An Implementation of Atomic Form Factors for Non-equal Masses

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Winter Nuclear and Particle Physics Conference, 2022

Outline

Form Factor

Transition form factor of hydrogen like atoms have a wide variety of applications such as in situations involving the Coulomb bound states of two elementary particles.

Definition of Form Factor

The calculation of transition probability of bound pion to bound muon decay requires computation of discrete-discrete atomic form factors, which is just the Fourier transform of $\phi^*_{n_2 l_2 m_2}(\overrightarrow{r})\varphi_{n_1 l_1 m_1}(\overrightarrow{r})$ with respect to transferred momentum $\vec{q}$ [2].

$$F^{n_2 l_2 m_2}_{n_1 l_1 m_1}(\overrightarrow{q}) = \int d\overrightarrow{r}\,\varphi^*_{n_2 l_2 m_2}(\overrightarrow{r}) e^{i\overrightarrow{q}\cdot\overrightarrow{r}} \varphi_{n_1 l_1 m_1}(\overrightarrow{r})$$

- $$\varphi_{n_1 l_1 m_1}(\overrightarrow{r}) = R_{n_1 l_1}(\overrightarrow{r}) Y_{l_1 m_1}(\Omega)$$
- $R_{n_1 l_1}(\overrightarrow{r})$ and $Y_{l_1 m_1}(\Omega)$ are the radial part and angular part of hydrogen like wave function and

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Radial Wave Function

$$R_{nl} = \frac{2}{a^{3/2} n^2} \sqrt{\frac{(n-l-1)!}{(n+l)!}} e^{-\frac{r}{an}} \left(\frac{2r}{na}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right)$$

- n, l are quantum numbers.
- Bohr radius $a \propto \frac{1}{mass}$.
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Plane Wave Expansion

$$e^{i\overrightarrow{q}\cdot\overrightarrow{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(qr) Y_{lm}(\Omega_q) Y^*_{lm}(\Omega_r)$$

Plugging the plane wave expansion in

$$F^{n_2 l_2 m_2}_{n_1 l_1 m_1}(\overrightarrow{q}) = \int d\overrightarrow{r} R^*_{n_2 l_2}(\overrightarrow{r}) Y_{l_2 m_2}(\Omega) e^{i\overrightarrow{q}\cdot\overrightarrow{r}} R_{n_1 l_1}(\overrightarrow{r}) Y_{l_1 m_1}(\Omega)$$

$$F^{n_2 l_2 m_2}_{n_1 l_1 m_1} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int_0^{\infty} r^2 dr R^*_{n_2 l_2}(r) R_{n_1 l_1}(r) i^l j_l(qr) Y_{lm}(\Omega_q) I^{m_1 m_2 m}_{l_1 l_2 l}$$

where $I^{m_1 m_2 m}_{l_1 l_2 l} = \int d\Omega Y^*_{l_2 m_2}(\Omega) Y^*_{lm}(\Omega) Y_{l_1 m_1}(\Omega)$

Angular Integral

$I_{l_1 l_2 l}^{m_1 m_2 m}$ can be expressed in terms of Wigner's 3j-symbols [3]

$$I_{l_1 l_2 l}^{m_1 m_2 m} = (-1)^{m_2+m}\sqrt{\frac{(2l_1+1)(2l_2+1)(2l+1)}{4\pi}}\begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & l_2 & l \\ m_1 & -m_2 & -m \end{pmatrix}$$

Radial Integral

Using the radial wave function the form factor becomes

$$F_{n_1 l_1 m_1}^{n_2 l_2 m_2} = \frac{4\pi 2^{2+l_1+l_2} i^l}{a_1^{3/2} a_2^{3/2} n_1^2 n_2^2} \sqrt{\frac{(n_1 - l_1 - 1)!}{(n_1 + l_1)!}} \sqrt{\frac{(n_2 - l_2 - 1)!}{(n_2 + l_2)!}} Y_{lm}(\Omega_q)$$

$$I_{l_1 l_2 l}^{m_1 m_2 m} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int_0^{\infty} r^2 dr e^{-\frac{r}{a_1 n_1}} \left(\frac{r}{a_1 n_1}\right)^{l_1} L_{n_1 - l_1 - 1}^{2l_1+1} \left(\frac{2r}{a_1 n_1}\right)$$

$$j_l(qr) e^{-\frac{r}{a_2 n_2}} \left(\frac{r}{a_2 n_2}\right)^{l_2} L_{n_2 - l_2 - 1}^{2l_2+1} \left(\frac{2r}{a_2 n_2}\right)$$

The integral involves the product of Bessel function and associated Laguerre polynomials.

Result of the Integral

The integral is calculated using mathematical result involving the product of Bessel function and associated Laguerre polynomials [1]

$$\int_0^\infty e^{-\delta x} J_\nu(\mu x) x^\gamma L_n^\alpha(\beta x)dx =$$

$$\sum_{k=0}^{n} \frac{(-\beta)^k \mu^\nu \Gamma(n+\alpha+1)\Gamma(\nu+\gamma+k+1)}{k!\Gamma(n-k+1)\Gamma(\alpha+k+1)2^\nu\Gamma(\nu+1)\delta^{\nu+\gamma+k+1}}$$

$$\times_2 F_1\left(\frac{\nu+\gamma+k+1}{2}, \frac{\nu+\gamma+k+2}{2}; 1+\nu; -\frac{\mu^2}{\delta^2}\right)$$

- ${}_2F_1$ is Gauss hypergeometric function. $L_n^m(x) = (n+m)! \sum_{k=0}^{n} \frac{(-1)^k}{k!(n-k)!(k+m)!} x^k$

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Final Formula for Form Factor

$$F_{n_1 l_1 m_1}^{n_2 l_2 m_2} = \frac{(-1)^{m_2+m} 2^{2+l_1+l_2}}{\left(\frac{a_2}{a_1}\right)^{3/2+l_2} n_1^{2+l_1} n_2^{2+l_2}} \delta_{m0} \sqrt{\frac{\pi}{2q}} \sqrt{\frac{(2l_1+1)(2l_2+1)(n_1+l_1)!(n_2+l_2)!(n_1-l_1-1)!}{(n_2-l_2-1)!}}$$

$$\sum_{l=|l_1-l_2|}^{l_1+l_2} \frac{i^l q^\nu (2l+1)}{2^\nu \Gamma(\nu+1)} \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & -m_2 & -m \end{pmatrix}$$

$$\sum_{k=0}^{n_2-l_2-1} \frac{(-2)^k}{\left(\frac{n_2 a_2}{a_1}\right)^k k!\,(2l_2+k+1)!}$$

$$\sum_{k_1=0}^{n} \frac{(-\beta)^{k_1} \Gamma(\nu+\gamma+k_1+1)}{k_1! \Gamma(n-k_1+1) \Gamma(\alpha+k_1+1) \delta^{\nu+\gamma+k_1+1}}$$

$$\times {}_2F_1\left(\frac{\nu+\gamma+k_1+1}{2}, \frac{\nu+\gamma+k_1+2}{2}; 1+\nu; -\frac{q^2}{\delta^2}\right)$$

with

$$\gamma = l_1 + l_2 + k + \frac{3}{2} \qquad \delta = \frac{n_2 \frac{a_2}{a_1} + n_1}{\frac{a_2}{a_1} n_1 n_2}$$

$$\nu = l + \frac{1}{2} \qquad \beta = \frac{2}{n_1}$$

$$n = n_1 - l_1 - 1 \qquad \alpha = 2l_1 + 1$$

Testing and Implementation

- The numerical integration agrees with the form factor formula.
- This formula can be used in any standard computer language.
- A Julia package is created by using this formula.

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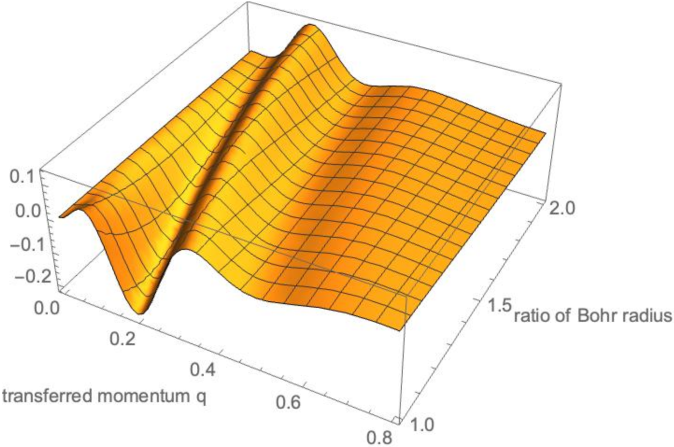
Illustration

The following figure is for $F^{5,0,0}_{4,2,0}(q)$, we can see that the discrete-discrete atomic form factors evaluated at zero transferred momentum should be 0 or 1.



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