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Correction of some formulas of Agarwal's fast Fourier transform least-squares algorithm — Source link <a> ☑

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Abstract

The formulas (34), (37) and (38) of Agarwal [Acta Cryst. (1978), A34, 791-809] should be changed to:

$$H_2(B_m, B_n) = \sum_{s} + \frac{1}{2} g_m(s) g_n(s) (s^4/16) W(s)$$

$$\times \exp[i2\varphi(s)] \exp[-i2\pi s \cdot (\mathbf{r}_m + \mathbf{r}_n)] \qquad (34)$$

$$H_1(x_m, B_n) = \sum_{s} -\frac{1}{4}g_m(s)g_n(s)(i\pi h s^2)W(s)$$

$$\times \exp[+i2\pi \mathbf{s} \cdot (\mathbf{r}_m - \mathbf{r}_n)]$$

$$H_2(\mathbf{x}_m, B_n) = \sum_{\mathbf{s}} + \frac{1}{4} g_m(\mathbf{s}) g_n(\mathbf{s}) (i\pi h s^2) W(\mathbf{s})$$

$$\times \exp[i2\varphi(\mathbf{s})] \exp[-i2\pi \mathbf{s} \cdot (\mathbf{r}_m + \mathbf{r}_n)].$$
(38)

All the information is contained in the Abstract.