Magnetic Pair Distribution Function Analysis Supplementary Information

Benjamin A. Frandsen,[a] Xiaohao Yang[b] and Simon J.L. Billinge [b,c*]

[a]Department of Physics, Columbia University, New York, NY 10027, USA, [b]Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027, USA, and [c]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973, USA. E-mail: sb2896@columbia.edu

Abstract

In this supplementary information, we present the detailed calculation of various integrals involved in the derivation of the magnetic pair distribution function.

1. Evaluation of relevant integrals

1.1. First integral in Eq. 18

$$\int_0^\infty d\kappa \sin\kappa r_{ij} \sin\kappa r = \int_0^\infty d\kappa \frac{1}{2i}(e^{i\kappa r_{ij}} - e^{-i\kappa r_{ij}})\frac{1}{2i}(e^{i\kappa r} - e^{-i\kappa r}) \quad (1)$$

$$= -\frac{1}{4}\int_0^\infty d\kappa[(e^{i\kappa(r+r_{ij})} + e^{-i\kappa(r+r_{ij})}) - (e^{i\kappa(r-r_{ij})} + e^{-i\kappa(r-r_{ij})})] \quad (2)$$

$$= -\frac{1}{8}[\int_{-\infty}^{\infty} d\kappa(e^{i\kappa(r+r_{ij})} + e^{-i\kappa(r+r_{ij})}) - \int_{-\infty}^{\infty}(e^{i\kappa(r-r_{ij})} + e^{-i\kappa(r-r_{ij})})] \quad (3)$$

$$= -\frac{1}{8}(2[2\pi\delta(r+r_{ij}) - 2\pi\delta(r-r_{ij})]) \quad (4)$$

$$= \frac{\pi}{2}[\delta(r-r_{ij}) - \delta(r+r_{ij})]. \quad (5)$$

The physically meaningless $\delta(r + r_{ij})$ may be ignored, since r_{ij} is defined as the magnitude of a vector and is therefore nonnegative.

1.2. Second integral in Eq. 18

$$\int_0^\infty d\kappa \frac{\sin\kappa r_{ij}\sin\kappa r}{\kappa^2} = \frac{1}{2}\int_{-\infty}^{\infty} d\kappa \frac{\sin\kappa r_{ij}}{\kappa}\frac{\sin\kappa r}{\kappa}. \tag{6}$$

Since $\frac{\sin x}{x}$ is a square-integrable function, the above expression may be viewed as an inner product in Hilbert space:

$$\int_0^\infty d\kappa \frac{\sin\kappa r_{ij}\sin\kappa r}{\kappa^2} = \frac{1}{2}\langle f_1(\kappa), f_2(\kappa)\rangle, \tag{7}$$

where $f_1(\kappa) = \frac{\sin\kappa r}{\kappa}$ and $f_2(\kappa) = \frac{\sin\kappa r_{ij}}{\kappa}$. If a symmetric Fourier transform is employed, then we have the result

$$\langle f_1(\kappa), f_2(\kappa)\rangle = \langle \mathscr{F}[f_1(\kappa)], \mathscr{F}[f_2(\kappa)]\rangle = \langle g_1(y), g_2(y)\rangle = \int_{-\infty}^{\infty} dy g_1(y) g_2(y). \tag{8}$$

In this case, the Fourier transform is easier to work with, since the well-known Fourier transform of the sinc function is a “top hat” or “window” function, as shown in the following:

$$g_1(y) = \mathscr{F}[f_1(\kappa)] = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\kappa \frac{\sin\kappa r}{\kappa} e^{-i\kappa y} \tag{9}$$

$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\kappa \frac{\sin\kappa r\cos\kappa y}{\kappa} \tag{10}$$

$$= \frac{1}{\sqrt{2\pi}}\frac{1}{2}\left[\int_{-\infty}^{\infty} \frac{\sin[\kappa(r+y)]}{\kappa} + \int_{-\infty}^{\infty} d\kappa \frac{\sin[\kappa(r-y)]}{\kappa}\right] \tag{11}$$

$$= \begin{cases} \sqrt{\frac{\pi}{2}} & \text{if} -r < y < r \\ 0 & \text{otherwise} \end{cases}. \tag{12}$$

In the last equality, we have made use of the fact that

$$\int_{-\infty}^{\infty} dx \frac{\sin ax}{x} = \begin{cases} \pi & \text{if } a > 0 \\ -\pi & \text{if } a < 0 \end{cases}. \tag{13}$$

Similarly, we have

$$g_2(y) = \mathscr{F}[f_2(\kappa)] = \begin{cases} \sqrt{\frac{\pi}{2}} & \text{if } -r_{ij} < y < r_{ij} \\ 0 & \text{otherwise} \end{cases}. \tag{14}$$

Therefore,

$$\langle g_1(y), g_2(y) \rangle = \int\limits_{-\infty}^{\infty} dy g_1(y) g_2(y) = \begin{cases} \frac{\pi}{2} \cdot 2r & \text{if } r < r_{ij} \\ \frac{\pi}{2} \cdot 2r_{ij} & \text{if } r > r_{ij} \end{cases}. \tag{15}$$

Notice that

$$\frac{\pi}{2}(r + r_{ij} - |r - r_{ij}|) = \begin{cases} \frac{\pi}{2}[r + r_{ij} - (r - r_{ij})] = \frac{\pi}{2} \cdot 2r & \text{if } r > r_{ij} \\ \frac{\pi}{2}[r + r_{ij} - (r_{ij} - r)] = \frac{\pi}{2} \cdot 2r_{ij} & \text{if } r < r_{ij} \end{cases} = \langle g_1(y), g_2(y) \rangle. \tag{16}$$

Putting this all together, we have

$$\int\limits_{0}^{\infty} d\kappa \frac{\sin \kappa r \sin \kappa r_{ij}}{\kappa^2} = \frac{1}{2} \langle f_1(\kappa), f_2(\kappa) \rangle = \frac{1}{2} \langle g_1(y), g_2(y) \rangle = \frac{\pi}{4}(r + r_{ij} - |r - r_{ij}|). \tag{17}$$

1.3. Third integral in Eq. 18

$$\int\limits_{0}^{\infty} d\kappa \frac{\sin \kappa r \cos \kappa r_{ij}}{\kappa} = \frac{1}{2} \int\limits_{-\infty}^{\infty} d\kappa \frac{\sin \kappa r \cos \kappa r_{ij}}{\kappa} \tag{18}$$

$$= \frac{1}{4} [\int\limits_{-\infty}^{\infty} d\kappa \frac{\sin[\kappa(r + r_{ij})]}{\kappa} + \int\limits_{-\infty}^{\infty} d\kappa \frac{\sin[\kappa(r - r_{ij})]}{\kappa}] \tag{19}$$

$$= \frac{1}{4} \begin{cases} 0 & \text{if } r < r_{ij} \\ 2\pi & \text{if } r > r_{ij} \end{cases} = \frac{\pi}{2} \Theta(r - r_{ij}). \tag{20}$$