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 $[\text{Ar}]3d^6 4s^{21}$, 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:

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

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

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

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[1] Linus Pauling argues in [2] that a better model for metallic Fe is $[\text{Ar}]3d^5 4s^1 4p^2$. 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:

$$C_0^1(x) = 1$$
$$C_1^1(x) = 2x$$
$$C_2^1(x) = 4x^2 - 1$$
$$C_3^1(x) = 8x^3 - 4x$$
$$C_0^2(x) = 1$$
$$C_1^2(x) = 4x$$
$$C_0^3(x) = 1.$$

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

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

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

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

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

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

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

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

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

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

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

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

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

$$= 275.01974 \times \frac{1}{(9p^2+1)^4}\left(4\frac{(9p^2-1)^2}{(9p^2+1)^2}-1\right)^2 \tag{13}$$

$$|\phi_{3,1}|^2 = \frac{248832p^2}{\pi}\left(\frac{(9p^2-1)}{(9p^2+1)^3}\right)^2 = 79205.686 \times p^2\left(\frac{(9p^2-1)}{(9p^2+1)^3}\right)^2 \tag{14}$$

$$|\phi_{3,2}|^2 = \frac{8957952}{5\pi}\frac{p^4}{(9p^2+1)^8} = 570280.94 \times \frac{p^4}{(9p^2+1)^8} \tag{15}$$

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

$$= 10430.378 \times \left(\frac{(16p^2-1)}{(16p^2+1)^3}\right)^2\left(2\frac{(16p^2-1)^2}{(16p^2+1)^2}-1\right)^2 \tag{17}$$

or alternately $\tag{18}$

$$= 651.89865 \times \left(\frac{(16p^2-1)}{(16p^2+1)^3}\right)^2\left(8\frac{(16p^2-1)^2}{(16p^2+1)^2}-4\right)^2 \tag{19}$$

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. Zolotorev. 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.