The Atomic Structure Factor in Coordinate and Momentum Space

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The following expression for the atomic structure factor in the coordinate and momentum representations can be found in a paper by Fearnside and Matthew [AJP 65(8), 795-796 (1997)].

$$f(\mu) = \int \exp(i\mu \cdot r)|\Psi(r)|^2\, dr = \int \Psi(p)\Psi^*(p+\mu)dp$$

The purpose of this tutorial is to establish the validity of this equation using Dirac notation and actual calculations using the hydrogen atom ground state eigenfunction in the position and momentum representations. See the Appendix for a graphical representation of what follows.

$$\int \exp(i\mu \cdot r)|\Psi(r)|^2\, dr = \int \langle \Psi | r \rangle \langle r | \mu \rangle \langle r | \Psi \rangle dr = \int\int \langle \Psi | r \rangle \langle r | \mu \rangle \langle r | p \rangle \langle p | \Psi \rangle drdp$$

$$\int\int \langle \Psi | r \rangle \langle r | \mu \rangle \langle r | p \rangle \langle p | \Psi \rangle drdp = \int\int \langle p | \Psi \rangle \langle \Psi | r \rangle \langle r | p+\mu \rangle drdp = \int\int \langle p | \Psi \rangle \langle \Psi | p+\mu \rangle dp$$

The following expressions have been used in mathematical manipulations above.

$$\int |p\rangle \langle p| dp = 1 \qquad \int |r\rangle \langle r| dr = 1 \qquad \langle r | \mu \rangle \langle r | p \rangle = \langle r | p+\mu \rangle$$

Detail on the latter relationship is as follows.

$$\langle r | \mu \rangle \langle r | p \rangle = \exp(i\mu \cdot r)\exp(ip \cdot r) = \exp(i(p+\mu)\cdot r) = \langle r | p+\mu \rangle$$

Now for the actual calculations (in atomic units) using the hydrogen atom ground state.

Ground state in the coordinate representation: $\Psi(r) := \frac{1}{\sqrt{\pi}} \cdot \exp(-r)$

$$f(\mu) := \int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \Psi(r)^2 \cdot \exp(i\cdot\mu\cdot r\cdot\cos(\theta))\cdot r^2 \cdot \sin(\theta)\, d\phi\, d\theta\, dr \ \Big|\begin{matrix}\text{complex}\\ \text{simplify}\end{matrix} \rightarrow \frac{16}{16 + 8\cdot\mu^2 + \mu^4}$$

Ground state in the momentum representation: $\Psi(p) := \frac{2\cdot\sqrt{2}}{\pi} \cdot \frac{1}{(1+p^2)^2}$

$$f(\mu) := \frac{8}{\pi^2} \cdot \int_0^{\infty}\int_0^{\pi}\int_0^{2\cdot\pi} \frac{1}{(1+p^2)^2 \cdot \left[1 + (p^2 + \mu^2 + 2\cdot p\cdot\mu\cdot\cos(\theta))\right]^2} \cdot p^2 \cdot \sin(\theta)\, d\phi\, d\theta\, dp \ \Big|\begin{matrix}\text{complex}\\ \text{simplify}\end{matrix} \rightarrow \frac{16}{16 + 8\cdot\mu^2 + \mu^4}$$

where $\Psi(p+\mu) = \frac{2\cdot\sqrt{2}}{\pi} \cdot \frac{1}{\left[1 + (p^2 + \mu^2 + 2\cdot p\cdot\mu\cdot\cos(\theta))\right]^2}$

Appendix

$$\begin{array}{ccc}
\int \Psi(p)\Psi^*(p+\mu)dp & = & \int \Psi^*(r)\exp(i\mu r)\Psi(r)dr \\
\updownarrow (Dirac) & & \updownarrow (Dirac) \\
\int \langle p|\Psi\rangle\langle\Psi|p+\mu\rangle dp & & \int \langle\Psi|r\rangle\langle r|\mu\rangle\langle r|\Psi\rangle dr \\
\updownarrow \left(\int |r\rangle\langle r| dr = 1\right) & & \updownarrow \left(\int |p\rangle\langle p| dp = 1\right) \\
\int\int \langle\Psi|r\rangle\langle r|p+\mu\rangle\langle p|\Psi\rangle dpdr & \xleftrightarrow{\langle r|p+\mu\rangle = \langle r|\mu\rangle\langle r|p\rangle} & \int\int \langle\Psi|r\rangle\langle r|\mu\rangle\langle r|p\rangle\langle p|\Psi\rangle dpdr
\end{array}$$