Notes On Pair Distribution Function

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- Combining the formulation given by (11) in D. Keen's paper (J. Appl. Cryst. (2001). 34, 172-177) and the expression (J.5) in M. Dove's book (Structure and dynamics: an atomic view of materials), we know that how the pair distribution function is linked with the scattering intensity. The usually seen sinc fucntion form appearing in the calculation from S(Q) to PDF actually comes from the isotropic average of the Fourier transform expression (refer to the appendix J in Martin's book). According to the aforementioned equation (11) in D. Keen's paper, the F(Q) function and the r-space function ($4\pi r^2 G(r)$) is a Fourier transform pair. According to the basic Fourier transform theory, the Q-space range determines the basic frequency component (thus the r-space resolution). Specifically for the transform between F(Q) and r-space function, we know from (11) that the r-space function ($4\pi r^2 G(r)$) is the angular frequency function in terms of the Fourier transform – refer to the aforementioned (J.5) in Martin's book, and from there we can see that r is actually the *angular frequency* if comparing to the frequency based Fourier transform (for which we should have a 2π pre-factor). Furthermore, since the Q-space range determines the r-space resolution in such a way that the smallest possible interval between frequency space point is given by $1/Q_{max}$. Therefore, when talking about the angular frequency resolution – the r-space PDF resolution for $4\pi r^2 G(r)$, we know that the corresponding resolution should be $2\pi/Q_{max}$.

- From section-(J.3) in Martin's book, we can understand how the definition of PDF can be linked up with the scattering intensity which is given as:

$$S(\mathbf{Q}) = \frac{1}{N} \sum_{j,k} b_j b_k exp[i\mathbf{Q} \cdot (\mathbf{r}_j - \mathbf{r}_k)] \tag{0.1}$$

according to the basic scattering theory (refer to Martin's book for detailed illustration based on the two-atoms simple system). In (J.8), the sinc function comes from the isotropic average for the Fourier transform part as mentioned above. the $\rho c_k 4\pi r^2 g_{jk}(r)dr$ refers to the number of k-type atoms within the shell $r \rightarrow r + dr$. c_j refers to the number density of the centering atom. Together this gives the contribution to the scattering intensity from the shell surrounding the centering atoms j with c_j serving as the normalization factor. Imaging we have n_j atoms in the system and we can take each of them as the centering atoms and we can do the same thing for all the other types of atoms. Summing them all up and divide through the total number of atoms in the system we get the finally normalized PDF.

- In stog program for preparing the input experimental data for RMCProfile, the equation-(46) in D. Keen's paper is used, through which we can obtain the equation (43) in that paper (but without the $4\pi r$ pre-factor). This is equivalent to the situation when we divide $4\pi r$ on both sides of the right two terms in (44) of that paper. Accordingly from (46) we can obtain $\rho^{PDF}(r) - \rho_0$ (which is done in stog by giving the program the $S(Q)$ data). Then through the equation-(42), we can calculate $G(r)$, to do which we need to know the number density and the Fiber-Ziman coefficient (which is called the 'final scale factor' in stog).