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 $[\mathrm{Ar}]3d^6 4s^2$[1], 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:

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

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

$$\begin{aligned} C^{\alpha}_0(x) &= 1 \\ C^{\alpha}_1(x) &= 2\alpha x \\ C^{\alpha}_0\beta(x) &= \frac{1}{n}\left[2x(\beta+\alpha-1)C^{\alpha}_{\beta-1}(x) - (\beta+2\alpha-2)C^{\alpha}_{\beta-2}(x)\right]. \end{aligned}$$

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

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

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

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

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

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

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

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

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

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

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 (18)

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

Using the procedure in the Swartz paper[1], the polarized and unpolarized momentum distributions for a pure elemental target foil are given by

$$f_{unp} = \sum_{n,l}\frac{C_{n,l}}{P_n}\left(\frac{p}{P_n}\right)^2\left|\phi_{n,l}\left(\frac{p}{P_n}\right)\right|^2, \tag{20}$$

where p is the radial momentum, $C_{n,l}$ is the fraction of the total unpolarized electron population in the n, l orbital and $P_n = Z_n m_e \alpha$ is an atomic momentum scale associated with the given orbital. The term Z_n is adjusted to account for screening assuming that a given electron is fully screened by electrons in inner orbitals and by half of its neighboring electrons in the same orbital. It is given explicitly by

$$Z_n = Z - \frac{N_n - 1}{2} - sum_i^{n-1} N_i,$$

where N_i is the number of electrons in the i^{th} shell. If the polarized distribution is assumed to come solely from D-wave, M-shell electrons, this polarized distribution is given by

$$f_{pol} = \sum_{n,l} \frac{1}{P_n} \left(\frac{p}{P_3}\right)^2 \left|\phi_{3,2}\left(\frac{p}{P_3}\right)\right|^2 .$$

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 møller 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.