INVESTIGATION OF THEORETICAL APPROACHES FOR COMPUTING RELATIVISTIC ATOMIC FORM FACTORS

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EXAMPLES OF USEFULNESS OF ATOMIC FORM FACTORS: f

- Crystallography: Structure Factors

$$F(hkl) = \sum_j f_j e^{-M_j} e^{2\pi i(hx_j + ky_j + lz_j)}$$

- Materials Science: Optical Properties of Materials

  (Refractive Index n_r and Dielectric Constant ϵ)

$$n_r = n + ik = \sqrt{\epsilon} = 1 - \delta - i\beta = 1 - \frac{r_0}{2\pi}\lambda^2 \sum_j n_j f_j$$

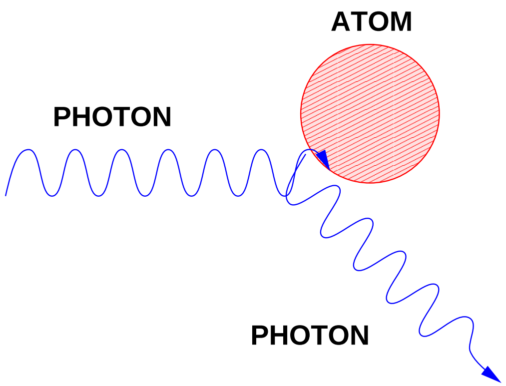
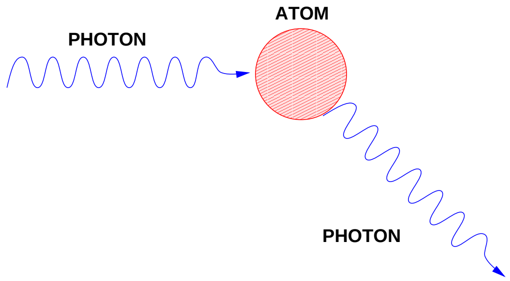
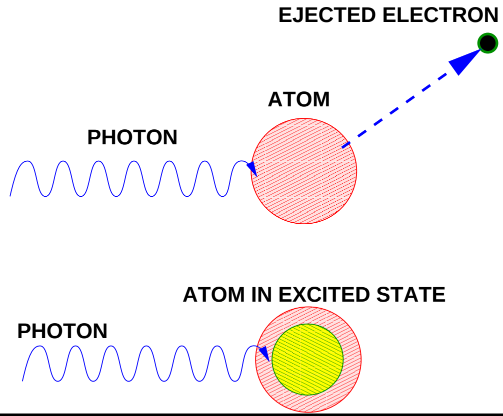
- Applications in X Ray Optics

  Including experimental work undertaken in School of Physics X Ray lab

THE ATOMIC FORM FACTOR f: WHAT IS IT?

Photon-Atom interactions are described by QFT.

$$f = f_0 + f' + if''$$

$f_0(q)$	$f'(\omega)$	$f''(\omega)$
		
NORMAL	ANOMALOUS	ANOMALOUS

HOW DO WE CALCULATE $f = f_0 + f' + if''$?

- **NORMAL FORM FACTOR:** The scattering power of an atom relative to the scattering power of a free electron.

$$f_0(q) = \int \rho(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}}\, d\mathbf{r} \qquad ; \qquad q = |\mathbf{k_f} - \mathbf{k_i}| = \frac{4\pi \sin(\theta/2)}{\lambda}\ \text{Å}^{-1}$$

- **IMAGINARY COMPONENT OF ANOMALOUS FORM FACTOR:** Related to the total photoionisation cross section $\sigma(\omega)$. ($r_0 = e^2/mc^2$)

$$f''(\omega) = \frac{\omega}{4\pi c r_0} \sigma(\omega)$$

- **REAL COMPONENT OF ANOMALOUS FORM FACTOR:** $f'(\omega)$ can be calculated from $f''(\omega)$ using a Kramers-Kronig dispersion relation.

THEORETICAL LIMITATIONS AND ASSUMPTIONS

- Isolated Atom
- Electromagnetic Field: Classical. Electric Dipole, Electric Quadrupole, All Poles, RMP
- Atomic Structure: Schrödinger, Dirac
- Perturbation Theory: 1st order relativistic, S-Matrix (QFT)
- Numerical and Computational Issues: singularities, convergence

PROJECT AIM AND RESULTS

AIM: *Investigate the issues, assumption and limitations in atomic form factor theory by a critical analysis and study of hydrogenic atoms*

- New analytic result for relativistic normal form factor
- New semi analytic results for first and second order photoionisation amplitudes.
- New numerical results for $f''(\omega)$ using S-matrix theory and relativistic perturbation theory.
- Calculated bound-bound relativistic transition amplitudes for the first three excited states for hydrogenic atoms.
- Angular dependent results

NORMAL FORM FACTOR $f_0(q)$ FOR HYDROGENIC ATOMS ANGULAR DEPENDENT CONTRIBUTION

- ANALYTIC NON RELATIVISTIC RESULT (has been done before)

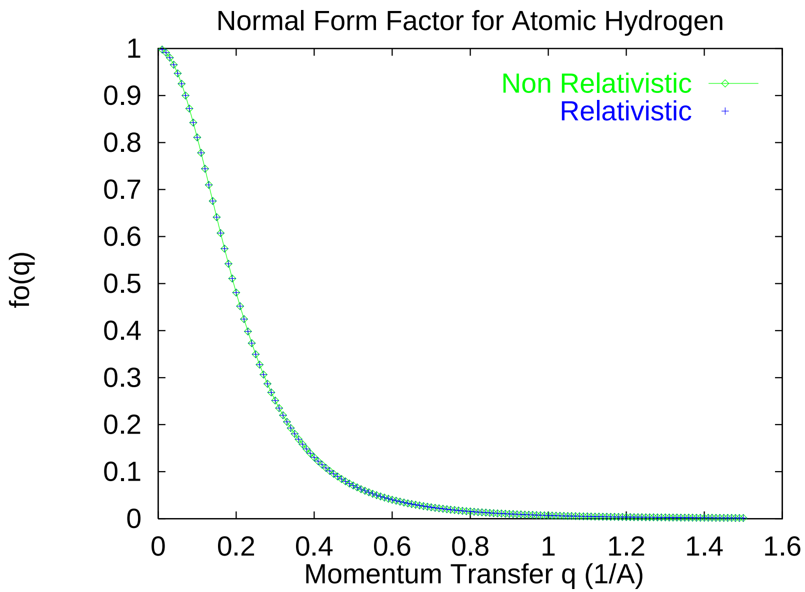
$$f_0(q) = \left(\frac{2Z}{a_0}\right)^4 \left[\left(\frac{2Z}{a_0}\right)^2 + q^2\right]^{-2}$$

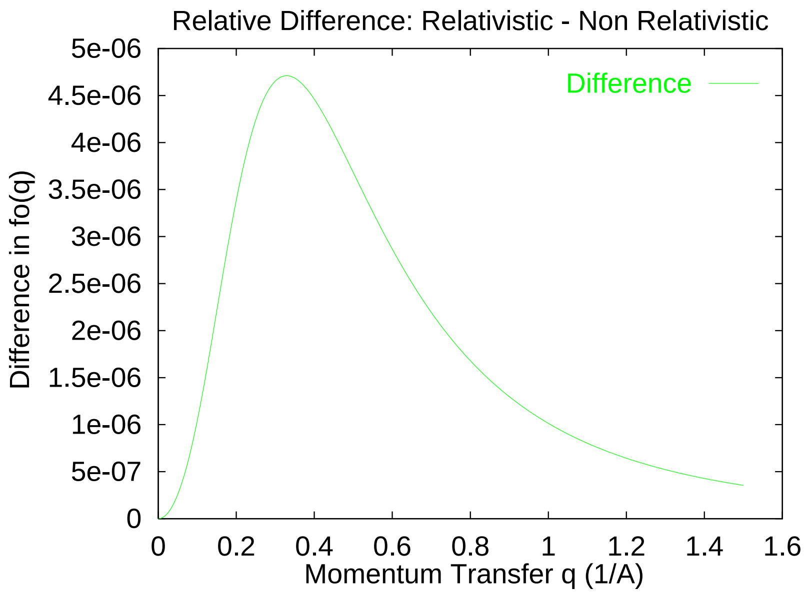
- **NEW** ANALYTIC RELATIVISTIC RESULT

$$\boxed{f_0(q) = \frac{\Gamma(2\gamma_1)}{2iq\Gamma(2\gamma_1+1)} \left(\frac{2Z}{a_0}\right)^{2\gamma_1+1} \left[\frac{\left(\frac{2Z}{a_0}+iq\right)^{2\gamma_1} - \left(\frac{2Z}{a_0}-iq\right)^{2\gamma_1}}{\left[\left(\frac{2Z}{a_0}\right)^2 + q^2\right]^{2\gamma_1}}\right]}$$

- $\gamma_1 = \sqrt{1-(\alpha Z)^2}$, $\alpha =$ fine structure constant, $a_0 =$ Bohr radius, $Z =$ Atomic Number. For low Z, $\gamma_1 \approx 1$.

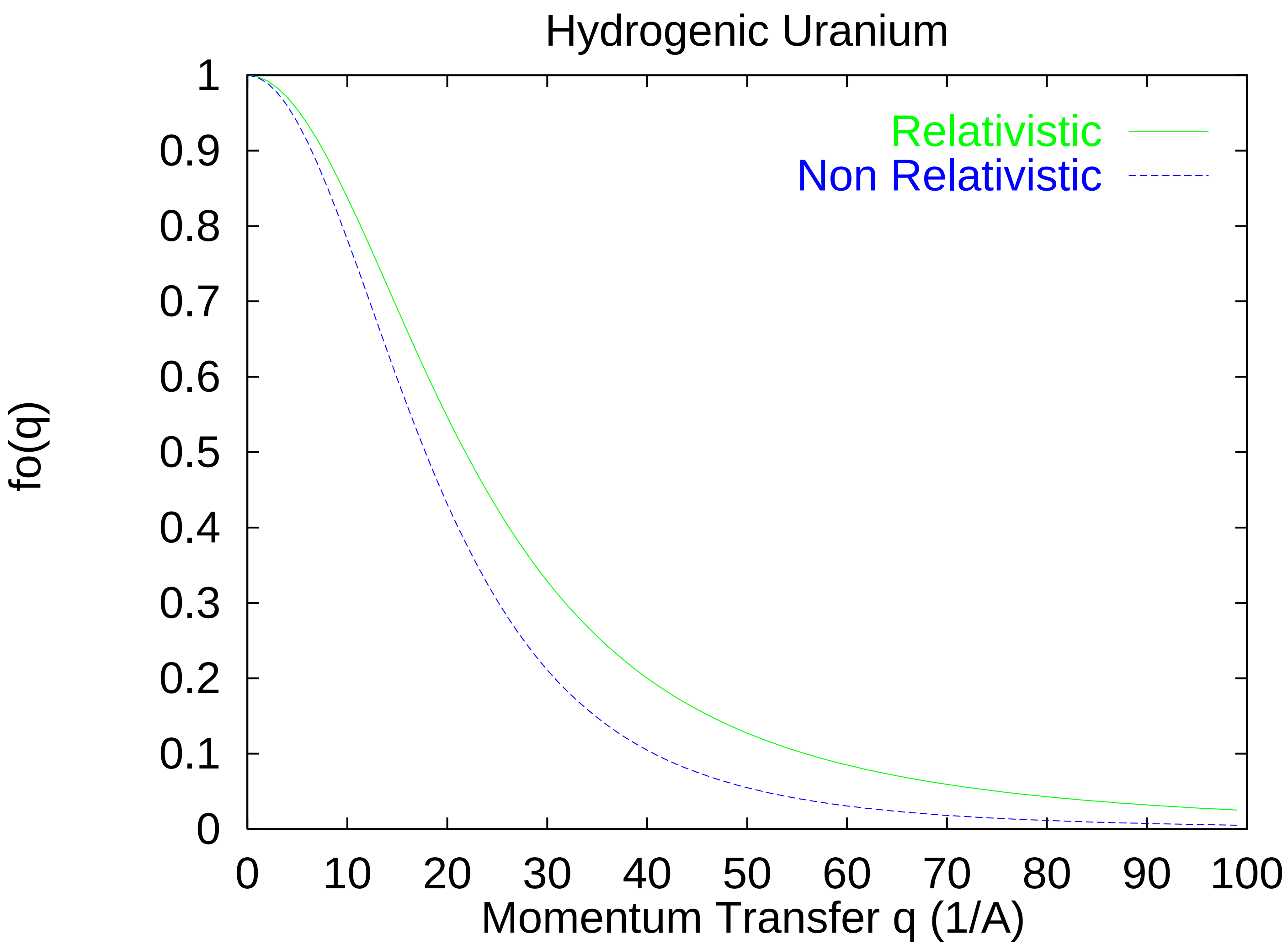
ATOMIC HYDROGEN



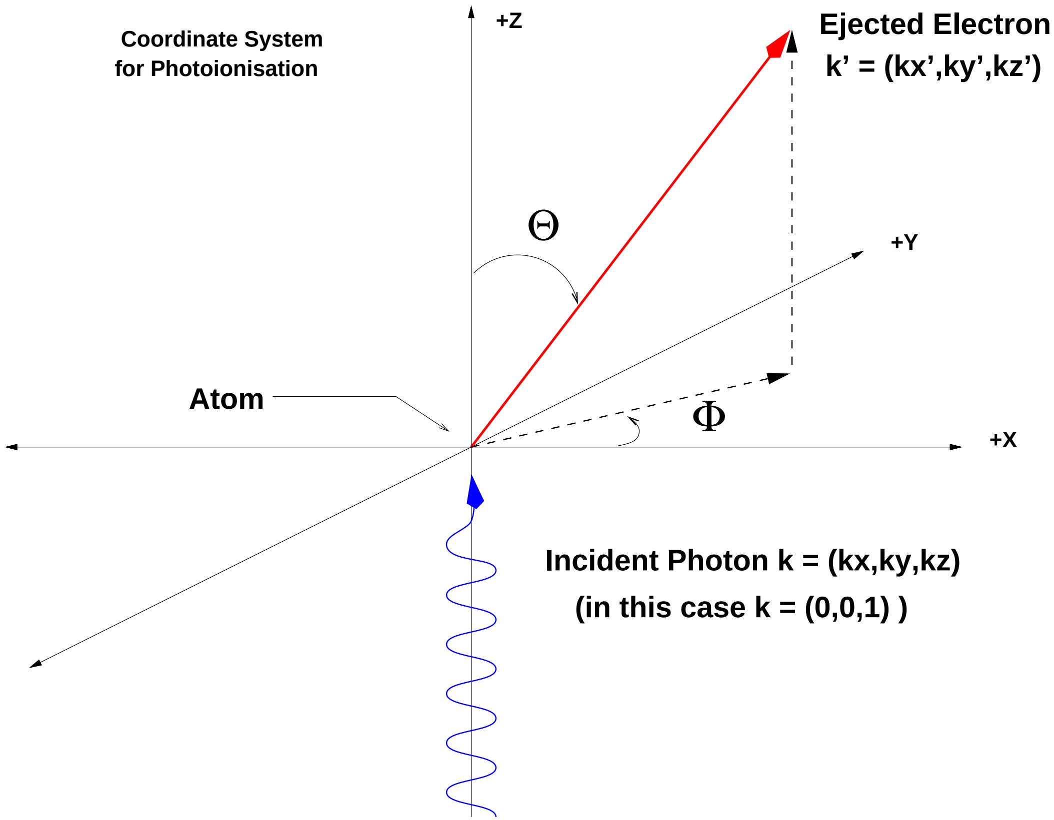


- Approximately 0.015% difference between reltativistic and non relativistic results.
- Current experimental precision: 0.1% – 1%

HYDROGENIC URANIUM



PHOTOIONISATION COORDINATE SYSTEM



$$k'_x = |k'| \sin(\Theta) \cos(\Phi) \ , k'_y = |k'| \sin(\Theta) \sin(\Phi) \ , k'_z = |k'| \cos(\Theta)$$

IMAGINARY ANOMALOUS ATOMIC FORM FACTOR $f''(\omega)$

- **APPROACHES TO CALCULATING $f''(\omega)$**: Standard Perturbation Theory, Relativistic Perturbation Theory, Relativistic S-Matrix Theory

- **RELATIVISTIC PHOTON ABSORPTION AND EMISSION OPERATORS (QFT)**

$$\mathcal{A}_i = \sum_j \bar{\alpha} \cdot \hat{\epsilon}_j e^{i\mathbf{k_i}\cdot\mathbf{r_j}} \qquad \mathcal{A}_f^\dagger = \sum_j \bar{\alpha} \cdot \hat{\epsilon}_j e^{-i\mathbf{k_f}\cdot\mathbf{r_j}}$$

Sum over j electrons, $\bar{\alpha}$ = Dirac alpha matrix, $\hat{\epsilon}_j$ = photon polarisation, $\mathbf{k}$ = photon wavevector, $\mathbf{k}'$ = ejected electron wave vector, r_j = coordinate of j-th electron.

- **RELATIVISTIC PHOTOIONISATION AMPLITUDE: HYDROGEN**

$$A_1(\mathbf{k}, \mathbf{k}') = \langle \psi_c | \mathcal{A}_i | \psi_0 \rangle = \langle \psi_c | e^{i\mathbf{k}\cdot\mathbf{r}} \bar{\alpha}_j | \psi_0 \rangle$$

ALL POLES AND ELECTRIC DIPOLE RESULTS

$$A_1(\mathbf{k},\mathbf{k}')_{\binom{x}{y}} = \frac{G_0\Gamma(\gamma_1+2)}{\sqrt{4\pi}} \times$$

$$\int_0^{2\pi}\int_0^{\pi}\left[\frac{\binom{1}{i}\sin(\theta)[\xi(k'_x - ik'_y) \pm iF_0\sin(\theta)e^{i\phi}]}{(\frac{1}{2}\sigma_1 - i\mu(\mathbf{q},\theta,\phi))^{\gamma_1+2}}\right]\, d\theta\, d\phi$$

$$A_1^{E1}(\mathbf{k},\mathbf{k}')_j = A_1(0,\mathbf{k}')_j$$

$$\mu(\mathbf{q},\theta,\phi) = q_x\sin\phi\cos\theta + q_y\sin\phi\sin\theta + q_z\cos\phi$$

THE FORWARD SCATTERING DIRECTION

$$A_1(k,k')_x = \frac{\pi}{\sqrt{\pi}} \left(\frac{2Z}{a_0}\right)^{3/2} \sqrt{\frac{1-\epsilon_1}{2\Gamma(2\gamma_1+1)}} \times$$

$$\left[\left(\frac{Z}{a_0}\right)^{-(\gamma_1+2)} \Gamma(\gamma_1+2)\ {}_2F_1\left(\frac{\gamma_1+2}{2}, \frac{\gamma_1+3}{2}; 1; -\left(\frac{2a_0}{Z}\right)^2 (k-k')^2\right)\right.$$

$$+ \frac{1}{8}(k-k')^2 \left(\frac{Z}{a_0}\right)^{-(\gamma_1+4)} \Gamma(\gamma_1+4) \times$$

$$\left. {}_2F_1\left(\frac{\gamma_1+4}{2}, \frac{\gamma_1+5}{2}; 1; -\left(\frac{2a_0}{Z}\right)^2 (k-k')^2\right)\right]$$

$$A_1(k,k')_y = -iA_1(k,k')_x \quad ; \quad |A_1(k,k')_y|^2 = |A_1(k,k')_x|^2$$

RELATIVISTIC S-MATRIX THEORY APPLIED TO ATOMIC FORM FACTOR CALCULATIONS

$$\mathrm{Im}A_2(\omega) = r_0 f''(\omega) = \frac{\omega}{4\pi c}\sigma^{TOT}(\omega)$$

$$A_2 = -r_0 mc^2 \sum_p \left[\frac{\langle m|\mathcal{A}_f^\dagger|p\rangle\langle p|\mathcal{A}_i|n\rangle}{E_n - E_p + \hbar\omega_f + i0_+} + \frac{\langle m|\mathcal{A}_i|p\rangle\langle p|\mathcal{A}_f^\dagger|n\rangle}{E_n - E_p - \hbar\omega_i + i0_+} \right]$$

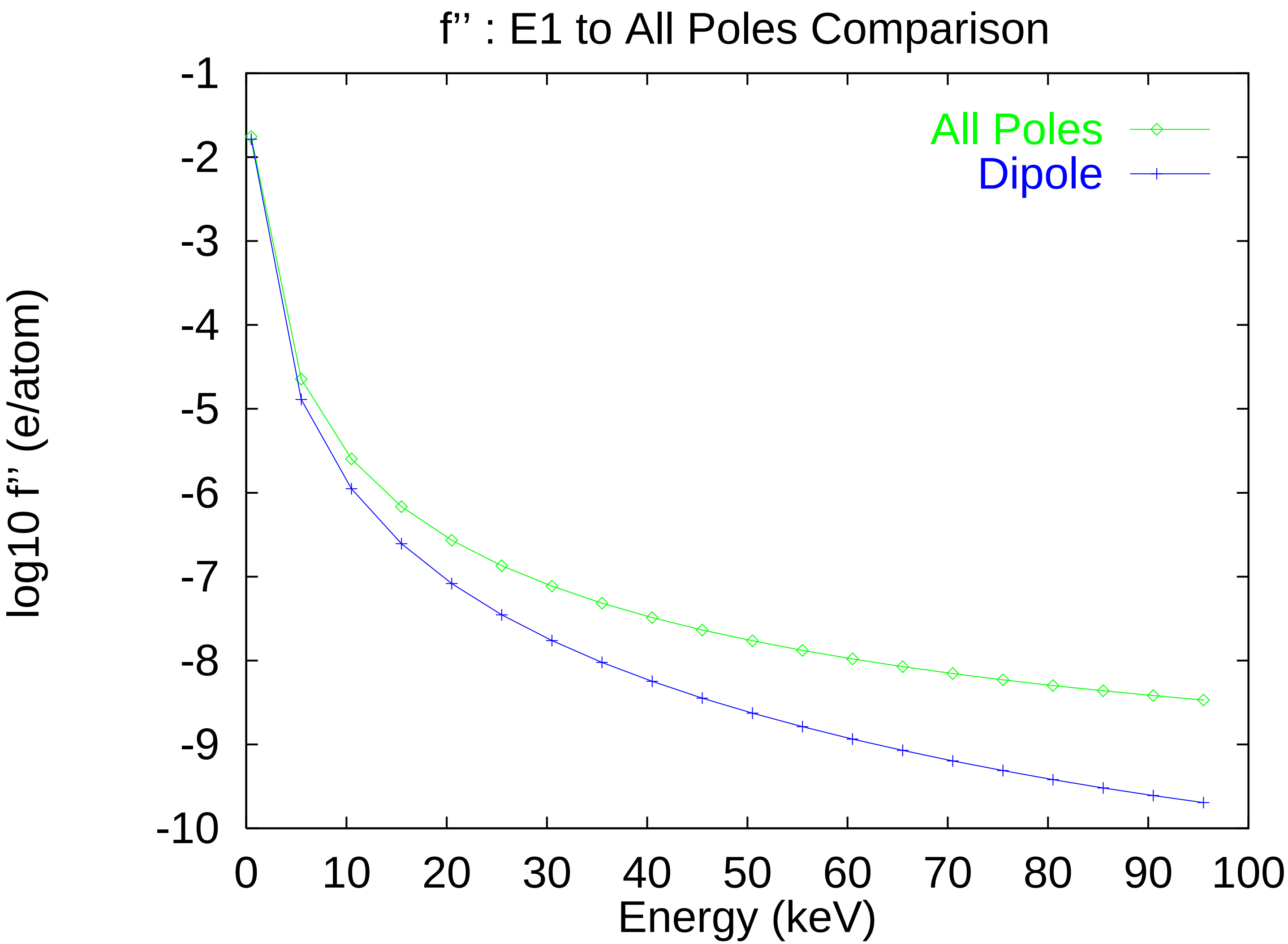
$$A_2^R(\omega) = A_2(\mathbf{k},\mathbf{k}')_j = -r_0 mc^2 \int_0^\infty \frac{|A_1(\mathbf{k},\mathbf{k}')_j|^2}{E_0 - E_c + \hbar\omega + i0_+} dE_c$$
$$- r_0 mc^2 \int_0^\infty \frac{|A_1(-\mathbf{k},\mathbf{k}')_j|^2}{E_0 - E_c - \hbar\omega - i0_+} dE_c$$

$$A_2^{E1}(\mathbf{k},\mathbf{k}')_j = A_2(0,\mathbf{k}')_j$$

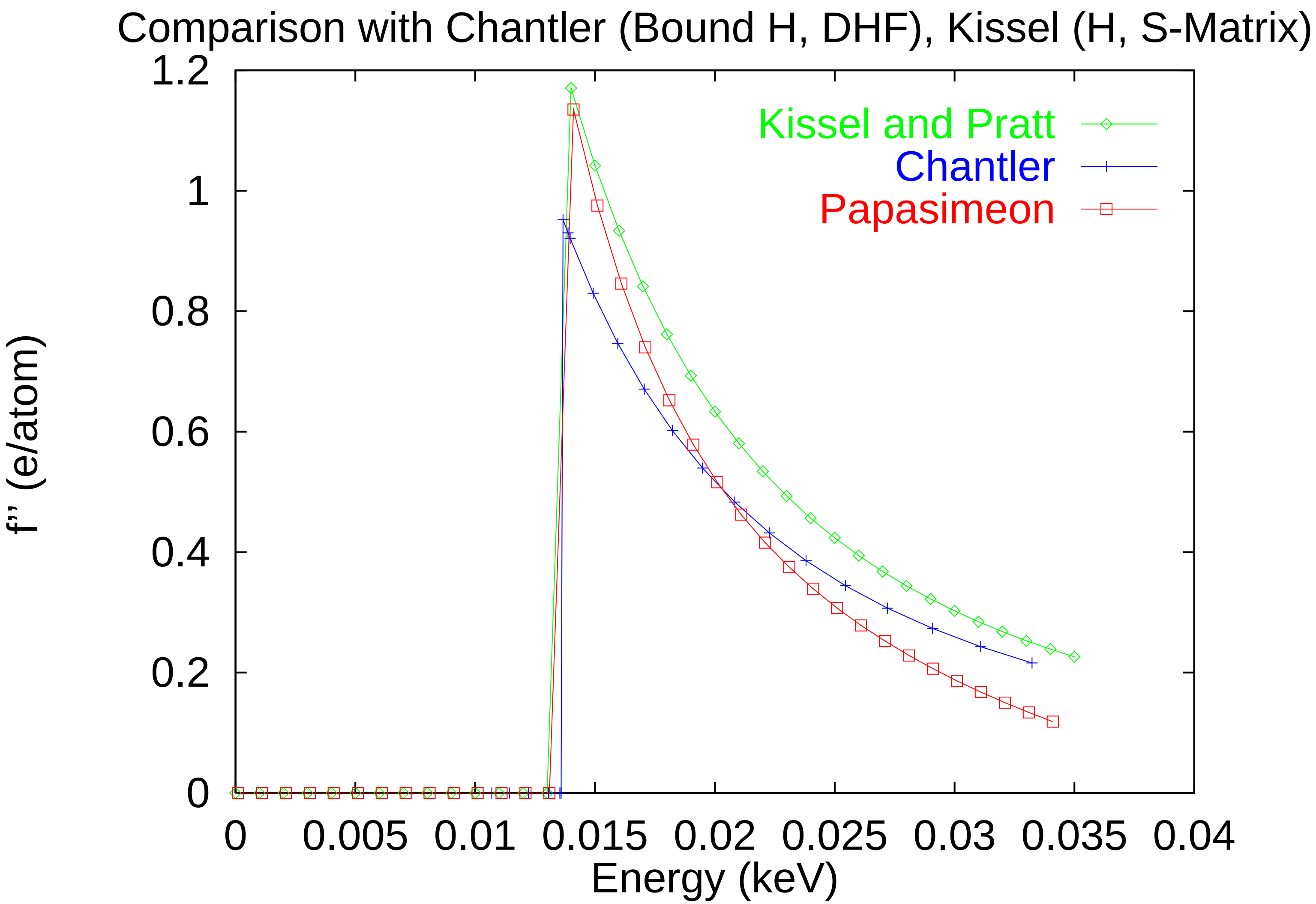
NUMERICAL CALCULATIONS

- Approximately 5000 lines of C++
- Approximately 2000 lines of Mathematica
- Quadrature Methods
  - Simpson, Trapezoidal
  - Gauss-Legendre (10 point)
  - Converging Romberg
- Intensive/Expensive Computation: Triple Integrals θ,ϕ, and Energy
- Singularities, open interval and numerical Cauchy Principal value integrations
- Parameters: Bound-Bound $i0_+ = i\frac{\Gamma}{2}$
  Continuum $i0_+$ = small value.

RESULTS - ALL POLES AND ELECTRIC DIPOLE



COMPARISON: CHANTLER (BOUND H), KISSEL (ATOMIC H)



CONCLUSIONS AND FURTHER WORK

- Summary of Results: Hydrogenic Atoms
  - New analytic result for relativistic normal form factor
  - New Semi analytic results for first and second order photoionisation amplitudes.
  - New Numerical results for $f''(\omega)$ using S-matrix theory and relativistic perturbation theory.
  - Calculated bound-bound relativistic transition amplitudes for the first three excited states for hydrogenic atoms.
  - Angular dependent results
- Further Work: Refine convergence, develop relativistic perturbation theory computation of $f'(\omega)$, XAFS (X Ray Anomalous Fine Structure) - multiple scattering processes off multiple atoms (eg: molecular hydrogen).

QUESTIONS?