Spherically-symmetric constant-density object

Peter C. Doerschuk

June 5, 2015

Let R_o ("o" for "object") be the radius of the object and ρ_0 be the density of the object:

$$\rho(\mathbf{x}) = \begin{cases} \rho_0 & |\mathbf{x}| \le R_o \\ 0 & \text{otherwise} \end{cases} . \tag{1}$$

From Ref. [1, Eq. 16.127],

$$\begin{aligned}
\exp(i\mathbf{k}^T\mathbf{x}) &= 4\pi \sum_{l=0}^{\infty} i^l j_l(kx) \sum_{m=-1}^{+l} Y_{l,m}^*(\theta', \phi') Y_{l,m}(\theta, \phi) & (2) \\
\Leftrightarrow \exp(i2\pi\mathbf{k}^T\mathbf{x}) &= 4\pi \sum_{l=0}^{\infty} i^l j_l(2\pi kx) \sum_{m=-1}^{+l} Y_{l,m}^*(\theta', \phi') Y_{l,m}(\theta, \phi) & (3) \\
\Leftrightarrow \exp(-i2\pi\mathbf{k}^T\mathbf{x}) &= 4\pi \sum_{l=0}^{\infty} (-i)^l j_l(2\pi kx) \sum_{m=-1}^{+l} Y_{l,m}(\theta', \phi') Y_{l,m}^*(\theta, \phi). & (4)
\end{aligned}$$

Therefore,

$$\begin{aligned}
P(\mathbf{k}) &= \int_{\mathbf{x}\in\mathbb{R}^3} \rho(\mathbf{x}) \exp(-i2\pi\mathbf{k}^T\mathbf{x}) \mathrm{d}\mathbf{x} & (5) \\
&= \int_{\mathbf{x}\in\mathbb{R}^3} \rho(\mathbf{x}) \left[4\pi \sum_{l=0}^{\infty} (-i)^l j_l(2\pi kx) \sum_{m=-1}^{+l} Y_{l,m}(\theta', \phi') Y_{l,m}^*(\theta, \phi) \right] \mathrm{d}\mathbf{x} & (6) \\
&= \int_{x=0}^{R_o} \int \rho_0 \left[4\pi \sum_{l=0}^{\infty} (-i)^l j_l(2\pi kx) \sum_{m=-1}^{+l} Y_{l,m}(\theta', \phi') Y_{l,m}^*(\theta, \phi) \right] x^2 \mathrm{d}x \mathrm{d}\Omega & (7) \\
&= \rho_0 4\pi \sum_{l=0}^{\infty} (-i)^l \left[\int_{x=0}^{R_o} j_l(2\pi kx) x^2 \mathrm{d}x \right] \sum_{m=-1}^{+l} Y_{l,m}(\theta', \phi') \left[\int Y_{l,m}(\theta, \phi) \mathrm{d}\Omega \right]^* & (8) \\
&= \rho_0 4\pi \sum_{l=0}^{\infty} (-i)^l \left[\int_{x=0}^{R_o} j_l(2\pi kx) x^2 \mathrm{d}x \right] \sum_{m=-1}^{+l} Y_{l,m}(\theta', \phi') \left[\sqrt{4\pi} \delta_{l,0} \delta_{m,0} \right]^* & (9) \\
&= \rho_0 4\pi (-i)^0 \left[\int_{x=0}^{R_o} j_0(2\pi kx) x^2 \mathrm{d}x \right] Y_{0,0}(\theta', \phi') \sqrt{4\pi} & (10)
\end{aligned}$$

$$= \rho_0 4\pi \left[\int_{x=0}^{R_o} j_0(2\pi k x) x^2 \mathrm{d}x\right] \frac{1}{\sqrt{4\pi}}\sqrt{4\pi} \tag{11}$$

$$= \rho_0 4\pi \int_{x=0}^{R_o} j_0(2\pi k x) x^2 \mathrm{d}x. \tag{12}$$

Replace x by γ defined by

$$\gamma = 2\pi k x \tag{13}$$

$$\mathrm{d}\gamma = 2\pi k \mathrm{d}x \tag{14}$$

$$x = 0 \Leftrightarrow \gamma = 0 \tag{15}$$

$$x = R_o \Leftrightarrow \gamma = 2\pi k R_o \tag{16}$$

to get

$$P(\mathbf{k}) = \rho_0 4\pi \int_{\gamma=0}^{2\pi k R_o} j_0(\gamma) \left(\frac{\gamma}{2\pi k}\right)^2 \frac{\mathrm{d}\gamma}{2\pi k} \tag{17}$$

$$= \rho_0 4\pi \frac{1}{(2\pi k)^3} \int_{\gamma=0}^{2\pi k R_o} \gamma^2 j_0(\gamma) \mathrm{d}\gamma. \tag{18}$$

Ref. [2, Eq. 10.47.3] is

$$j_n(z) = \sqrt{\frac{\pi}{2z}} J_{n+\frac{1}{2}}(z). \tag{19}$$

Therefore ($n = 0$ and $z = \gamma$),

$$P(\mathbf{k}) = \rho_0 4\pi \frac{1}{(2\pi k)^3} \int_{\gamma=0}^{2\pi k R_o} \gamma^2 \sqrt{\frac{\pi}{2\gamma}} J_{0+\frac{1}{2}}(\gamma) \mathrm{d}\gamma \tag{20}$$

$$= \rho_0 4\pi \frac{1}{(2\pi k)^3} \sqrt{\frac{\pi}{2}} \int_{\gamma=0}^{2\pi k R_o} \gamma^{(\frac{1}{2}+1)} J_{\frac{1}{2}}(\gamma) \mathrm{d}\gamma. \tag{21}$$

Ref. [2, Eq. 10.22.1] is the indefinite integral

$$\int z^{\nu+1} \mathcal{C}_\nu(z) \mathrm{d}z = z^{\nu+1} \mathcal{C}_{\nu+1}(z). \tag{22}$$

Therefore ($\mathcal{C} = J$, $\nu = \frac{1}{2}$),

$$P(\mathbf{k}) = \rho_0 4\pi \frac{1}{(2\pi k)^3} \sqrt{\frac{\pi}{2}}\, \gamma^{(\frac{1}{2}+1)} J_{1+\frac{1}{2}}(\gamma)\Big|_{\gamma=0}^{2\pi k R_o} \tag{23}$$

$$= \rho_0 4\pi \frac{1}{(2\pi k)^3} \sqrt{\frac{\pi}{2}} (2\pi k R_o)^{(\frac{1}{2}+1)} J_{1+\frac{1}{2}}(2\pi k R_o). \tag{24}$$

Ref. [2, Eq. 10.47.3] in the reverse direction is

$$J_{n+\frac{1}{2}}(z) = \sqrt{\frac{2z}{\pi}} j_n(z). \tag{25}$$

Therefore ($n = 1$ and $z = 2\pi k R_o$),

$$\begin{aligned}
P(\mathbf{k}) &= \rho_0 4\pi \frac{1}{(2\pi k)^3} \sqrt{\frac{\pi}{2}} (2\pi k R_o)^{(\frac{1}{2}+1)} \sqrt{\frac{2 \times 2\pi k R_o}{\pi}} j_1(2\pi k R_o) && (26) \\
&= \rho_0 4\pi \frac{1}{(2\pi k)^3} (2\pi k R_o)^2 j_1(2\pi k R_o) && (27) \\
&= \rho_0 4\pi R_o^3 \frac{1}{(2\pi k R_o)^3} (2\pi k R_o)^2 j_1(2\pi k R_o) && (28) \\
&= \rho_0 4\pi R_o^3 \frac{1}{2\pi k R_o} j_1(2\pi k R_o). && (29)
\end{aligned}$$

Except for the replacement of "k" by "$2\pi k$", this formula matches Ref. [3, formula between Eqs. 20 and 21].

References

[1] J. D. Jackson. *Classical Electrodynamics*. John Wiley, New York, 2nd edition, 1975.

[2] F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark, editors. *NIST Handbook of Mathematical Functions*. Cambridge University Press, Cambridge, UK, 2010. `http://dlmf.nist.gov`.

[3] Y. Zheng, P. C. Doerschuk, and J. E. Johnson. Determination of three-dimensional low-resolution viral structure from solution x-ray scattering data. *Biophys. J.*, 69(2):619–639, Aug. 1995.