Real Space wavefunctions

$\psi_1(x, y, z) =$

$$\sin(1x) + \sin(3x) + \sin(2y) + \sin(1z)$$

$\psi_2(x, y, z) =$

$$\sin(2x) + \sin(1y) + \sin(2y)$$

Reciprocal Space wavefunctions

$\psi_1(G_x, G_yG_z) =$

$$\frac{i}{2}\delta(G_x - 1)\delta(G_y)\delta(G_z) - \frac{i}{2}\delta(G_x + 1)\delta(G_y)\delta(G_z) + \frac{i}{2}\delta(G_x - 3)\delta(G_y)\delta(G_z) - \frac{i}{2}\delta(G_x + 3)\delta(G_y)\delta(G_z)$$
$$+ \frac{i}{2}\delta(G_x)\delta(G_y - 2)\delta(G_z) - \frac{i}{2}\delta(G_x)\delta(G_y + 2)\delta(G_z) + \frac{i}{2}\delta(G_x)\delta(G_y)\delta(G_z - 1) - \frac{i}{2}\delta(G_x)\delta(G_y)\delta(G_z + 1)$$

$\psi_2(G_x, G_yG_z) =$

$$\frac{i}{2}\delta(G_x - 2)\delta(G_y)\delta(G_z) - \frac{i}{2}\delta(G_x + 2)\delta(G_y)\delta(G_z) + \frac{i}{2}\delta(G_x)\delta(G_y - 1)\delta(G_z) - \frac{i}{2}\delta(G_x)\delta(G_y + 1)\delta(G_z)$$
$$+ \frac{i}{2}\delta(G_x)\delta(G_y - 2)\delta(G_z) - \frac{i}{2}\delta(G_x)\delta(G_y + 2)\delta(G_z)$$

Real Space Convolution Functions

$f_1(x, y, z) =$

$$2 + \frac{1}{2}\cos(2x) - \cos(4x) - \frac{1}{2}\cos(6x) - \frac{1}{2}\cos(4y) - \frac{1}{2}\cos(2z) + 2\sin(1x)\sin(2y) + 2\sin(1x)\sin(1z) + 2\sin(3x)\sin(2y) + 2\sin(3x)\sin(1z) + 2\sin(2y)\sin(1z)$$

$f_2(x, y, z) =$

$$\frac{3}{2} - \frac{1}{2}\cos(4x) + \cos(y) - \frac{1}{2}\cos(2y) - \cos(3y) - \frac{1}{2}\cos(4y) + 2\sin(2x)\sin(y) + 2\sin(2x)\sin(2y)$$

$f_3(x, y, z) =$

$$\frac{1}{2} + \cos(x) - \frac{1}{2}\cos(3x) - \frac{1}{2}\cos(5x) + \frac{1}{2}\cos(y) - \frac{1}{2}\cos(3y) - \frac{1}{2}\cos(4y) + \sin(x)\sin(2y) + \sin(2x)\sin(2y) + \sin(3x)\sin(2y) + \sin(x)\sin(y) + \sin(3x)\sin(y) + \sin(2x)\sin(z) + \sin(y)\sin(z) + \sin(2y)\sin(z)$$

Reciprocal Space Convolution Functions

$f_1(G_x, G_yG_z) =$

$$2\delta(G_x)\delta(G_y)\delta(G_z) - \frac{1}{4}\delta(G_x - 6)\delta(G_y)\delta(G_z) - \frac{1}{2}\delta(G_x - 4)\delta(G_y)\delta(G_z) - \frac{1}{4}\delta(G_x)\delta(G_y - 4)\delta(G_z) + \frac{1}{4}\delta(G_x - 2)\delta(G_y)\delta(G_z) - \frac{1}{2}\delta(G_x - 3)\delta(G_y - 2)\delta(G_z) - \frac{1}{2}\delta(G_x - 1)\delta(G_y - 2)\delta(G_z) + \frac{1}{2}\delta(G_x + 1)\delta(G_y - 2)\delta(G_z) + \frac{1}{4}\delta(G_x + 2)\delta(G_y)\delta(G_z) + \frac{1}{2}\delta(G_x - 3)\delta(G_y + 2)\delta(G_z) + \frac{1}{2}\delta(G_x - 1)\delta(G_y + 2)\delta(G_z) - \frac{1}{2}\delta(G_x + 1)\delta(G_y + 2)\delta(G_z) + \frac{1}{2}\delta(G_x + 3)\delta(G_y - 2)\delta(G_z) - \frac{1}{2}\delta(G_x + 3)\delta(G_y + 2)\delta(G_z) - \frac{1}{2}\delta(G_x + 4)\delta(G_y)\delta(G_z) - \frac{1}{4}\delta(G_x)\delta(G_y + 4)\delta(G_z) - \frac{1}{4}\delta(G_x + 6)\delta(G_y)\delta(G_z) - \frac{1}{4}\delta(G_x)\delta(G_y)\delta(G_z - 2) - \frac{1}{2}\delta(G_x - 3)\delta(G_y)\delta(G_z - 1) - \frac{1}{2}\delta(G_x)\delta(G_y - 2)\delta(G_z - 1) - \frac{1}{2}\delta(G_x - 1)\delta(G_y)\delta(G_z - 1) + \frac{1}{2}\delta(G_x + 1)\delta(G_y)\delta(G_z - 1) + \frac{1}{2}\delta(G_x - 3)\delta(G_y)\delta(G_z + 1) + \frac{1}{2}\delta(G_x)\delta(G_y - 2)\delta(G_z + 1) + \frac{1}{2}\delta(G_x - 1)\delta(G_y)\delta(G_z + 1) - \frac{1}{2}\delta(G_x + 1)\delta(G_y)\delta(G_z + 1) + \frac{1}{2}\delta(G_x)\delta(G_y + 2)\delta(G_z - 1) - \frac{1}{2}\delta(G_x)\delta(G_y + 2)\delta(G_z + 1) - \frac{1}{4}\delta(G_x)\delta(G_y)\delta(G_z + 2) + \frac{1}{2}\delta(G_x + 3)\delta(G_y)\delta(G_z - 1) - \frac{1}{2}\delta(G_x + 3)\delta(G_y)\delta(G_z + 1)$$

$$f_2(G_x, G_yG_z) =$$

$$\begin{aligned}
&\frac{3}{2}\delta(G_x)\delta(G_y)\delta(G_z) - \frac{1}{4}\delta(G_x-4)\delta(G_y)\delta(G_z) - \frac{1}{4}\delta(G_x)\delta(G_y-4)\delta(G_z) - \frac{1}{2}\delta(G_x)\delta(G_y-3)\delta(G_z) - \frac{1}{4}\delta(G_x)\delta(G_y-2)\delta(G_z)\\
&- \frac{1}{2}\delta(G_x-2)\delta(G_y-2)\delta(G_z) + \frac{1}{2}\delta(G_x)\delta(G_y-1)\delta(G_z) - \frac{1}{2}\delta(G_x-2)\delta(G_y-1)\delta(G_z) + \frac{1}{2}\delta(G_x)\delta(G_y+1)\delta(G_z)\\
&+ \frac{1}{2}\delta(G_x-2)\delta(G_y+1)\delta(G_z) + \frac{1}{2}\delta(G_x+2)\delta(G_y-2)\delta(G_z) + \frac{1}{2}\delta(G_x+2)\delta(G_y-1)\delta(G_z) - \frac{1}{2}\delta(G_x+2)\delta(G_y+1)\delta(G_z)\\
&- \frac{1}{4}\delta(G_x)\delta(G_y+2)\delta(G_z) + \frac{1}{2}\delta(G_x-2)\delta(G_y+2)\delta(G_z) - \frac{1}{2}\delta(G_x+2)\delta(G_y+2)\delta(G_z) - \frac{1}{2}\delta(G_x)\delta(G_y+3)\delta(G_z)\\
&- \frac{1}{4}\delta(G_x+4)\delta(G_y)\delta(G_z) - \frac{1}{4}\delta(G_x)\delta(G_y+4)\delta(G_z)
\end{aligned}$$

$$f_3(G_x, G_yG_z) =$$

$$\begin{aligned}
&\frac{1}{2}\delta(G_x)\delta(G_y)\delta(G_z) - \frac{1}{4}\delta(G_x-5)\delta(G_y)\delta(G_z) - \frac{1}{4}\delta(G_x)\delta(G_y-4)\delta(G_z) - \frac{1}{4}\delta(G_x-3)\delta(G_y)\delta(G_z) - \frac{1}{4}\delta(G_x)\delta(G_y-3)\delta(G_z)\\
&- \frac{1}{4}\delta(G_x-3)\delta(G_y-2)\delta(G_z) - \frac{1}{4}\delta(G_x-2)\delta(G_y-2)\delta(G_z) + \frac{1}{2}\delta(G_x-1)\delta(G_y)\delta(G_z) - \frac{1}{4}\delta(G_x-1)\delta(G_y-2)\delta(G_z)\\
&+ \frac{1}{4}\delta(G_x)\delta(G_y-1)\delta(G_z) - \frac{1}{4}\delta(G_x-3)\delta(G_y-1)\delta(G_z) - \frac{1}{4}\delta(G_x-1)\delta(G_y-1)\delta(G_z) + \frac{1}{2}\delta(G_x+1)\delta(G_y)\delta(G_z)\\
&+ \frac{1}{4}\delta(G_x+1)\delta(G_y-2)\delta(G_z) + \frac{1}{4}\delta(G_x+1)\delta(G_y-1)\delta(G_z) + \frac{1}{4}\delta(G_x)\delta(G_y+1)\delta(G_z) + \frac{1}{4}\delta(G_x-3)\delta(G_y+1)\delta(G_z)\\
&+ \frac{1}{4}\delta(G_x-1)\delta(G_y+1)\delta(G_z) - \frac{1}{4}\delta(G_x+1)\delta(G_y+1)\delta(G_z) + \frac{1}{4}\delta(G_x+2)\delta(G_y-2)\delta(G_z) + \frac{1}{4}\delta(G_x-3)\delta(G_y+2)\delta(G_z)\\
&+ \frac{1}{4}\delta(G_x-2)\delta(G_y+2)\delta(G_z) + \frac{1}{4}\delta(G_x-1)\delta(G_y+2)\delta(G_z) - \frac{1}{4}\delta(G_x+1)\delta(G_y+2)\delta(G_z) - \frac{1}{4}\delta(G_x+2)\delta(G_y+2)\delta(G_z)\\
&- \frac{1}{4}\delta(G_x+3)\delta(G_y)\delta(G_z) + \frac{1}{4}\delta(G_x+3)\delta(G_y-2)\delta(G_z) + \frac{1}{4}\delta(G_x+3)\delta(G_y-1)\delta(G_z) - \frac{1}{4}\delta(G_x+3)\delta(G_y+1)\delta(G_z)\\
&- \frac{1}{4}\delta(G_x+3)\delta(G_y+2)\delta(G_z) - \frac{1}{4}\delta(G_x)\delta(G_y+3)\delta(G_z) - \frac{1}{4}\delta(G_x)\delta(G_y+4)\delta(G_z) - \frac{1}{4}\delta(G_x+5)\delta(G_y)\delta(G_z)\\
&- \frac{1}{4}\delta(G_x-2)\delta(G_y)\delta(G_z-1) - \frac{1}{4}\delta(G_x)\delta(G_y-2)\delta(G_z-1) - \frac{1}{4}\delta(G_x)\delta(G_y-1)\delta(G_z-1) + \frac{1}{4}\delta(G_x)\delta(G_y+1)\delta(G_z-1)\\
&+ \frac{1}{4}\delta(G_x-2)\delta(G_y)\delta(G_z+1) + \frac{1}{4}\delta(G_x)\delta(G_y-2)\delta(G_z+1) + \frac{1}{4}\delta(G_x)\delta(G_y-1)\delta(G_z+1) - \frac{1}{4}\delta(G_x)\delta(G_y+1)\delta(G_z+1)\\
&+ \frac{1}{4}\delta(G_x+2)\delta(G_y)\delta(G_z-1) - \frac{1}{4}\delta(G_x+2)\delta(G_y)\delta(G_z+1) + \frac{1}{4}\delta(G_x)\delta(G_y+2)\delta(G_z-1) - \frac{1}{4}\delta(G_x)\delta(G_y+2)\delta(G_z+1)
\end{aligned}$$