) are generally different, the two eigenwaves have different indexes of refraction in the crystal, giving a Faraday effect. For instance, if the beam is incident along the axis of magnetic polarization, then for MI transitions \( |K^o_o, \hat{E}_{\omega}^{(\lambda)} \rangle \) is an eigenwave coupling only to the two (+1) transitions (neglecting reflections), and \( |K^o_o, \hat{E}_{\omega}^{(\lambda)} \rangle \) is an eigenwave coupling only to the two (-1) transitions. The two (0) transitions are unexcited. The \( K' \) corresponding to the two eigenwaves are, for \( |K_{\lambda}, \hat{E}_{\omega}^{(\lambda)} \rangle \)

\[
(36) \quad \begin{align*}
(i) & \quad K'_{(\lambda)} = g_0 + \frac{i}{2} \left( \frac{C_{\lambda}^{(\alpha, o)}}{Q_{\omega}^{(\alpha, l)}} \right) (C_{\lambda}^{(\alpha, l)} + C_{\lambda}^{(-\alpha, l)}) \frac{g_1}{\Delta} + \frac{g_2}{\Delta} \\
(ii) & \quad K'_{(\lambda)} = g_0 + \frac{i}{2} \left( \frac{C_{\lambda}^{(\alpha, o)}}{Q_{\omega}^{(\alpha, l)}} \right) (C_{\lambda}^{(\alpha, l)} + C_{\lambda}^{(-\alpha, l)}) \frac{g_1}{\Delta} + \frac{g_2}{\Delta}
\end{align*}
\]

and for \( |K_{\lambda}, \hat{E}_{\omega}^{(\lambda)} \rangle \)

\[
(\hat{2}) \quad \begin{align*}
(i) & \quad K'_{(\lambda)} = g_0 + \frac{i}{2} \left( \frac{C_{\lambda}^{(\alpha, o)}}{Q_{\omega}^{(\alpha, l)}} \right) (C_{\lambda}^{(\alpha, l)} + C_{\lambda}^{(-\alpha, l)}) \frac{g_1}{\Delta} + \frac{g_2}{\Delta}
\end{align*}
\]

where \( f_\ell \) is given by (28), (III-54), \( \left( 1^+, 1^+ \right) \) label the two \( \ell^+ \) transitions

\[
Q_{\lambda}^{(\alpha, l)} = \left[ \Delta E(\lambda) - K_{\lambda} - \frac{\ell}{2} \right] , \quad \text{and} \quad C_{\lambda}^{(\alpha, \ell)}
\]

is the squared Clebsch-Gordon coefficient for the transition. By Doppler shifting an unsplit, unpolarized source so that it is in resonance with one of the transitions, as will have strong absorption in an enriched crystal of the two waves. For instance if the incident wave is in resonance with the \( 1_{1}, 1_{2} \leftrightarrow 1_{1}, 1_{2} \) transition, then

\[
K' = g_0 + \frac{i}{2} \frac{C_{\lambda}^{(\alpha, o)}}{Q_{\omega}^{(\alpha, l)}} \left( \frac{g_1}{\Delta} + \frac{g_2}{\Delta} \right)
\]
For \( F = \sin \phi = .5 \), after \( 10^4 \) layers the intensities of the right- and left-hand circularly polarized waves are down by .025, .8.6 respectively, so that the initially unpolarized photon is now essentially left hand polarized (assuming that the magnetic field at the nucleus is in the direction of the wave propagation \( \vec{K}_o \). If the field is in the opposite direction, the senses of the polarization are reversed).

For incident linear polarization and small fractions we will have a type of Faraday rotation. If the incident polarization is \( \hat{E}_o = \alpha \hat{E}_g + \alpha \hat{E}_e \), then the transmitted wave is \( \hat{E}_o = e^{i[\mu \cdot \vec{K}_o + \alpha]t} \left[ \alpha \hat{E}_g + \alpha e^{i(\gamma_{ne} \mu \cdot \vec{K}_o) t} \hat{E}_e + \alpha^2 \hat{E}_e + \alpha \hat{E}_e e^{i(\gamma_{ne} \mu \cdot \vec{K}_o) t} \right] \)

For \( F = .04 \), \( \hat{E}_o = \hat{E}_g \), \( K_o \) in resonance with \( 1\frac{1}{2}, \frac{1}{2} \leftrightarrow 1\frac{1}{2}, \frac{1}{2} \) then after \( 10^4 \) layers \( \hat{E}_e = \hat{E}_g - .04 \left( \hat{E}_g + e^{i \psi} \hat{E}_e \right) \)

This is not actually a rotation of the plane of polarization, but a change from linear polarization to elliptical polarization.

(ii) **Bragg Scattering:**

The solution for the reflection and transmission coefficients for Bragg scattering from a Mössbauer crystal involves solving the dispersion equation (33) for the four \( K' \), and then solving the sixteen linear equations (30-iv), (30-v), (32) for \( R_{\alpha}^{(\alpha)} \), \( T_{\alpha}^{(\alpha)} \). The reflection and transmission coefficients are then given by

\[
R_{(\alpha)} = |\sum_{\alpha'} R_{(\alpha')}(\alpha' \alpha)|^2, \quad T_{(\alpha)} = |\sum_{\alpha'} T_{(\alpha')}(\alpha' \alpha) e^{i \alpha \cdot \alpha'}| \n
The formal solution in terms of determinants can be written down immediately, but this gives no particular insight into the physics. There are certain simplifications which can be made in the general solution, and these will be given in a forthcoming publication. Here however, we will restrict our attention to the cases where equation (32) separates into two equations of the Darwin-Prin type. This occurs when the non-diagonal elements of the \( 2 \times 2 \) scattering matrices \( \tilde{\mathbf{f}}^{(C_2)}(\alpha_1, \alpha_2) \) vanish - that is, when there exist a polarization basis such that \( \hat{E}_{(\alpha_1)} \) couples only to \( \hat{E}_{(\alpha_2)} \), and \( \hat{E}_{(\alpha_1)} \) couples only to \( \hat{E}_{(\alpha_2)} \). As we will see below, there are several situations where this will occur.

When such a separation is possible, equations (30) reduce to
\[(37) \quad (1 - e^{-i (g - \kappa')\lambda} + i f(\lambda, 0)) \phi_{\lambda'}(\lambda) + i f(\lambda, \kappa') \phi_{\kappa'}(\lambda) = 0\]

\[i f(\lambda, 0) \phi_{\lambda'}(\lambda) + (1 - e^{i (g + \kappa')\lambda} + i f(\lambda, \kappa') \phi_{\kappa'}(\lambda) = 0\]

for \(\lambda = 1, 2\), and in addition we have the two boundary conditions

\[(38) \quad (i) \quad \sum \phi_{\lambda'}(\lambda) = \sum \phi_{\lambda}(\lambda) = 0 \quad \text{(in units of} \ \alpha_0 = \sqrt{\frac{4\pi c^3}{\omega_0}})\]

\[(ii) \quad \sum \phi_{\lambda'}(\lambda) e^{ik\lambda} = 0\]

The dispersion equation for \(\kappa'_{\lambda}\) is given by setting the coefficient determinant of (37) equal to zero. Since we are near Bragg, \(g d = \pi n + s\), where \(s = k_0 d \sin \phi \Delta \phi\), and \(\phi\) is the angle of incidence. Making the substitution \(\kappa'_{\lambda} d = \pi n + \alpha_{\lambda}\), we obtain

\[(39) \quad \alpha'_{\lambda} = -(\frac{f(\lambda, 0) - f(\lambda, \kappa')}{2}) \pm \sqrt{\left(\frac{f(\lambda, 0) - f(\lambda, \kappa')}{2}\right)^2 + \left[(s + f(\lambda, 0))(s + f(\lambda, \kappa')) - f(\lambda, 0) f(\lambda, \kappa')\right]}\]

In all the cases considered below, we have symmetry about the scattering planes, so that \(f(\lambda, 0) = f(\lambda, \kappa')\), and (39) reduces to

\[(40) \quad \alpha'_{\lambda} = \pm \sqrt{(s + f(\lambda, 0)^2 - f(\lambda, 0) f(\lambda, \kappa')}\]

the square root is to be taken so that

\[I(\alpha'_{\lambda}) > 0\]

Setting \(\kappa'_{\lambda} = \pi n + \alpha'_{\lambda}\), \(\kappa'_{\lambda} = \pi n + \alpha'_{\lambda}\).
and solving for the reflection and transmission coefficients from (37), (38), we obtain

\[ R_{(A)}^{\pm} = \sum_{\kappa_{(A)}^{\pm}} C_{(A)}^{\kappa_{(A)}^{\pm}} \left( \frac{i M_{(A)} - \alpha_{(A)}^{\kappa_{(A)}^{\pm}}}{1 - i M_{(A)} \alpha_{(A)}^{\kappa_{(A)}^{\pm}}} \right) \left( \hat{e}_{(A)}^{\kappa_{(A)}^{\pm}} \cdot \hat{e}_{o} \right) \]

\[ T_{(A)}^{\pm} = \sum_{\kappa_{(A)}^{\pm}} e^{-i \kappa_{(A)}^{\pm} t} M_{(A)} T_{(A)}^{\kappa_{(A)}^{\pm}} \]

\[ = \left( \frac{-e^{i M_{(A)} \alpha_{(A)}^{\pm}}}{1 - i M_{(A)} \alpha_{(A)}^{\pm}} \right) \left( \frac{e^{-i \kappa_{(A)}^{\pm} t} - e^{i \kappa_{(A)}^{\pm} t}}{e^{-i \kappa_{(A)}^{\pm} t} - e^{i \kappa_{(A)}^{\pm} t}} \right) \left( \frac{e^{-i \kappa_{(A)}^{\pm} t} - e^{i \kappa_{(A)}^{\pm} t}}{e^{-i \kappa_{(A)}^{\pm} t} - e^{i \kappa_{(A)}^{\pm} t}} \right) \]

\[ \Rightarrow \left( \frac{-e^{i M_{(A)} \alpha_{(A)}^{\pm}}}{1 - i M_{(A)} \alpha_{(A)}^{\pm}} \right) \left( \frac{2 \alpha_{(A)}^{\pm}}{(s + \alpha_{(A)}^{\pm}) - e^{i M_{(A)} \alpha_{(A)}^{\pm}} \alpha_{(A)}^{\pm}} \right) \left( \hat{e}_{(A)}^{\kappa_{(A)}^{\pm}} \cdot \hat{e}_{o} \right) \]

where \( M_{(A)} \) is given by

\[ M_{(A)} = \left( \frac{\alpha_{(A)}^{\pm}}{1 - e^{-2i M_{(A)} \alpha_{(A)}^{\pm}} \alpha_{(A)}^{\pm}} \right) \left( \frac{\alpha_{(A)}^{\pm}}{\alpha_{(A)}^{\pm} - e^{-2i M_{(A)} \alpha_{(A)}^{\pm}} \alpha_{(A)}^{\pm} \alpha_{(A)}^{\pm}} \right) \]

It is easy to see that for thin films, very near Bragg, such that \( |M_{(A)}^{(B)}| \ll 1 \) then \( M_{(A)} = M \), the number of layers; while for thick crystals, such that \( e^{i M_{(A)}^{(B)} \alpha_{(A)}^{\pm}} \approx 0 \), then \( M_{(A)} = \alpha_{(A)}^{\pm} / (s + \alpha_{(A)}^{\pm}) \). Thus the two limiting cases for the reflection coefficient are given by

\[ R_{(A)}^{\pm} = \left( \frac{i M_{(A)} - \alpha_{(A)}^{\kappa_{(A)}^{\pm}}}{1 - i M_{(A)} \alpha_{(A)}^{\kappa_{(A)}^{\pm}}} \right) \left( \hat{e}_{(A)}^{\kappa_{(A)}^{\pm}} \cdot \hat{e}_{o} \right) \]
for a thin film, very near Bragg, and

\[
R_{\lambda}^{(i)} = \left( -\frac{\alpha_{\lambda,\lambda}^{(i)}}{(\delta + \alpha_{\lambda,\lambda}^{(i)})} \right) \left( \hat{e}_{\lambda}^{(i)} \cdot \hat{e}_{\lambda} \right)
\]

for a thick crystal.

If the incident beam has an angular distribution of energy \( I(\delta) \) (normalized to unity), we are experimentally interested in the integrated intensities

\[
I_{\lambda}(\kappa) = \int_{-\infty}^{\infty} R_{\lambda}(\kappa, \delta) I(\delta) d\delta
\]

This should also be integrated over the frequency distribution \( I_{\lambda} \) of the incident wave

\[
I_{\lambda}(\omega) = \int_{-\infty}^{\infty} I_{\lambda}(\omega; \omega, \omega' + \frac{\omega_{s}}{c}) I_{\lambda}(\omega)
\]

where \( I_{\lambda}(\omega) \) is given by (46),

\[
I_{\lambda}(\omega, \omega' + \frac{\omega_{s}}{c}) = \frac{1}{2\pi} \frac{l}{(\omega - \omega' - \omega_{s})^2 + (\frac{\omega_{s}}{c})^2}
\]

\( \gamma_{s} \) is the total width for the source gamma ray, \( \omega_{s} = \Delta E_{s} \), is the natural frequency of the source transition, and \( \omega_{s} \) is the source velocity which doppler shifts the incident radiation. Because of the large imaginary part of \( I_{\lambda} \), the integrals (45), (46) are difficult to evaluate explicitly, and the expressions must usually be computerized.

(a) Isotropic Resonant Scattering:

We will now consider several cases for which the above formula hold, and we consider from non-Zeeman split Fe\(^{57}\) nuclei. The basis which allows us diagonalize equation (32) is shown in figure (12)
and is given explicitly by

\[(47) \quad \hat{\mathbf{E}}_c (\mathbf{R}_c) = (\hat{\mathbf{R}}_2 \times \hat{\mathbf{R}}_3) / |\hat{\mathbf{R}}_2 \times \hat{\mathbf{R}}_3| = \hat{\mathbf{E}}_c (\mathbf{R}_c) = (\hat{\mathbf{R}}_2 \times \hat{\mathbf{R}}_3) / |\hat{\mathbf{R}}_2 \times \hat{\mathbf{R}}_3|\]
\[\hat{\mathbf{E}}_a (\mathbf{R}_c) = \hat{\mathbf{E}}_c (\mathbf{R}_c) \times \mathbf{R}_c / |\mathbf{R}_c|, \quad \hat{\mathbf{E}}_a (\mathbf{R}_a) = \hat{\mathbf{E}}_c (\mathbf{R}_c) \times \mathbf{R}_2 / |\mathbf{R}_2|\]

With this basis, we find from expressions (28), (III-53) - (III-55), that

\[(48) (i) \quad f_{(\lambda, A)}^{(\lambda, A)} = \frac{4 \pi \mathcal{F} e^{-\frac{\mathbf{R}_2^2}{4\sigma_0^2}}}{(2\gamma_0 + 1)(\lambda a)^3 \sin \phi} \left( \frac{\mathbf{R}_2}{\sigma_0} \right) = \frac{4 \pi \mathcal{F} \lambda a^2 e^{-\frac{\mathbf{R}_2^2}{4\sigma_0^2}}}{(2\gamma_0 + 1)(\lambda a)^3 \sin \phi} \left( \frac{\mathbf{R}_2}{\sigma_0} \right) \frac{1}{2 \sigma_0} \frac{\mathbf{R}_2}{\sigma_0} \right) \frac{2 \sigma_0}{\sigma_0} \]
\[= \frac{4 \pi \mathcal{F} \lambda a^2 e^{-\frac{\mathbf{R}_2^2}{4\sigma_0^2}}}{(2\gamma_0 + 1)(\lambda a)^3 \sin \phi} \frac{1}{2 \sigma_0} \frac{\mathbf{R}_2}{\sigma_0} \]
\[\equiv f_{\lambda, A} \]

for \( \lambda = a, b, \) and \( A = a, b \). We also have

\[(48) (ii) \quad f_{(a, c)}^{(c, a)} = f_{(a, c)}^{(a, b)} = f_{(b, a)}^{(a, b)} \]
\[(iii) \quad f_{(c, c)}^{(c, c)} = f_{(c, c)}^{(c, c)} = f_{(c, c)}^{(a, c)} = f_{(c, c)}^{(a, b)} \]

The \( \cos(2\phi) \) dependence of (48)-(iii) is a geometrical factor, which, from a classical viewpoint, gives the component of the vibrating magnetic dipole perpendicular to the direction of scattering. Except for this geo-
metrical factor, we see that the amplitudes for scattering the radiation an angle $2\phi$ are equal to the forward scattering amplitudes. This is an important feature of Mössbauer scattering and is due to the fact that the Mössbauer phonon factor is angularly independent, and because there is no nuclear form factor. For the fast electronic scattering however, the Dybye phonon factor $\mathcal{F}(\vec{R}_c - \vec{R}_c')$ is a rapidly decreasing function of angle. Also since the electrons are spread over an angstrom or more, the electronic form factor decreases rapidly with angle for the short wavelength Mössbauer gamma rays. For a $60^\circ$ scattering angle of 14.4 KeV radiation in iron, the electronic scattering is down by an order of magnitude. Thus by doing large angle scattering one can greatly reduce the electronic effects with respect to the nuclear.

Substituting expressions (48) into (40), we have explicitly

\begin{equation}
\alpha^{(\pm)}(\alpha) = \pm \sqrt{\delta^2 + 2\delta \mathcal{H}}
\end{equation}

(ii) \[ \alpha^{(\pm)}(\alpha) = \pm \sqrt{\delta^2 + 2\delta \mathcal{H} + \mathcal{H}^2 \sin^2(2\phi)} \]

It is interesting to note that $\alpha^{(\pm)}(\alpha) \rightarrow 0$ as $\delta \rightarrow 0$, and thus at exact Bragg $\vec{R}_c' = \vec{R}_c$. This can never happen for electronic scattering since $\mathcal{F}(2\phi)$ is always smaller than $\mathcal{F}(0)$ because of the phonon- and form-factor.

The reflection and transmission coefficients are given by the general expressions (41), (42), with $M$ defined by (43). We will examine only the limiting cases of thin films and thick crystals.

First for a thin film such that $|M\phi| \ll 1$, we have from (43) that $M \gg M$, the actual number of layers. The reflection and transmission coefficients are then given by

\begin{equation}
R^{(\pm)}(\phi) = \left| \frac{\mathcal{M} \mathcal{H} \cos(2\phi)}{1 - \mathcal{M} \mathcal{H}} \right|^2 = \frac{(\mathcal{M} \mathcal{H})^2/(\xi^2 + 1)}{[1 + (\mathcal{M} \mathcal{H})/(\xi^2 + 1)]^2 + [\mathcal{M} \mathcal{H}^2/(\xi^2 + 1)]^2}
\end{equation}
The reflection coefficient as a function of the incident frequency is symmetrical about the nuclear resonance frequency $\omega_0 = \Delta \varepsilon$, passing through a maximum at resonance. The transmission coefficient is also symmetrical and minimizes at resonance. This minimization is partly due to the maximization of the reflected wave, and also because the coefficient $A$ for absorptive and inelastic processes maximizes at resonance.

\[
A(\varepsilon) = 1 - (R + T) = \frac{2M \varepsilon G_0 + i M F_0}{|1 - i M F_0|^2}
\]

It should be noted however, that the transmission coefficient at Bragg is much greater than that obtained off Bragg, and the coefficient $A$ is much smaller at Bragg. For incident $G_0$ (for which equations (50), (51) are strictly valid for any thickness at exact Bragg since $\delta = 0$), $\omega_0 = \Delta \varepsilon$, $M = 10^4$, and setting $F_0 \sin \phi = 1$, then at a Bragg angle $T \approx 0.04$, $R \approx 0.7$, and $A \approx 29$; while off Bragg $T \approx 2 \times 10^{-4}$, $R \approx 2 \times 10^{-4}$, and $A \approx 1$.

This suppression of inelastic processes at Bragg can also be viewed as due to an enhanced coherent scattering width. Returning to expression (50) and multiplying though by $\delta$

\[
Q_0(\delta) = [\Delta \varepsilon - \kappa_0 - i \gamma/2]
\]

we have

\[
R(\varepsilon) = \left| \frac{i M \left( \frac{2\pi}{k_0} \sin \phi \right) \left( \frac{\kappa_0}{2} \right) \left( \cos 2\phi \right)}{\Delta \varepsilon - \kappa_0 - i \gamma/2 - i \left[ M \left( \frac{2\pi}{k_0} \sin \phi \right) \left( \frac{\kappa_0}{2} \right) \right]} \right|^2
\]
From this form we see that the coherent scattering width for the system is

\[ \Gamma_{\text{int}} = M \left( \frac{2\pi F}{k^2} \right) \Gamma_{\text{coh}} \]

where \( \Gamma_{\text{coh}} = \frac{F}{(2\pi)^{1/2}} \Gamma' \). The width is proportional to the number of layers, and for enriched samples is much greater than the elastic scattering width \( \Gamma' \) for an isolated nucleus. For sufficiently large \( M \), \( \Gamma_{\text{int}} \gg \Gamma' \), the width for absorptive and inelastic processes, and there is an enhancement of the coherent scattering processes, and a suppression of the incoherent. This enhancement of the coherent width at Bragg angles and suppression of inelastic processes was first pointed out in references (1), (3) and corresponds to the superradiant states of Dicke (4). The coherent width for emission of a photon from a crystal is also given by (54) as shown by these authors and by Zaretskii (5) in a recent paper on multiphoton emission. It is interesting to note that since the lifetime is inversely proportional to the width, a photon incident at a Bragg angle escapes from the crystalline system faster than from an isolated nucleus.

The condition \(|m\delta| < 1\) for which (50) - (52) are valid, restricts the beam collimation as well as the film thickness, and requires that \( M < 1 \) (\( \delta < 1 \)). In terms of a beam collimation \( 2\delta \), this requirement is \( (2\delta) < \frac{\lambda_0}{(2\pi\text{cos} \theta)} \) where \( \theta \) is the angle of incidence, and \( \lambda_0 \) the incident wavelength. For a 400 A film, \( \lambda_0 = 0.5 \), \( \theta = 45^\circ \), then \( \lambda_0 / (2\pi\text{cos} \theta) \approx 10^{-3} \) radians.

For a thick crystal such that \( |m\delta| > 1 \) or if the beam collimation \( (2\delta) > \frac{\lambda_0}{(2\pi\text{cos} \theta)} \), we can set the exponential factor \( e^{2im\delta \phi} \) in (43) equal to zero, and \( M(\delta) = \frac{i}{(s + \alpha^{(n)})} \), and \( R(\delta) \) is given by (44-i)

\[ R(\delta) = \frac{1}{(s + \lambda_0^2 + 2s\lambda_0)} \left[ \hat{\varepsilon}(\delta) \cdot \hat{\varepsilon}_{\delta} \right]^2 \]

\[ R(\delta) = \frac{1}{(s + \lambda_0^2 + 2s\lambda_0)} \left[ \hat{\varepsilon}(\delta) \cdot \hat{\varepsilon}_{\delta} \right]^2 \]
The behaviour of these curves is more complicated than in the X-ray case because of the rapid frequency dependence of the \( f_N \), and because the \( f_N \) are almost purely imaginary in the resonance region. As a function of \( \delta \), \( R(x, \delta) \) maximizes at \( \delta = 0 \) to \( R(x, 0) = 1 \). There is no region of total reflection as in the Darwin solution because \( f_N \) is almost purely imaginary in the near resonance region. The positive and value of the maximum of \( R(x, \delta) \) depends on the frequency. If \( \omega_0 = \Delta \omega \), such that \( f_N \) is purely imaginary, the maximum occurs for \( \delta = 0 \)

\[
R(x, \Delta \omega, 0) = \left| \frac{\cos(\Delta \omega)}{i + \sin(\Delta \omega)} \right|^2
\]

If \( \omega_0 > \Delta \omega \) such that the real part of \( f_N \) is negative, the maximum occurs for \( \delta > 0 \) as in the electronic case. For \( \omega_0 < \Delta \omega \) such that \( R(x) > 0 \) the maximum occurs for \( \delta < 0 \). Of actual interest of course are the integrated intensities (45), (46). We have presently only carried out such integrations for the isotropic Mössbauer case considered below.

(b) Isotropic Mössbauer Scattering:

We will now consider isotropic Mössbauer scattering, and we will take as an example Fe\(^{57}\) in stainless steel. We will assume that the electronic scattering amplitudes for Fe\(^{56}\) and Fe\(^{57}\) are equal. It is easy to verify that the same polarization basis used in part (a) will diagonalize the isotropic Mössbauer case, and we have explicitly

\[
\begin{align*}
(f(\lambda, A)) & = f_N + f_R \\
(f(\alpha, \alpha)) & = f(\alpha, R) = f_N + f_R \cos(\alpha) \\
(f(\lambda, \alpha)) & = f(\lambda, R) = f_N \cos(\alpha) + f_R
\end{align*}
\]
(57) \( f_\lambda = \frac{4\pi N_d \lambda^2}{\sin \phi} \left( \frac{F(0) e^2}{m c^2} \right) \left( \frac{1 + \frac{F(0)}{m c^2}}{2 \sin \phi} \right)^2 \)

(ii) \( f_e = -\left( \frac{4\pi N_d \lambda^2}{\sin \phi} \right) \left( \frac{F(0) e^2}{m c^2} \right) + \frac{i N d \lambda^2}{2 \sin \phi} \)

(iii) \( f_R = -\left( \frac{4\pi N_d \lambda^2}{\sin \phi} \right) \left( \frac{F(2\phi) e^2}{m c^2} \right) + \frac{i N d \lambda^2}{2 \sin \phi} f(2\phi) \)

For an iron lattice with \( N = 8.47 \times 10^{22} \) atoms/cm\(^3\) scattering 14.4 KeV radiation, with \( F(0) = 24 \) (the effective number of tightly bound electrons per atom in the metal), then

(58) \( f_e = \frac{1}{\sin \phi} \left( -7.0 \times 10^{-5} + i \ 3.5 \times 10^{-6} \right) \)

(i) \( f_\lambda = \frac{\delta F}{x^4} \left( \frac{r}{r^2+1} \right) \left( 1 + \frac{F(0)}{m c^2} \right)^2 \)

For a 30° angle of incidence, \( F(2\phi)/F(0) = .27 \), \( f_e(2\phi) = .9 \) and \( f_e(\phi=30^\circ) = -3 \times 10^{-5} + 3.1 \times 10^{-6} \)

Substituting expressions (56) into (39) we obtain

(59) \( \alpha(\phi) = \pm \sqrt{[\delta + f_\lambda + f_e]^2 - (f_\lambda + f_e \cos(2\phi))^2] \)}

(ii) \( \alpha(\phi) = \pm \sqrt{[\delta + f_\lambda + f_e]^2 - (f_\lambda \cos(2\phi) + f_e)^2] \)}

From (41) the fourier transform reflection coefficient is given by

(60) \( R(\phi, \psi) = \left| \frac{i M(\phi) \left[ f_\lambda \left( \cos(2\phi) \right) + f_e \left( \cos(2\phi) \right) \right]}{1 - i M(\phi) \left[ f_\lambda + f_e \right]} \right|^2 \)

where \( M(\phi) \) is defined by (43) with the new values of \( \alpha(\phi) \), and the transmission coefficient from (42) is given by

(61) \( T(\phi, \psi) = \left| \frac{\cos(2\phi) M(\phi)}{1 - i M(\phi) \left[ f_\lambda + f_e \right]} \right|^2 \left| \frac{2 \alpha(\phi)}{(\alpha(\phi) + \delta) + (\alpha(\phi) - \delta) e^{2iM(\phi)}} \right|^2 \)
We are primarily interested in the reflection coefficient (60). The reflection coefficient contains both the real and imaginary parts of \( \gamma \), \( \bar{\epsilon}_{\alpha} \), and the electronic, nuclear interference can be either constructive or destructive depending upon whether \( \kappa_{\alpha} \leq \Delta \epsilon \), and whether \( \cos(2\phi) > 0 \).

If \( \kappa_{\alpha} > \Delta \epsilon \) (in which case the real part of the nuclear response denominator \( \kappa_{\alpha} - \Delta \epsilon + i \kappa_{\beta} \) has the same sign as the electronic response denominator \( Q_{\alpha} = \kappa_{\alpha} - (\epsilon_{e,m} - \epsilon_{e}) = 2mc^2 \)) the interference is constructive for a scattering angle \( (2\phi) < \frac{\pi}{2} \), and destructive for \( (2\phi) > \frac{\pi}{2} \), as given by the \( \cos(2\phi) \) dependence in (60). It is easy to see why this is the case. If we consider a plane wave \( \zeta \hat{z} e^{i \kappa_{\gamma} y} \) incident upon superimposed electric and magnetic dipoles, then the \( \vec{E} \)-field from the electric dipole, which vibrates in the \( \hat{z} \) direction, goes as \( (\hat{z} \times \hat{z}) \times \hat{z} \) and the \( \vec{E} \)-field from the magnetic dipole, which vibrates in the \( \hat{x} \) direction, goes as \( (\hat{x} \times \hat{z}) \).

As shown in figure (13), this gives constructive interference in the forward direction and destructive in the backward direction. If \( \kappa_{\alpha} < \Delta \epsilon \) such that the response denominators have opposite sign, the constructive interference occurs for \( \cos(2\phi) < 0 \) and destructive for \( \cos(2\phi) > 0 \). For 90° scattering, \( \cos(2\phi) = 0 \) and there is no interference at all between the waves scattered by the nuclei and electrons. This is because for incident \( |\vec{R}_{i}, \hat{z}_{\alpha} \rangle \), the electric dipoles vibrate in the direction of the scattered wave, and hence give no contribution, while the magnetic dipoles give a scattered field \( |\vec{R}_{\alpha}, \hat{z}_{\alpha} \rangle \). Similarly for incident \( |\vec{R}_{i}, \hat{\epsilon}_{z} \rangle \) the electric dipoles scatter \( |\vec{R}_{\alpha}, \hat{\epsilon}_{z} \rangle \), and the magnetic dipoles give no contribution. The waves scattered by the electric and magnetic dipoles
are thus polarized at right angles, and there is no interference. This 
\cos(2\phi) dependence of the interference between Rayleigh and Mössbauer 
scattering was first pointed out by Black, Moon, etc. (21)-(23).

Returning to expressions (60) and (61), \( M_{\alpha} \) is replaced by \( M \), the 
number of layers, in the thin film region \( |M_{\alpha}| \ll 1 \) for a well \textit{colimated} 
incident beam \( 25d < \frac{\lambda \cos \phi}{\pi} \). In figure (14) we plot \( R, T \) as a function 
of the incident frequency for unpolarized, unsplit 14.4 KeV Mössbauer 
radiation incident on a 300 A\(^\circ\) stainless steel film containing 65 % Fe\(^{57}\). 
For all three angles, the transmission minimum occurs at resonance, 
and \( T \) is slightly asymmetrical about the resonance, with smaller values 
in the region \( \kappa > \Delta \varepsilon \) because of the constructive interference of the 
\( \Sigma + \Sigma_{\varepsilon} \) term in the denominator. The reflection coefficient is 
governed primarily by the numerator, and has the general interference 
feature discussed above. For a 30\(^\circ\) angle of incidence, the maximum is 
shifted in the \( \kappa > \Delta \varepsilon \) direction due to constructive interference, and 
\( R \) is slightly asymmetrical about the maximum with larger values in the 
\( \kappa > \Delta \varepsilon \) region. At 45\(^\circ\) the interference effects are minimized and 
the maximum occurs at resonance. Because of the \( \Sigma + \Sigma_{\varepsilon} \) term 
in the denominator, \( R(\phi > 0) < R(\phi < 0) \). For \( \phi = 60\(^\circ\) \) the maximum is 
shifted in the \( \kappa < \Delta \varepsilon \) region and \( R(\phi > 0) < R(\phi < 0) \).
Thin film $R, T$

$M = 200$

$F = .65$

$\phi = 45^\circ$

$T(\kappa)$

$R(\kappa)$

$(\kappa - \Delta \kappa)/(\kappa_{fl})$
For the thick crystal or uncollimated cases, such that \(|M_N| \gg 1\), the Fourier transform reflection coefficients are

\[
R_{(i)}(k, \delta) = \left| \frac{t_{\theta} + t_{\theta} \cos(2\phi)}{(\delta + t_{\theta} + t_{\theta}) \pm \sqrt{(\delta + t_{\theta} + t_{\theta})^2 - (t_{\theta} \cos(2\phi) + t_{\theta})}} \right|^2
\]

\[
R_{(ii)}(k, \delta) = \left| \frac{t_{\theta} \cos(2\phi) + t_{\theta}}{(\delta + t_{\theta} + t_{\theta}) \pm \sqrt{(\delta + t_{\theta} + t_{\theta})^2 - (t_{\theta} \cos(2\phi) + t_{\theta})}} \right|^2
\]

In figure (15) we take a Mössbauer gamma ray from a stainless source with collimation \(25\phi = 2 \times 10^{-3}\) radians incident on an iron crystal containing a fraction \(F\) of \(^{57}\text{Fe}\), and plot the partially integrated intensity

\[
R(k, \delta) = \int ds I(s) \int \frac{e^{-|\mathbf{k}|^2 <x^2>} \left[ \frac{1}{2} R_{(i)}(k, \delta) + \frac{1}{2} R_{(ii)}(k, \delta) \right]}{\left[ 1 - e^{-|\mathbf{k}|^2 <x^2>} \right] \left[ \frac{1}{2} R_{(i)}(s) + \frac{1}{2} R_{(ii)}(s) \right]}
\]

as a function of an incident frequency \(\omega_0\). In the last part of expression (63), \(R_{(ii)}(s)\) is obtained from (62) by setting \(f_N = 0\). This gives the scattering of the non-Mössbauer fraction of the incident beam which is significant as pointed out by Cambell and Bernstein.

In figures 15(a)-(d) we take \(F = .65\) and angles of incidence \(\phi = 10^0, 30^0, 45^0, 60^0\). The nuclear electronic interference effects again have a \(\cos(2\phi)\) dependence and for highly enriched, well collimated beams the reflection coefficients behave qualitatively as discussed before. The most pronounced interference effects occur for the small scattering angles, where the electronic scattering amplitude \(t_{se}\) is of comparable magnitude to the nuclear amplitude \(f_N\). For large scattering angles the interference effects are almost negligible because the \(t_{se}\) are greatly decreased by the phonon - and form factors (for \(\phi = 60^0, F(2\phi)/F(0) = .17, f_p(2\phi) = .5\)).

An interesting feature of (62), (63) is that the reflection does not necessarily maximize near resonance, but instead may minimize depending upon the angle of incidence, the beam collimation, and the
fraction $F$ of $\text{Fe}^{57}$. In figure (15-a - 15-e) for $\phi = 10^0$, $F = .02$ (the natural fraction of $\text{Fe}^{57}$) we see that the reflection coefficient goes through a minimum at a frequency $\omega_c \leq \Delta E - .4 (\gamma E)$ Similarly for grazing incidence from a 90 % enriched film as shown in figures (19), the reflection coefficient minimizes near resonance (below the critical angle). The possibility of obtaining either a maximum or minimum at resonance was predicted by Black and O'Connor(22), (23) using a kinematical approach. The condition they obtained for obtaining a maxima scattering uncollimated incident radiation was that $\left( \frac{\nu}{\nu} \right)^2 \left( \frac{\nu}{\nu} \right) \left( \frac{\nu}{\nu} \right) > 1$, where $N$ is the peak value of the amplitude per unit cell for coherent elastic nuclear resonant scattering, $A$ is the amplitude per unit cell for coherent elastic electronic scattering, $\mathcal{N}$ is the peak value of the linear absorption coefficient for nuclear resonance, $\mathcal{A}$ the linear absorption coefficient for all other processes, $\mathcal{F}$ is the ideal linewidth of the resonance and $\mathcal{E}$ the effective linewidth. Qualitatively this states that the most favourable conditions for obtaining a maxima are for large scattering angles and highly enriched scatterers. For collimated beams (or even uncollimated, $\mathcal{E}(\theta) \equiv 1$ in (63)) it is difficult to give a similar criteria for a maxima of (62) because the integrals involved are elliptic. As we see from figures (15), (17)-(19) however, the general behaviour is that minima occur for small scattering angles, small functions $F$ of the resonant nuclei (for sufficiently small angles, such as at grazing incidence, a minima will occur regardless of $F$), and maxima will occur for large scattering angles and large fractions $F$. Also highly collimated beams are a more favourable condition for obtaining a maxima, as we saw in the thin film, high collimation limit of the reflective coefficient ($\mathcal{N} = \mathcal{M}$). Finally, polarization can also be important. For example, if the angle of incidence is $\phi = 45^0$, then the reflection coefficient $\mathcal{R}$ will always minimize at resonance. This occurs because $\mathcal{N} = \mathcal{E}(\theta) = 0$, so that the numerator only contains $f_e$ and is frequency independent. The denominator however, contains $f_N$ and maximizes at resonance, so $\mathcal{R}$ minimizes at resonance. The physical reason for this is that for $\phi = 45^0$ and incident $\mathcal{E}$, the magnetic dipoles vibrate in the direction and hence do not contribute to the scattered field, and the reflected wave is due entirely to electronic scattering. However, the reflected wave from a layer will interact with the magnetic dipoles in upper layers, and this absorbs energy from the reflected wave.
Since the reflected wave is only due to electronic scattering, and since the energy dissipated by the reflected wave in driving the magnetic dipoles will maximize at resonance, the reflection coefficient $R_e$ will minimize at resonance.
Bragg Integrated Intensity

$\phi = 10^\circ$

$8\phi = 10^{-3}$ radians

$F = 0.65$
Bragg Integ. Int. $R(k_0)$

$\phi = 30^\circ$

$F = 0.65$

$\delta \phi = 10^{-3}$ radians

FIG 15 (b)
Bragg Integ. Int. \( R(k_0) \)

- \( \phi = 60^\circ \)
- \( F = 0.65 \)
- \( \delta \phi = 10^{-3} \) radians

**Fig 15(a)**
(c) Polarized Ferromagnetic:

To treat the scattering from a polarized ferromagnetic M"ossbauer crystal, we must generally work with the non-diagonalized equations (32). A general treatment of the ferromagnetic case will be given in a following publication. However, for one particular case, the diagonalized equations (37) hold. This occurs when the direction of magnetic polarization lies in the scattering planes and perpendicular to the incident beam. In this case, the previous bases \( \hat{\mathcal{E}}_s(\mathbf{r}_s) \), \( \hat{\mathcal{E}}_t(\mathbf{r}_t) \), and \( \hat{\mathcal{E}}_r(\mathbf{r}_r) \) again diagonalize the \((2 \times 2)\) scattering matrices.

Classically this is easy to see. An incident \(|\mathbf{r}_s, \hat{\mathcal{E}}_s>\) photon corresponds to having an incident classical wave \( \mathcal{E}_s \hat{\mathcal{E}}_s(\mathbf{r}_s) \), and corresponding magnetic field \( \mathcal{H}_s \hat{\mathcal{E}}_s \), which in this case is in the direction of the axis of magnetic polarization for the crystal. The electronic oscillators vibrate in the \((\mathbf{r}_s, \hat{\mathcal{E}}_s)\) plane (but not in general in the \( \hat{\mathcal{E}}_s \) direction because of coupling with reflected waves), and hence in the forward direction they scatter an E-field with polarization \( \mathcal{E}_s(\mathbf{r}_s) \) \((\mathbf{r}_s \times \mathbf{r}_s)\), and in the reflected direction an \( \mathcal{E}_s(\mathbf{r}_s) \) field. In both directions the scattered H-field is in the \( \hat{\mathcal{E}}_s \) direction. The only magnetic dipoles which couple to \( \mathcal{H}_s \hat{\mathcal{E}}_s \) are the ones constrained to vibrate along the axis of polarization \( \hat{\mathcal{E}}_s \). These oscillators correspond to the two (0) M1 transitions. In the forward direction these oscillators give an \( \mathcal{E}_s \hat{\mathcal{E}}_s(\mathbf{r}_s) \) field \((\mathcal{H}_s \hat{\mathcal{E}}_s \times \mathbf{r}_s)\), and \( \mathcal{E}_s \hat{\mathcal{E}}_s(\mathbf{r}_s) \) in the reflected direction. Similarly for incident \( \mathcal{E}_s \hat{\mathcal{E}}_s \), the reflected and transmitted waves have polarization \( \hat{\mathcal{E}}_s \), and the oscillators excited are all orthogonal to the ones excited by \( \mathcal{E}_s \hat{\mathcal{E}}_s \). In this case the magnetic dipoles excited are the right and left hand circularly polarized magnetic dipoles lying in the \((\mathbf{r}_s, \hat{\mathcal{E}}_s)\) plane. These correspond to the two (+), and two (-) transitions.

From expressions (28), (III-53) - (III-55), we obtain explicitly for this case

\[
(64) \hspace{1cm} \left( x, x^2 \right) \equiv \mathcal{N}_x + \mathcal{F}_x = \frac{3\pi}{2} \frac{x^2}{(x_0+1)^2} \frac{\mathcal{H}_s \mathcal{E}_s}{2 \sin \phi} \left( \frac{\mathcal{C}\left(\phi \right)}{\mathcal{Q}(\phi)} + \frac{\mathcal{C}\left(\phi \right)}{\mathcal{Q}(\phi)} \right) \frac{1}{x_0 + 1} + \frac{1}{x_0 + 1}
\]
(ii) \[ f(\alpha,0) = f(\alpha,\lambda) = f_{0} + f_{R} \cos(2\phi) \]

(iii) \[ f(\kappa,0) = f_{\kappa(0)} + f_{\kappa(-1)} + f_{2} = \frac{\alpha_{0}^{2} \mu_{0} \mu_{F} e^{-2\phi}}{2(\sqrt{2} \lambda_{0}) \sin \phi} \left( \frac{C_{\kappa(0)}}{Q_{\kappa(0)}} + \frac{C_{\kappa(-1)}}{Q_{\kappa(-1)}} \right) \frac{1}{2} + f_{2} \]

(iv) \[ f(\kappa,\lambda) = f_{\kappa(0)} e^{2\phi} + f_{\kappa(-1)} e^{-2\phi} + f_{R} \]

(v) \[ f(\kappa,\lambda) = f_{\kappa(0)} e^{-2\phi} + f_{\kappa(-1)} e^{2\phi} + f_{R} \]

In expressions (iv) and (v), we have assumed that the magnetic field at the nucleus is in the \((+\varepsilon_{z})\)-direction. If the field were in the \((-\varepsilon_{z})\)-direction, \(e^{2\phi}\) should be replaced by \(e^{-2\phi}\), and vice-versa. Substituting (64) into (40) we obtain

\[ (65) \]

\[ \chi_{(\kappa)}^{\pm} = \pm \sqrt{(\delta + f_{0} + f_{2})^{2} - (f_{0} + f_{R} \cos(2\phi))^{2}} \]

\[ (66) \]

\[ R_{\kappa}(\kappa,0) = \frac{i \left( \frac{\mu_{0}}{\mu_{F}} \left[ f_{0} + f_{R} \cos(2\phi) \right] \right)}{1 - i \left( \frac{\mu_{0}}{\mu_{F}} \left[ f_{0} + f_{2} \right] \right)} \]

\[ R_{\kappa}(\kappa,\lambda) = \frac{i \left( \frac{\mu_{0}}{\mu_{F}} \left[ f_{0} \cos(2\phi) + f_{0} \cos(2\phi) + f_{2} + \frac{2}{\mu_{0}} \left( f_{0} + f_{2} \right) \sin(2\phi) \right] \right)}{1 - i \left( \frac{\mu_{0}}{\mu_{F}} \left[ f_{0} + f_{2} \right] \right)} \]

where \(M_{(\lambda)}\) is obtained by (43) and where \(2 = \pm \) if the field at the nucleus is in the \((\pm \varepsilon_{z})\)-direction. From (42) we have the transmission coefficients
\[
(i) \quad \mathcal{T}_\alpha(k, \delta) = \left| \frac{e^{i M k \delta}}{1 - e^{i M k \delta}} \right|^2 \left| \frac{i \alpha}{\alpha\delta + i (\alpha - \delta)} \right|^2
\]
\[
(ii) \quad \mathcal{T}_\alpha(k, \delta) = \left| \frac{e^{i M k \delta}}{1 - e^{i M k \delta}} \right|^2 \left| \frac{i \alpha}{\alpha\delta + i (\alpha - \delta)} \right|^2
\]

In the thin film, well collimated limit \( \alpha \ll 1, 2\delta \phi < \left[ \frac{X_\alpha}{n \cos \theta} \right] \), then \( N_\alpha \to M \) in (66), (67), and for the thick crystal, uncollimated limit \( M_\alpha \approx i \), we have \( M_\alpha = \frac{i}{\delta + \delta_\alpha} \), or explicitly

\[
(i) \quad R_\alpha(k, \delta) = \left| \frac{f_{00} + f_{er} \cos(2\phi)}{(\delta + f_{nc} + f_{er}) + \sqrt{(\delta + f_{nc} + f_{er})^2 - (f_{nc} + f_{er} \cos(2\phi))^2}} \right|^2
\]
\[
(ii) \quad R_\alpha(k, \delta) = \left| \frac{f_{er} + (f_{nc} + f_{er} \cos(2\phi)) + i \sqrt{(f_{nc} + f_{er} \sin(2\phi))^2 - (f_{nc} + f_{er} \cos(2\phi))^2}}{(\delta + f_{nc} + f_{er}) + \sqrt{(\delta + f_{nc} + f_{er})^2 - (f_{nc} + f_{er} \cos(2\phi))^2}} \right|^2
\]

As a function of the incident frequency, expressions (66)-(68) behave qualitatively like the single resonance case. For incident \( | \vec{E}_o, \vec{E}_n > \) which interacts with the two \( (0) \) transitions, the reflection will maximize (or minimize - see discussion following (62)) near both of the resonances, with the position of the maxima and the asymmetry again determined by the \( \cos(2\phi) \) interference term as for the single resonance case in figure(15). For incident \( | \vec{E}_o, \vec{E}_n > \), which interacts with the two \( (+) \) and two \( (-1) \) transitions, there will be four maxima (or minima). The interference term no longer has a \( \cos(2\phi) \) angular dependence, but instead is \( \sum f_{er}(f_{nc} + f_{er}) \cos(2\phi) \). Away from \( \phi = \frac{\pi}{4} \), such that \( \cos(2\phi) \approx \sin(2\phi) \), then \( \sum f_{er}(f_{nc} + f_{er}) \cos(2\phi) \approx \sum f_{er}(f_{nc} + f_{er}) \sin(2\phi) \). Thus for small scattering angles, all four maxima (minima) are shifted to the right (left) of the respective resonances as shown in figures (15 a, b, d), while for large scattering angles the shifts occur in the opposite
direction. For $\Phi = \frac{\pi}{4}$ such that $\sin(2\Phi) \approx 1$, $\cos(2\Phi) \approx 0$, then

$$\left(\alpha_{k_0} + \beta_{k_0} e^{2i\Phi} + \gamma_{k_0} e^{-2i\Phi}\right) \approx 2 \left(\alpha_{k_0} + \gamma_{k_0} e^{i\phi} \right) \approx 2 \left[ \alpha_{k_0} \right] \approx 2 \left[ \alpha_{k_0} + \gamma_{k_0} e^{i\phi} \right] \approx 2 \left[ \alpha_{k_0} + \gamma_{k_0} e^{i\phi} \right]$$

where $\Phi = 2(\Delta E - K)/\gamma$. Examining this dependence we see that the maxima for the (+) transition will be shifted to the region $K_0 < \Delta E(x)$, while the maxima for the (-) transitions will be shifted in the opposite direction $K_0 > \Delta E(x)$. If the field at the nuclei is reversed to lie in the (-) direction (for a polarized domain, simply a rotation by $180^\circ$), then the maxima will be shifted in the opposite direction.

For unpolarized incident radiation, the reflected wave has six maxima (minima) with relative strengths 3:4:1:1:4:3 (in the sequence $+, 0, -, +, 0, -$ of increasing energy) determined by the corresponding Clebsch-Gordon coefficients and angular factors. In the limit that all resonance denominators coalesce, all the results (64)-(68) go into the isotropic, single resonance results as they should.

(d) Antiferromagnetic Scattering:

Finally we will consider scattering from an antiferromagnetic Mössbauer crystal. In an antiferromagnetic system the magnetic cell is larger than the electronic, and it is possible to eliminate the Rayleigh scattering and obtain purely nuclear scattered radiation of certain Bragg angles.

![Fig. (16).]

As a particular example, we work out the case where the axis of polarization is in the plane of the film perpendicular to $\vec{K}_0$ as shown in figure (16). The bases $\left\{ \vec{K}_0, \vec{\epsilon}_a \right\}$ $\leftrightarrow$ $\left\{ \vec{K}_0, \vec{\epsilon}_a \right\}$ diagonalize the scattering matrices and we have
(69) (i) \[
\sum_{m} T_{m}^{(n)} = e^{2i\alpha d} T_{m-1}^{(n)} - e^{2i\beta d} \frac{1}{\rho} \sum_{\alpha} \gamma_{\alpha}^{(n)}(\rho) T_{m-1}^{(n)} - e^{2i\gamma d} \frac{1}{\rho} \sum_{\alpha} \gamma_{\alpha}^{(n)}(\rho) T_{m+1}^{(n)}
\]

(ii) \[
\sum_{m} R_{m}^{(n)} = e^{2i\alpha d} R_{m-1}^{(n)} - e^{2i\beta d} \frac{1}{\rho} \sum_{\alpha} \gamma_{\alpha}^{(n)}(\rho) R_{m-1}^{(n)} - e^{2i\gamma d} \frac{1}{\rho} \sum_{\alpha} \gamma_{\alpha}^{(n)}(\rho) R_{m+1}^{(n)}
\]

plus the usual boundary condition (38). The unit cell sums of the scattering amplitudes are explicitly

(70) (i) \[
\sum_{\phi} f_{(a,\phi)}^{(x,\phi)} = \sum_{\phi} f_{(a,\phi)}^{(y,\phi)} = \left[ 2f_{(a)} \cos(2\phi) + 2f_{(b)} \cos(4\phi) \right], \lambda = c
\]

(ii) \[
\sum_{\phi} f_{(a,\phi)}^{(x,\phi)} e^{i(2\phi d)} = \sum_{\phi} f_{(a,\phi)}^{(y,\phi)} e^{i(2\phi d)} = 2f_{(a)} \cos(2\phi) \cos(2\phi d) + 2f_{(b)} \cos(4\phi) \cos(2\phi d)
\]

(iii) \[
\sum_{\phi} f_{(a,\phi)}^{(x,\phi)} e^{i(2\phi d)} = \sum_{\phi} f_{(a,\phi)}^{(y,\phi)} e^{i(2\phi d)} = 2f_{(a)} \cos(2\phi) \cos(2\phi d) + 2f_{(b)} \cos(4\phi) \cos(2\phi d)
\]

where \( f_{(a)}, f_{(b)}, f_{(c)}, f_{(d)}, f_{(e)} \) are defined as before. Near a Bragg angle \( 2\phi d = m\pi \), the dispersion equations give

(71) (i) \[
\lambda_{x}^{(a)}(\phi) = \pm \sqrt{\left[ (\delta + f_{(a)} + f_{(b)} \cos(2\phi))^2 - (f_{(a)} + f_{(b)} \cos(2\phi)) \right]}
\]

(ii) \[
\lambda_{y}^{(a)}(\phi) = \pm \sqrt{\left[ (\delta + f_{(a)} + f_{(b)} \cos(2\phi))^2 - (f_{(a)} + f_{(b)} \cos(2\phi)) \right]}
\]

With these values of \( \lambda_{y}^{(a)} \), the reflection coefficient is given by

(72) (i) \[
R_{c}^{(n)} = \frac{2i M_{(c)}}{1 - 2i M_{(c)} [f_{(a)} \cos(2\phi + \gamma d) + f_{(b)} \cos(4\phi + \gamma d) + f_{(c)} \cos(2\phi + \gamma d)]}
\]

(ii) \[
R_{c}^{(n)} = \frac{2i M_{(c)}}{1 - 2i M_{(c)} [f_{(a)} + f_{(b)} \cos(2\phi)] \cos(2\phi)}
\]

where \( M_{(c)} \) is given by (43).

Of particular interest are the Bragg conditions \( g_{(2d)} = (m+1)\pi \)
for which the electronic scattering will be minimized. Then and we have from (72)
(73) (i) \[ R_{(e)} = \left| \frac{2 M(e) (\frac{\mathbf{f}_{(e)}}{\mathbf{f}_{(e+1)}}) \sin (2\phi)}{1 - \varepsilon^2 M(e) (\mathbf{f}_{(e+1)} + \mathbf{f}_{(e+1)} \times \mathbf{e})} \right|^2 \]

(ii) \[ R_{(e)} = 0 \]

or explicitly for a thick crystal

(iii) \[ R_{(e)} = \left| \frac{(\mathbf{f}_{(e+1)} - \mathbf{f}_{(e)}) \sin (2\phi)}{(s + \mathbf{f}_{(e+1)} + \mathbf{f}_{(e+1)} \times \mathbf{e}) \sqrt{(\mathbf{f}_{(e+1)} + \mathbf{f}_{(e+1)} \times \mathbf{e})^2 - (\mathbf{f}_{(e)} - \mathbf{f}_{(e+1)})^2 \sin^2 (2\phi)}} \right|^2 \]

There are several interesting features of (73). First we note that the scattered radiation is polarized in the \( \mathbf{e} \) direction. Although the magnetic field at the nucleus is reviewed for each adjacent level, the scattering depends on \( \hat{M}^2 \), so that for any M1 transition which behaves as a linear oscillator, such as the (0) transition of \( R_{(e)} \), we have

\[ \hat{M}^2 (\hat{e} \times \mathbf{r}_e) \cdot (\hat{e} \times \mathbf{r}_e) + e^{-2igd} (-\hat{e} \times \mathbf{r}_e) \cdot (-\hat{e} \times \mathbf{r}_e) = 0 \text{ for } g(d = \frac{\pi}{2}) \]

\( R_{(e)} \) is non zero because the transitions involved behave as circularly polarized magnetic dipoles. If we are near one of the resonances, the magnetic dipoles of adjacent layers are circularly polarized in the opposite sense. For \( g(d = \frac{\pi}{2}) \), the reflected wave from the lower layer is retarded by \( e^{i\pi} \) with respect to that from the first layer, and as shown in figure (17) this corresponds to a wave scattered from a linear oscillator which vibrate in the \( \mathbf{e} \) direction. This is the origin of the \( \sin (2\phi) \) dependence.
\[ \sin(2\phi) \] dependence which maximizes for a Bragg angle near \( \phi = \frac{\pi}{4} \) and minimizes near \( \phi = 0, \frac{\pi}{2} \). As a function of the incident frequency, the reflection will have four maxima (minima). Since there is no electronic interference in the numerator, these maxima will occur at the resonances of the \( ^+ \) transitions and be essentially symmetric. In the non Zeeman split limit, in which case \( \nu_{\text{ev}} = \nu_{\text{ec}} \), then \( R \to 0 \) as it should.

Finally, we note an interesting optical property which occurs if the axis of magnetic polarization is perpendicular to the scattering planes. For a \( (2m+1)\pi \) Bragg angle, and near resonance with one of the \( ^+ \) transitions, a 90° rotation of the plane of polarization occurs. We will not work this out in detail here, but this effect is easy to see classically. If a wave \( \mathbf{E}_0 \hat{\mathbf{z}} e^{i \mathbf{k} \cdot \mathbf{r}} \) is incident normally upon two electric dipole oscillators, right- and left-hand circularly polarized respectively, then the reflected wave is

\[
\begin{align*}
\mathbf{A}_r &= e^{i \mathbf{k} \cdot \mathbf{r}} \mathbf{A}_{\text{ev}} (\hat{\mathbf{x}}^+ \hat{\mathbf{z}}^0) + e^{i \mathbf{k} \cdot \mathbf{r} - \omega t} \mathbf{A}_{\text{ec}} (\hat{\mathbf{x}}^- \hat{\mathbf{z}}^0) e^{i \mathbf{k} \cdot \mathbf{r}} \hat{\mathbf{z}}^0 \\
&= e^{i \mathbf{k} \cdot \mathbf{r} - \omega t} \mathbf{A}_{\text{ev}} (\hat{\mathbf{x}}^- \hat{\mathbf{z}}^0) e^{i \mathbf{k} \cdot \mathbf{r}} \hat{\mathbf{z}}^0
\end{align*}
\]

which is rotated 90° with respect to the incident polarization.
(iii) Laue Diffraction - Bormann Transmission:

As we saw in section (ii), at Bragg the radiation penetrates much more deeply into the crystal, and there is a suppression of inelastic processes. This is the basis of the anomalous Bormann transmission.

We have considered scattering from the \((x,y)\) planes, but we could equally well have taken any other set of planes, such as the \((x,z)\) planes shown in figure (18). This is the Laue geometry usually used in the analysis of the Bormann effect. The incident radiation is now near a Bragg angle for the \(K^\circ\) component of \(\vec{k}\), \(K^\circ \alpha = \pi - \delta\), and in addition to the \((0+)\) channel, the \(\vec{e}_{0+} = -\frac{2\pi}{\lambda} \vec{e}_y\) channel is open.

The set of coupled equations which determine the field amplitudes \(T_{K'}^{(\lambda,s^\dagger)}\), \(T_{K'}^{(\lambda,1^+)}\) are given by equations (32) with \(T_{K'}^{(\lambda)}\) replaced by \(T_{K'}^{(\lambda,1^+)}\), and the boundary conditions are now

\[
\begin{align*}
(i) & \quad \sum_{K'} T_{K'}^{(\lambda,0^+)} = \vec{E}_0^* \cdot \vec{E}_0 \\
(ii) & \quad \sum_{K'} T_{K'}^{(\lambda,1^+)} = 0
\end{align*}
\]

As in the Bragg case, we will again restrict our attention to the cases where the \((2 \times 2)\) scattering matrices can be diagonalized. We then
have in analogy to equation (37)

\[
(1 - e^{-i G_0 d - \kappa' d'}) + ie \mathcal{F}(\lambda_1, 0) T_{\lambda_1} - i e \mathcal{F}(\lambda_1, 0') T_{\lambda_1} = 0
\]

\[
e^{-i G_1 d - \kappa' d'} \mathcal{F}(\lambda_1, 0') \mathcal{T}_{\lambda_1} - (1 - e^{-i G_1 d - \kappa' d'}) + ie \mathcal{F}(\lambda_1, 1') \mathcal{T}_{\lambda_1} = 0
\]

For \( \kappa' d = m \pi - \delta \), where \( \delta = \kappa d \sin \phi \), then

\[
G_0 d = \sqrt{(k a)^2 - (m - \delta)^2}
\]

\[
G_1 d = \sqrt{(k a)^2 - (m + \delta)^2}
\]

Letting \( \kappa' = G_2 + \kappa' \), and defining \( \Delta g = G_2 - G_1 = \frac{2 \pi m}{a} \delta \), then we obtain from the dispersion equation of (75)

\[
\alpha_{\lambda}^{(2)} = -\frac{i}{2} \left( \Delta g - \mathcal{F}_{\lambda_0} - \mathcal{F}_{\lambda_1} \right) \pm \frac{i}{2} \sqrt\left( (\Delta g - \mathcal{F}_{\lambda_0} - \mathcal{F}_{\lambda_1})^2 \right)
\]

\[
-\left( \mathcal{F}_{\lambda_0} \mathcal{F}_{\lambda_1} \right) + 4 \Delta g \mathcal{F}_{\lambda_0} \mathcal{F}_{\lambda_1}
\]

If \( \mathcal{F}_{\lambda_0} = \mathcal{F}_{\lambda_1} \) and \( \mathcal{F}_{\lambda_0} = \mathcal{F}_{\lambda_1} \), which will usually hold in cases where (75) is applicable, then

\[
\alpha_{\lambda}^{(2)} = -\frac{i}{2} \left( \Delta g - 2 \mathcal{F}_{\lambda_0} \right) \pm \frac{i}{2} \sqrt{(\Delta g)^2 + 4 \left( \mathcal{F}_{\lambda_1} \right)^2}
\]

Solving equations (75), (74) for the \( \mathcal{T}_{\kappa'} \), we obtain for the transmission coefficients in the channel:

\[
\mathcal{T}_{\lambda_1}^{(2)} = \sum_{\kappa'} \mathcal{T}_{\lambda_1}^{(2)} e^{i \kappa' m}
\]

\[
= e^{i \mathcal{F}_{\lambda_1}} \left( \frac{e^{i \Delta g + \alpha_{\lambda}^{(2)} m}}{e^{i \Delta g + \alpha_{\lambda_0}^{(2)} m}} - e^{i \Delta g + \alpha_{\lambda_1}^{(2)} m} \right)
\]
For the cases where (77) holds, we then have

\[
\frac{1}{T_{\lambda}} = \left| \frac{\varepsilon \left[ \lambda^2 - \lambda_{\alpha} \sqrt{1 + (\beta^2 / \lambda^2 \lambda_{\alpha})^2} \right] m}{2 \sqrt{1 + (\beta^2 / \lambda^2 \lambda_{\alpha})^2}} - \varepsilon \left[ \lambda_{\alpha} + \lambda_{\beta} \sqrt{1 + (\beta^2 / \lambda^2 \lambda_{\alpha})^2} \right] m \right|^2
\]

Similarly, for the transmission coefficient in the \( \bar{\varepsilon} \) channel, we obtain

\[
T_{\lambda}^{\bar{\varepsilon}} = \sum_{\lambda'} \lambda' \varepsilon_{\lambda'} = \frac{1}{\kappa'} \lambda' \varepsilon_{\lambda'} m
\]

\[
= \lambda' \left( \frac{1 + \varepsilon_{\lambda'} - \varepsilon_{\lambda} - \varepsilon_{\lambda} \varepsilon_{\lambda'}}{\varepsilon_{\lambda'} - \varepsilon_{\lambda}} \right) \varepsilon_{\lambda'} m
\]

or for the cases where (77) holds, we obtain

\[
T_{\lambda}^{\bar{\varepsilon}} = \left\{ \begin{array}{l l}
\frac{1}{2} \left( \varepsilon \left[ \lambda^2 - \lambda_{\alpha} \sqrt{1 + (\beta^2 / \lambda^2 \lambda_{\alpha})^2} \right] m + \varepsilon \left[ \lambda_{\alpha} + \lambda_{\beta} \sqrt{1 + (\beta^2 / \lambda^2 \lambda_{\alpha})^2} \right] m \right)

\end{array} \right.
\]

\[
+ \left( \frac{\lambda_{\alpha}}{\sqrt{1 + X^2}} \right)^{1/2} \left( \varepsilon \left[ \lambda^2 - \lambda_{\alpha} \sqrt{1 + (\beta^2 / \lambda^2 \lambda_{\alpha})^2} \right] m - \varepsilon \left[ \lambda_{\alpha} + \lambda_{\beta} \sqrt{1 + (\beta^2 / \lambda^2 \lambda_{\alpha})^2} \right] m \right)
\]

where \( X = \frac{\alpha^2 / 2 \lambda_{\alpha}}{\lambda_{\alpha}} \).

The cases where (79) and (81) are applicable are the same as for the validity of (37) in the Bragg case. Also the appropriate values of 

\[
\lambda_{\alpha} \quad \lambda_{\alpha} \quad \lambda_{\alpha}
\]

for isotropic, ferromagnetic, and antiferro-
magnetic cases are given by equations (48), (56), (64), (70), but in these equations the Bragg scattering angle $2\phi$ must be replaced by $2(\pi - \phi)$, the Bormann scattering angle.

In order to examine the behaviour of expressions (79), (81) as a function of frequency and as a function of $\delta \phi$, these expressions must be computerized. This is being carried out presently. As a function of film thickness, we see that $\overline{\sigma}_{(\omega)} \rightarrow 1$, $\overline{\sigma}_{(\omega)} \rightarrow 0$ as $M \rightarrow 1$ as we would expect. For large $M$, and $\chi = \omega$, then

$$\overline{\sigma}_{(\omega)} \sim \frac{1}{4} \left| \sum_{\lambda} \left[ \frac{1}{\lambda_{\omega, \lambda}} \right] \right|^2$$

and we have anomalously large transmission $\lesssim 25\%$ in each channel.

(iv) Grazing Incidence:

At grazing incidence we can replace all scattering matrices $\overline{\sigma}_{(\omega)}^{(s)}$, $\lambda, \delta = \omega, \chi$ in (70), (69) by the forward scattering matrix $\overline{\sigma}_{(\omega)}^{(s)}$ with small error. The equations can then be simultaneously diagonalized, and separated into two Darwin sets of equations. The reflection coefficients for the two eigenwaves are then given by the form (41). We will give the explicit results only for three ferromagnetic cases in which the axis of magnetic polarization is symmetric with respect to the scattering planes.

For polarization in the plane of the film, $\perp \vec{h}$, the eigenwaves are $|\vec{h}, \vec{e}>$, $|\vec{h}', \vec{e}>$, and we have

\begin{align*}
(82) \ (i) \quad \overline{R}_{(\omega)}^{(s)}(\vec{k}, \phi) &= \left| \frac{1 - \sqrt{1 + \frac{2(\vec{h}_{\omega} + \vec{h}_\alpha) \cdot \vec{e}}{\phi K \alpha}}}{1 + \sqrt{1 + \frac{2(\vec{h}_{\omega} + \vec{h}_\alpha) \cdot \vec{e}}{\phi K \alpha}}} \right|^2 \\
(82) \ (ii) \quad \overline{R}_{(\omega)}^{(s)}(\vec{k}', \phi) &= \left| \frac{1 - \sqrt{1 + \frac{2(\vec{h}_{\omega} + \vec{h}_\alpha) \cdot \vec{e}}{\phi K \alpha}}}{1 + \sqrt{1 + \frac{2(\vec{h}_{\omega} + \vec{h}_\alpha) \cdot \vec{e}}{\phi K \alpha}}} \right|^2
\end{align*}
where \( \tau_{01}, \tau_{11}, \tau_{12}, \tau_{22} \) are defined in equations (64) (and \( \sin \phi = \phi \) in these equations).

For polarization in the plane of the film, \( \parallel \vec{K}_c \), the eigenwaves are \( | \vec{K}_c', \vec{E}_c >, | \vec{K}_c'', \vec{E}_c > \) and we have

\[
R^{(i)}(\vec{K}_c, \phi) = \left| \frac{1 - \sqrt{1 + \frac{2}{2}(\vec{K}_c', \vec{E}_c )/(\vec{K}_c, \vec{E}_c )} \phi}{1 + \sqrt{1 + \frac{2}{2}(\vec{K}_c', \vec{E}_c )/(\vec{K}_c, \vec{E}_c )} \phi} \right|^2
\]

\[
R^{(ii)}(\vec{K}_c, \phi) = \left| \frac{1 - \sqrt{1 + \frac{2}{2}(\vec{K}_c', \vec{E}_c )/(\vec{K}_c, \vec{E}_c )} \phi}{1 + \sqrt{1 + \frac{2}{2}(\vec{K}_c', \vec{E}_c )/(\vec{K}_c, \vec{E}_c )} \phi} \right|^2
\]

The (0) transitions are unexcited in this case.

Finally for magnetic polarization \( \perp \) to the scattering plane, the eigenwaves are \( | \vec{K}_c', \vec{E}_c >, | \vec{K}_c'', \vec{E}_c > \), and \( R_a(\vec{K}_c, \phi) \) is given by (82 ii), \( R_a(\vec{K}_c, \phi) \) by (82 i).

Off resonance, the critical angle is determined by \( 1 + R(\tau_{01}) = 0 \) which gives \( \phi_c = \sqrt{\frac{4 \pi N F(0)}{\lambda_c^2}} \). For iron scattering 14.4 KeV radiation, this gives \( \phi_c = 3.7 \times 10^{-3} \) radians. (Here \( F(0) \) has been taken as 21.6. For this value, \( R_{c}(\phi) \) gives 11% reflection at \( \phi = 4 \times 10^{-3} \) radians, the value experimentally observed by Cambell and Bernstein.)

In figure (19) we plot the reflection coefficient (82) as a function of frequency, for an incident unpolarized beam, at angles \( \phi = 2 \times 10^{-3} \) radians, \( 4 \times 10^{-3} \) radians which lie below and above the critical angle \( \phi_c = 3 \times 10^{-3} \) radians. The film is taken as 90% enriched (F = 0.9), and the electronic form factor \( F(2\phi) \) is taken as 21.6 in the forward direction, which gives the experimentally observed \( 11\% \) electronic reflection at \( \phi = 4 \times 10^{-3} \) radians. The arrows locate the nuclear resonances. For \( \phi = 2 \times 10^{-3} \) radians, shown in (5a), minima occur near each resonance, shifted to the left \( (\omega_c < \Delta \omega_{res} ) \) as occurred in the Bragg angle case (15e). The depths of the minima are determined by the relative strengths of the transition which depend upon the Clebsch-Gordon coefficients and angular factors. For the case being considered here, the relative strengths are 3:4:1:1:4:3 \( (+.,o,-,+.,o,-) \).
The asymmetry of each minimum is due primarily to the electronic-nuclear interference. The additional asymmetry between resonances of the same strength, the lower energy minimum being deeper, is due to interference between the various nuclear transitions. For \( \phi = 4 \times 10^{-3} \) radians the reflection maximizes to the right of each resonance as shown in (19 b). The asymmetries are again due to the electronic-nuclear interference, and to the interference between the transition, and the heights of the maxima are determined by the relative strengths of the transitions.

A qualitative way to see that a minimum should occur if \( \phi < \phi_c \) and a maximum if \( \phi > \phi_c \) is the following. The critical angle for Mössbauer scattering is actually a function of frequency determined by

\[
1 + R \left[ \frac{2(z_{\phi} + z_{\phi}')}{k_c \phi} \right] = 0 \quad \text{or} \quad \phi_c(y) = \sqrt{(\frac{2}{k_c \phi})^2 + \frac{y}{z_c}}
\]

where \( y = (\kappa - \Delta \varepsilon)/(4 \varepsilon) \) and \( z_c = \sin \phi z_c \), \( z_c = \sin \phi (\frac{\Delta \varepsilon + \eta}{\mu}) R G_c \)

(for a single resonance.) It is easy to see that \( \phi_c(y) \) maximizes for \( \kappa = \Delta \varepsilon + \eta/2 \), and minimizes for \( \kappa = \Delta \varepsilon - \eta/2 \) (assuming \( R^2 - z_c^2 > 0 \). If not, there is no true critical angle for this frequency).

Then if the angle of incidence is \( \phi < \phi_c \) (the Rayleigh scattering critical angle), we see that \( (\phi_c(\kappa) - \phi) \) minimizes for \( \kappa = \Delta \varepsilon - \eta/2 \) Thus at a frequency slightly less than the resonance frequency, \( \phi \) lies closest to the critical angle \( \phi_c(y) \) and the reflection minimizes. Similarly, for \( \phi > \phi_c \), \( (\phi - \phi_c(y)) \) minimizes for \( \kappa = \Delta \varepsilon + \eta/2 \) and the reflection thus maximizes slightly to the right of a resonance.

For a more detailed treatment of Mössbauer scattering at grazing incidence the reader is referred to the papers of Cambell and Bernstein. \(^{(7)}\)
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APPENDIX (A): Evaluation of $\kappa_0^2 |M_{\nu\sigma\ell}|^2$

As we saw in section (II), the radiative width of an excited level is given by

$$\frac{\Gamma}{2} = -\sum_{\nu\sigma\ell} \frac{1}{2\pi} \int \frac{d^3q}{q^2} F(q) \tilde{F}(q) \delta(p-q)$$

(1)

By analysis similar to that used in appendix (B), we find that the longitudinal and scalar parts give a contribution proportional to

$$\frac{\kappa_0^2}{\kappa_0^2} \frac{(\epsilon_{\nu\sigma} - \epsilon_{\mu\tau})^2}{\kappa_0^2} = 0$$

which vanishes. We are then left with the transverse current product, which for the MI case is explicitly

$$\frac{\Gamma}{2} = \sum_{\nu\sigma\ell} \frac{1}{2\pi} |M_{\nu\sigma\ell}|^2 \kappa_0^2 \int \omega_\sigma \left( \hat{e}_{\lambda,\nu\sigma\ell} \cdot \hat{\tau} \right) \cdot \left( \hat{e}_{\lambda,\mu\sigma\ell} \cdot \hat{\tau} \right)$$

(2)

Making use of the fact that

$$\left( \hat{e}_{\lambda} \times \hat{\tau} \right) \cdot \left( \hat{e}_{\lambda} \times \hat{\tau} \right) = 1 - \left( \hat{e}_{\lambda} \cdot \hat{\tau} \right)^2$$

and that

$$\left( \hat{e}_{\lambda,\nu\sigma\ell} \cdot \hat{\tau} \right) = \left( \hat{e}_{\lambda,\mu\sigma\ell} \cdot \hat{\tau} \right)^* = \sqrt{\frac{2\pi}{3}} Y_{1,\lambda}^* (\hat{\tau})$$

we obtain

$$\sum_{\nu\sigma\ell} \kappa_0^2 |M_{\nu\sigma\ell}|^2 \left( \frac{\omega_\sigma}{\kappa_0^2} \right) = \frac{\Gamma}{2}$$

(3)

By the Wigner-Eckhart theorem, we have $\kappa_0^2 |M_{\nu\sigma\ell}|^2 = c_{\gamma_0,\gamma_1; \mu, \lambda}(\omega_\sigma)$. Substituting into (3), we find that

$$\beta = \left( \frac{\omega_\sigma}{\kappa_0^2} \right) \left( \frac{\Gamma}{2} \right)$$

(4)

Finally

$$\kappa_0^2 |M_{\nu\sigma\ell}|^2 = \left( \frac{\omega_\sigma}{2\kappa_0^2} \right) c^2 (\gamma_0, \gamma_1; m_0, \lambda)(\gamma_\sigma)$$

(4)
APPENDIX (B): Behavior of Photon Potential at Large Distances.

For large \(|\vec{r} - \vec{r}_c|\), the photon potential \(A(\vec{r})\) corresponds to a purely transverse field. That is, there exists a gauge transformation such that \(\vec{A}^\text{el}(\vec{r}, t) + \nabla \times \chi = (\vec{A}^\text{el}(\vec{r}_c), 0, 0)\). To show this, we first show that for \(\kappa |\vec{r} - \vec{r}_c| \gg 1\), then \(A(\vec{r}) = A(\vec{r}_c)\). For \(\kappa_0 |\vec{r} - \vec{r}_c| \gg 1\), we do not need to treat \(\hat{k}\) as an operator, and we have

\[
(1) \quad \Delta(\vec{r}) - A(\vec{r}) = \sum_m \langle E_m | e(1 - \alpha \cdot \vec{r} / \kappa_0) e^{-i \vec{k} \cdot \vec{x}} \frac{E_m \times E_0}{[\kappa - (E_m - E_0)]} \frac{\alpha \cdot \vec{x}}{[\kappa + (E_m - E_0)]} \]

Noting that \(-\alpha \cdot \vec{k} e^{-i \vec{k} \cdot \vec{x}} = He^{-i \vec{k} \cdot \vec{x}} - e^{-i \vec{k} \cdot \vec{x}} H\), we have

\[
(2) \quad \Delta(\vec{r}) - A(\vec{r}) = \sum_m \langle E_m | e^{-i \vec{k} \cdot \vec{x}} \frac{E_m \times E_0}{[\kappa - (E_m - E_0)]} \frac{\alpha \cdot \vec{x}}{[\kappa + (E_m - E_0)]} \]

Carrying out the sum over the complete set of states \(|E_m\rangle\) we have

\[
(3) \quad \Delta(\vec{r}, t) = A(\vec{r}_c, t)
\]

It is now an easy problem to find the desired gauge transformation. In particular, \(\chi = \frac{\kappa}{\kappa_0} A(\vec{r}_c)\) satisfies the wave equation for \(\kappa |\vec{r} - \vec{r}_c| \gg 1\)

\[
(4) \quad \Delta \chi = \left[ \kappa_0^2 - \kappa^2 - \kappa_0^2 O\left(\frac{\kappa}{\kappa_0 |\vec{r} - \vec{r}_c|}\right) \right] \chi = 0
\]
Moreover,

\[
\frac{\partial X}{\partial t} = -A_x(r, t)
\]

and, using relation (3),

\[
-\frac{\partial X}{\partial t} = -A_x(r, t)
\]

Also, it is obvious that

\[
\nabla \cdot X = 0
\]

Hence

\[
\frac{\partial}{\partial t} A_x(r, t) + \nabla \cdot X = \bar{A}_x(r, t)
\]

We also note that result (8) is valid for the purely resonant transitions. Then \((A_x - \bar{A}_{\text{long}})\) is proportional to \(\langle \xi_0 | (1 - \frac{r - \xi'_m}{\xi_0}) e^{-\frac{i}{\xi_0} | \xi_m \rangle = 0\). This term is zero since for near resonance \([K-(\xi_0 - \xi'_m)]/\xi_0 = 0\). Thus \(A^{(4)} - \bar{A}_{\text{long}}\) and the analysis carries through as before.
APPENDIX (C): Green's Function Sum for Plane Layers.

In deriving the results of section (IV), we have transformed the sum
\[ \sum_{j} e^{\kappa_{j} 1 + 2 \pi \delta_{j}} \frac{\exp(i \kappa_{j} 1 + 2 \pi \delta_{j})}{1 + 2 \pi \delta_{j}} \]
to a sum over the (xy) reciprocal lattice vectors. Define
\[ Q(\vec{R}) = \sum_{j} e^{\kappa_{j} \dot{x}_y \cdot \dot{y}} \frac{\exp(i \kappa_{j} 1 + 2 \pi \delta_{j})}{1 + 2 \pi \delta_{j}} \]

Using the relation
\[ \frac{\exp(i \kappa_{j} 1 + 2 \pi \delta_{j})}{1 + 2 \pi \delta_{j}} = \frac{1}{2\pi} \int \frac{\delta(\vec{R} - \vec{R}_j) \overrightarrow{\alpha}}{\overrightarrow{\alpha}^2 - \kappa^2} \mathrm{d}^2 \overrightarrow{\alpha} \]
we can write
\[ Q(\vec{R}) = \frac{1}{2\pi} \int \sum_{j} e^{\kappa_{j} (\dot{x}_y \cdot \dot{y}) \dot{R}_j} \overrightarrow{\alpha} \cdot \overrightarrow{\alpha} \mathrm{d}^2 \overrightarrow{\alpha} \]

Noting that
\[ \sum_{j} e^{\kappa_{j} \dot{x}_y \cdot \dot{y}} = \frac{(2\pi)^2}{\alpha \alpha} \sum_{\mu} \overrightarrow{s}(\overrightarrow{\alpha}_{xy} - \overrightarrow{\alpha}_x^\mu) \]
where the \( \overrightarrow{\alpha}_{xy} \) are the (xy) reciprocal lattice vectors, we obtain from (3),
\[ Q(\vec{R}) = \sum_{\mu} \frac{(2\pi)^2}{\alpha \alpha} \int \overrightarrow{s}(\overrightarrow{\alpha}_{xy} - \overrightarrow{\alpha}_x^\mu) e^{\kappa_{j} \dot{x}_y \cdot \dot{y}} \mathrm{d}^2 \overrightarrow{\alpha} \]

\[ = \frac{2}{\alpha \alpha} \sum_{\mu} \overrightarrow{s}(\overrightarrow{\alpha}_{xy} - \overrightarrow{\alpha}_x^\mu) \int \frac{e^{\kappa_{j} \dot{x}_y \cdot \dot{y}}}{\overrightarrow{z}^2 - \kappa^2 - \overrightarrow{z}_{xy} \overrightarrow{z}_{xy}^\mu} \mathrm{d}^2 \overrightarrow{z} \]

The integral is evaluated simply by contour integration, and we finally obtain
\[ Q(\vec{R}) = \frac{2}{\alpha \alpha} \sum_{\mu} \overrightarrow{s}(\overrightarrow{\alpha}_{xy} - \overrightarrow{\alpha}_x^\mu) \cdot \overrightarrow{R} \frac{e^{\sqrt{\kappa^2 + \overrightarrow{z}_{xy}^\mu}}} {\sqrt{\kappa^2 - (\overrightarrow{z}_{xy} + \overrightarrow{z}_{xy}^\mu)^2}} \]