Explicit Hydrogen-like Momentum Wave Functions

Donald Jones
Temple University

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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:

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

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

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

[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:

$$
\begin{aligned}
\phi_{1,0} &= \frac{8}{\sqrt{2\pi}(p^2+1)^2} \\
\phi_{2,0} &= \frac{32(4p^2-1)}{\sqrt{\pi}(4p^2+1)^3} \\
\phi_{2,1} &= \frac{128p}{\sqrt{3\pi}(4p^2+1)^3} \\
\phi_{3,0} &= \frac{72}{\sqrt{6\pi}}\left(4\frac{(9p^2-1)^2}{(9p^2+1)^3} - 1\right) \\
\phi_{3,1} &= \frac{864p}{\sqrt{3\pi}}\frac{(9p^2-1)}{(9p^2+1)^3} \\
\phi_{3,2} &= \frac{5184}{\sqrt{15\pi}}\frac{p^2}{(9p^2+1)^4} \\
\phi_{4,0} &= \frac{256}{\sqrt{2\pi}}\frac{(16p^2-1)}{(16p^2+1)^3}\left(2\frac{(16p^2-1)^2}{(16p^2+1)^2} - 1\right)
\end{aligned}
$$

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.