

# Explicit Hydrogen-like Momentum Wave Functions

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Correcting for the Levchuk effect i.e. the presence of non-zero target energy due to the Fermi motion of the bound electrons requires knowing the momentum distribution of the electrons in the target material. The procedure applied in the Swartz *et al.* paper [1] used screened hydrogen-like wave functions to obtain the momentum distribution, by explicit summing over the wavefunctions for each shell weighted by its occupancy. Here I explicitly write the momentum wave functions  $\phi_{n,l}(p)$  required for an Fe foil, where  $p$  is in atomic units of  $\hbar/a_0$ . Since the electron configuration for atomic Fe is  $[\text{Ar}]3d^64s^2$ , at a minimum, the following wave functions are required:  $\phi_{1,0}$ ,  $\phi_{2,0}$ ,  $\phi_{2,1}$ ,  $\phi_{3,0}$ ,  $\phi_{3,1}$ ,  $\phi_{3,2}$ ,  $\phi_{4,0}$ . The momentum wave functions come from a reference written by Bethe [3], where equation 8.8 gives the following form for the radial momentum:

$$\phi_{n,l}(p) = \left( \frac{2(n-l-1)!}{\pi(n+l)!} \right)^{\frac{1}{2}} n^2 2^{2(l+1)} l! \frac{n^l p^l}{(n^2 p^2 + 1)^{l+2}} C_{n-l-1}^{l+1} \left( \frac{n^2 p^2 - 1}{n^2 p^2 + 1} \right), \quad (1)$$

where  $C_\beta^\alpha(x)$  is the Gegenbauer function. The Gegenbauer functions are given explicitly by

$$\begin{aligned} C_0^\alpha(x) &= 1 \\ C_1^\alpha(x) &= 2\alpha x \\ C_0^\alpha(x) C_\beta^\alpha(x) &= \frac{1}{n} \left[ 2x(\beta + \alpha - 1) C_{\beta-1}^\alpha(x) - (\beta + 2\alpha - 2) C_{\beta-2}^\alpha(x) \right]. \end{aligned}$$

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<sup>1</sup>Linus Pauling argues in [2] that a better model for metallic Fe is  $[\text{Ar}]3d^54s^14p^2$ . He suggests we can view Fe as having about 5.8 valence electrons in hybridized wave functions which are linear combinations of the 3d, 4s and 4p functions. This would require a further wave function  $\phi_{4,2}$  beyond that required for the simple atomic electron configuration.

The required Gegenbauer polynomials are:

$$\begin{aligned}
C_0^1(x) &= 1 \\
C_1^1(x) &= 2x \\
C_2^1(x) &= 4x^2 - 1 \\
C_3^1(x) &= 8x^3 - 4x \\
C_0^2(x) &= 1 \\
C_1^2(x) &= 4x \\
C_0^3(x) &= 1.
\end{aligned}$$

Substituting these polynomials into Eq. 1 gives the momentum wave functions:

$$\phi_{1,0} = \frac{8}{\sqrt{2\pi}(p^2 + 1)^2} \quad (2)$$

$$\phi_{2,0} = \frac{32(4p^2 - 1)}{\sqrt{\pi}(4p^2 + 1)^3} \quad (3)$$

$$\phi_{2,1} = \frac{128p}{\sqrt{3\pi}(4p^2 + 1)^3} \quad (4)$$

$$\phi_{3,0} = \frac{72}{\sqrt{6\pi}} \left( 4 \frac{(9p^2 - 1)^2}{(9p^2 + 1)^4} - 1 \right) \quad (5)$$

$$\phi_{3,1} = \frac{864p}{\sqrt{3\pi}} \frac{(9p^2 - 1)}{(9p^2 + 1)^3} \quad (6)$$

$$\phi_{3,2} = \frac{5184}{\sqrt{15\pi}} \frac{p^2}{(9p^2 + 1)^4} \quad (7)$$

$$\phi_{4,0} = \frac{256}{\sqrt{2\pi}} \frac{(16p^2 - 1)}{(16p^2 + 1)^3} \left( 2 \frac{(16p^2 - 1)^2}{(16p^2 + 1)^2} - 1 \right) \quad (8)$$

And since we need probability distributions let's just go ahead and square them all.

$$|\phi_{1,0}|^2 = \frac{32}{\pi(p^2 + 1)^4} = 10.185916 \times \frac{1}{(p^2 + 1)^4} \quad (9)$$

$$|\phi_{2,0}|^2 = \frac{1024(4p^2 - 1)^2}{\pi(4p^2 + 1)^6} = 325.94932 \times \frac{(4p^2 - 1)^2}{(4p^2 + 1)^6} \quad (10)$$

$$|\phi_{2,1}|^2 = \frac{16384p^2}{3\pi(4p^2 + 1)^6} = 1738.3964 \times \frac{p^2}{(4p^2 + 1)^6} \quad (11)$$

$$|\phi_{3,0}|^2 = \frac{864}{\pi} \left( 4 \frac{(9p^2 - 1)^2}{(9p^2 + 1)^4} - 1 \right)^2 = 275.01974 \times \left( 4 \frac{(9p^2 - 1)^2}{(9p^2 + 1)^4} - 1 \right)^2 \quad (12)$$

$$|\phi_{3,1}|^2 = \frac{248832p^2}{\pi} \left( \frac{(9p^2 - 1)}{(9p^2 + 1)^3} \right)^2 = 79205.686 \times p^2 \left( \frac{(9p^2 - 1)}{(9p^2 + 1)^3} \right)^2 \quad (13)$$

$$|\phi_{3,2}|^2 = \frac{8957952}{5\pi} \frac{p^4}{(9p^2 + 1)^8} = 570280.94 \times \frac{p^4}{(9p^2 + 1)^8} \quad (14)$$

$$|\phi_{4,0}|^2 = \frac{32768}{\pi} \left( \frac{(16p^2 - 1)}{(16p^2 + 1)^3} \right)^2 \left( 2 \frac{(16p^2 - 1)^2}{(16p^2 + 1)^2} - 1 \right)^2 \quad (15)$$

$$= 10430.378 \times \left( \frac{(16p^2 - 1)}{(16p^2 + 1)^3} \right)^2 \left( 2 \frac{(16p^2 - 1)^2}{(16p^2 + 1)^2} - 1 \right)^2 \quad (16)$$

$$\text{or alternately} \quad (17)$$

$$= 651.89865 \times \left( \frac{(16p^2 - 1)}{(16p^2 + 1)^3} \right)^2 \left( 8 \frac{(16p^2 - 1)^2}{(16p^2 + 1)^2} - 4 \right)^2 \quad (18)$$

## References

- [1] M. Swartz, H.R. Band, F.J. Decker, P. Emma, M.J. Fero, R. Frey, R. King, A. Lath, T. Limberg, R. Prepost, P.C. Rowson, B.A. Schumm, M. Woods, and M. Zolotarev. Observation of target electron momentum effects in single-arm mller polarimetry. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, 363(3):526 – 537, 1995.
- [2] Linus Pauling. A theory of ferromagnetism. *Proceedings of the National Academy of Sciences*, 39(6):551–560, 1953.
- [3] Hans A. Bethe and Edwin E. Salpeter. *Quantum Mechanics of One- and Two-Electron Atoms*. Springer Berlin Heidelberg, 1957.