SUPPLEMENTARY PUBLICATION MATERIAL

Algebraic direct methods for few-atoms structure models

Herbert A. Hauptman, D.Y. Guo, Hongliang Xu, and Robert H. Blessing

Hauptman-Woodward Medical Research Institute
73 High Street
Buffalo, New York 14203-1196, USA
and
Department of Structural Biology
School of Medicine and Biomedical Sciences
State University of New York at Buffalo

Email: guo@hwi.buffalo.edu

Abstract

As a basis for direct methods phasing at very low resolution for macromolecular crystal structures, normalized structure factor algebra is presented for few-atoms structure models with N = 1,2,3,… equal atoms or polyatomic globs per unit cell. Main results include:

For $N=1$, $(\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h}-\mathbf{k}}) \bmod 2\pi = 0$.

For $N=2$, $(\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h}-\mathbf{k}}) \bmod 2\pi = \begin{cases} 0 & \text{if} \quad |E_{\mathbf{h}}|^2+|E_{\mathbf{k}}|^2+|E_{-\mathbf{h}-\mathbf{k}}|^2-2>0, \\ \pi & \text{if} \quad |E_{\mathbf{h}}|^2+|E_{\mathbf{k}}|^2+|E_{-\mathbf{h}-\mathbf{k}}|^2-2<0. \end{cases}$

For $N=3$, $\cos(\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h}-\mathbf{k}})$ is obtained in an exact, closed form as a rational function of nine magnitudes $|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{h}+\mathbf{k}}|, |E_{\mathbf{h}-\mathbf{k}}|, |E_{\mathbf{h}+2\mathbf{k}}|, |E_{2\mathbf{h}+\mathbf{k}}|, |E_{2\mathbf{h}}|, |E_{2\mathbf{k}}|, |E_{2\mathbf{h}+2\mathbf{k}}|$.

For $N=1,2,3,...$,

$$\tan(\varphi_{\mathbf{h}}-\alpha_{\mathbf{h}}) \approx -\sum_{\mathbf{k}} W_{\mathbf{hk}} \sin(\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h}-\mathbf{k}}) \Big/ \sum_{\mathbf{k}} W_{\mathbf{hk}} \cos(\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h}-\mathbf{k}}),$$

$$\alpha_{\mathbf{h}} = \begin{cases} 0 & \text{if} \quad \sum_{\mathbf{k}} \Delta_{\mathbf{hk}} |\Delta_{\mathbf{hk}}| > 0 \\ \pi & \text{if} \quad \sum_{\mathbf{k}} \Delta_{\mathbf{hk}} |\Delta_{\mathbf{hk}}| < 0 \end{cases}, \qquad \Delta_{\mathbf{hk}} = |E_{\mathbf{h}}|^2+|E_{\mathbf{k}}|^2+|E_{-\mathbf{h}-\mathbf{k}}|^2-\frac{a}{N},$$

$$W_{\mathbf{hk}} = |\Delta_{\mathbf{hk}} E_{\mathbf{h}} E_{\mathbf{k}} E_{-\mathbf{h}-\mathbf{k}}| \left[1-\left(1-|\Delta_{\mathbf{hk}}|^{-1}\right)\tanh(N-b)\right].$$

Triplet discriminant $\Delta_{\mathbf{hk}}$ and triplet weight $W_{\mathbf{hk}}$ parameters, $a \approx 4.0$ and $b \approx 3.0$, respectively, were determined empirically in numerical error analyses. Tests with phases calculated for few-atoms "super-glob" models of the protein, apo-D-glyceraldehyde-3-phosphate dehydrogenase (~10,000 non-H atoms) showed that low-resolution phases from the new few-atoms tangent formula were much better than conventional tangent formula phases for $N=2$ and 3; phases from the two formulae were essentially the same for $N \geq 4$.

$$H + K + L = 0, \qquad N = 3$$

$\text{Cos}(\phi_H + \phi_K + \phi_L)$ is the Root of a Linear Equation with Coefficients that are Polynomials in Nine Magnitudes |E|.

Chapter I.

$\mathrm{Cos}(\phi_H + \phi_K + \phi_L)$

N=3

$$E_H = \frac{1}{N^{1/2}} \sum_{\mu=1}^{N} \exp 2\pi i H \bullet r_\mu \qquad \text{(N terms) (1)}$$

$$E_K = \frac{1}{N^{1/2}} \sum_{\mu=1}^{N} \exp 2\pi i K \bullet r_\nu \qquad \text{(N terms) (2)}$$

$$E_H E_K = \frac{1}{N} \sum_{\mu,\nu} \exp 2\pi i \left(H \bullet r_\mu + K \bullet r_\nu\right) \qquad \text{(N}^2\text{ terms)}$$

$$= \frac{1}{N} \sum_{\mu} \exp 2\pi i (H + K) \bullet r_\mu \qquad \text{(N terms)}$$

$$+ \frac{1}{N} \sum_{\mu \neq \nu} \exp 2\pi i \left(H \bullet r_\mu + K \bullet r_\nu\right) \qquad \text{(N(N-1) terms)}$$

$$E_H E_K = \frac{1}{N^{1/2}} E_{H+K} + \frac{1}{N} \sum_{\mu \neq \nu} \exp 2\pi i \left(H \bullet r_\mu + K \bullet r_\nu\right) \qquad (3)$$

$$\frac{1}{N} \sum_{\mu \neq \nu} \exp 2\pi i \left(H \bullet r_\mu + K \bullet r_\nu\right) = E_H E_K - \frac{1}{N^{1/2}} E_{H+K} \qquad (4)$$

$$\left|E_H\right|^2 - 1 = \frac{1}{N} \sum_{\mu \neq \nu} \exp 2\pi i H \bullet \left(r_\mu - r_\nu\right) \qquad (5)$$

No. of
<u>terms</u>

$$E_H E_K E_L = \frac{1}{N^{3/2}} \sum_{\mu,\nu,\rho} \exp 2\pi i \left(H \bullet r_\mu + K \bullet r_\nu + L \bullet r_\rho \right) \qquad (N^3) \qquad (6)$$

$\mu=\nu=\rho$ $$= \frac{1}{N^{3/2}} \sum_{\mu} \exp 2\pi i (H+K+L) \bullet r_\mu \qquad (N)$$

$\mu=\nu\neq\rho$ $$+ \frac{1}{N^{3/2}} \sum_{\mu\neq\rho} \exp 2\pi i \left((H+K) \bullet r_\mu + L \bullet r_\rho \right) \qquad (N(N-1))$$

$\mu=\rho\neq\nu$ $$+ \frac{1}{N^{3/2}} \sum_{\mu\neq\nu} \exp 2\pi i \left((H+L) \bullet r_\mu + K \bullet r_\nu \right) \qquad (N(N-1))$$

$\nu=\rho\neq\mu$ $$+ \frac{1}{N^{3/2}} \sum_{\mu\neq\nu} \exp 2\pi i \left(H \bullet r_\mu + (K+L) \bullet r_\nu \right) \qquad (N(N-1))$$

$\mu\neq\nu\neq\rho$ $$+ \frac{1}{N^{3/2}} \sum_{\mu\neq\nu\neq\rho} \exp 2\pi i \left(H \bullet r_\mu + K \bullet r_\nu + L \bullet r_\rho \right) \qquad (N(N-1)(N-2))$$

(7)

Counting check: $N+3N(N-1)+N(N-1)(N-2)=N+3N^2-3N+N^3-3N^2+2N=N^3$.

H+K+L = 0

$$E_H E_K E_L = \frac{1}{N^{1/2}} + \frac{1}{N^{1/2}} \left(|E_H|^2 + |E_K|^2 + |E_L|^2 - 3 \right) + \frac{1}{N^{3/2}} \sum_{\mu\neq\nu\neq\rho} \exp 2\pi i \left(H \bullet r_\mu + K \bullet r_\nu + L \bullet r_\rho \right) \qquad (8)$$

$$E_H E_K E_L = \frac{1}{N^{1/2}} \left(|E_H|^2 + |E_K|^2 + |E_L|^2 - 2 \right) + \frac{1}{N^{3/2}} \sum_{\mu\neq\nu\neq\rho} \exp 2\pi i \left(H \bullet r_\mu + K \bullet r_\nu + L \bullet r_\rho \right) \qquad (9)$$

H+K+L=0

$$\left|E_H E_K E_L\right| \cos(\phi_H + \phi_K + \phi_L) = \frac{1}{N^{1/2}}\left(\left|E_H\right|^2 + \left|E_K\right|^2 + \left|E_L\right|^2 - 2\right) + \frac{1}{N^{3/2}} \sum_{\mu \neq \nu \neq \rho} \cos 2\pi\left(H \bullet r_\mu + K \bullet r_\nu + L \bullet r_\rho\right) \tag{10}$$

$$\left|E_H E_K E_L\right| \sin(\phi_H + \phi_K + \phi_L) = \frac{1}{N^{3/2}} \sum_{\mu \neq \nu \neq \rho} \sin 2\pi\left(H \bullet r_\mu + K \bullet r_\nu + L \bullet r_\rho\right) \tag{11}$$

$$\frac{1}{N^{3/2}} \sum_{\mu \neq \nu \neq \rho} \exp 2\pi i\left(H \bullet r_\mu + K \bullet r_\nu + L \bullet r_\rho\right) = E_H E_K E_L - \frac{1}{N^{1/2}}\left(\left|E_H\right|^2 + \left|E_K\right|^2 + \left|E_L\right|^2 - 2\right) \tag{12}$$

N=2

$$E_H E_K E_L = \frac{1}{2^{1/2}}\left(\left|E_H\right|^2 + \left|E_K\right|^2 + \left|E_L\right|^2 - 2\right) \tag{13}$$

$$\left|E_H E_K E_L\right| \cos(\phi_H + \phi_K + \phi_L) = \frac{1}{2^{1/2}}\left(\left|E_H\right|^2 + \left|E_K\right|^2 + \left|E_L\right|^2 - 2\right) \tag{14}$$

$$\left|E_H E_K E_L\right| \sin(\phi_H + \phi_K + \phi_L) = 0 \tag{15}$$

H+K+L=0

$$\left(\left|E_H\right|^2-1\right)E_H E_K E_L$$

$$= \frac{1}{N^{1/2}}\left(\left|E_H\right|^2-1\right)\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2-2\right)$$
$$+\frac{1}{N^{5/2}}\sum_{\mu\neq\nu}\exp 2\pi i H\bullet\left(r_\mu - r_\nu\right)\sum_{\rho\neq\sigma\neq\tau}\exp 2\pi i\left(H\bullet r_\rho + K\bullet r_\sigma = L\bullet r_\tau\right) \qquad (16)$$

$$= \frac{1}{N^{1/2}}\left(\left|E_H\right|^2-1\right)\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2-2\right)$$

μ=ρ ν=σ	$+\frac{1}{N^{5/2}}\sum_{\rho\neq\sigma\neq\tau}\exp 2\pi i\left(2H\bullet r_\rho + (-H+K)\bullet r_\sigma + L\bullet r_\tau\right)$	N(N-1)(N-2)
μ=ρ ν=τ	$+\frac{1}{N^{5/2}}\sum_{\rho\neq\sigma\neq\tau}\exp 2\pi i\left(2H\bullet r_\rho + K\bullet r_\sigma + (-H+L)\bullet r_\tau\right)$	N(N-1)(N-2)
μ=σ ν=ρ	$+\frac{N-2}{N^{5/2}}\sum_{\sigma\neq\tau}\exp 2\pi i\left((H+K)\bullet r_\sigma + L\bullet r_\tau\right)$	N(N-1)(N-2)
μ=σ ν=τ	$+\frac{1}{N^{5/2}}\sum_{\rho\neq\sigma\neq\tau}\exp 2\pi i\left((H+K)\bullet r_\sigma + (-H+L)\bullet r_\tau + H\bullet r_\rho\right)$	N(N-1)(N-2)
μ=τ ν=ρ	$+\frac{N-2}{N^{5/2}}\sum_{\sigma\neq\tau}\exp 2\pi i\left((H+L)\bullet r_\tau + K\bullet r_\sigma\right)$	N(N-1(N-2)
μ=τ ν=σ	$+\frac{1}{N^{5/2}}\sum_{\rho\neq\sigma\neq\tau}\exp 2\pi i\left((H+L)\bullet r_\tau + (-H+K)\bullet r_\sigma + H\bullet r_\rho\right)$	N(N-1)(N-2)
μ=ρ	$+\frac{1}{N^{5/2}}\sum_{\nu\neq\rho\neq\sigma\neq\tau}\exp 2\pi i\left(-H\bullet r_\nu + 2H\bullet r_\rho + K\bullet r_\sigma + L\bullet r_\tau\right)$	N(N-1)(N-2)(N-3)

$$
\begin{array}{ll}
\mu=\sigma & +\frac{1}{N^{5/2}}\sum_{\nu\neq\sigma\neq\rho\neq\tau}\exp 2\pi i\big((H+K)\bullet r_\sigma - H\bullet r_\nu + H\bullet r_\rho + L\bullet r_\tau\big) \quad - \\
\mu=\tau & +\frac{1}{N^{5/2}}\sum_{\nu\neq\rho\neq\sigma\neq\tau}\exp 2\pi i\big((H+L)\bullet r_\tau - H\bullet r_\nu + H\bullet r_\rho + K\bullet r_\sigma\big) \quad - \\
\nu=\rho & +\frac{N-3}{N^{5/2}}\sum_{\mu\neq\sigma\neq\tau}\exp 2\pi i\big(H\bullet r_\mu + K\bullet r_\sigma + L\bullet r_\tau\big) \quad - \\
\nu=\sigma & +\frac{1}{N^{5/2}}\sum_{\mu\neq\rho\neq\sigma\neq\tau}\exp 2\pi i\big(H\bullet r_\mu + H\bullet r_\rho + (-H+K)\bullet r_\sigma + L\bullet r_\tau\big) \quad - \\
\nu=\tau & +\frac{1}{N^{5/2}}\sum_{\mu\neq\rho\neq\sigma\neq\tau}\exp 2\pi i\big(H\bullet r_\mu + (-H+L)\bullet r_\tau + H\bullet r_\rho + K\bullet r_\sigma\big) \quad N(N-1)(N-2)(N-3) \\
 & +\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho\neq\sigma\neq\tau}\exp 2\pi i\big(H\bullet r_\mu - H\bullet r_\nu + H\bullet r_\rho + K\bullet r_\sigma + L\bullet r_\tau\big) \quad N(N-1)(N-2)(N-3)(N-4)
\end{array}
\tag{17}
$$

Check: $6N(N-1)(N-2)+6N(N-1)(N-2)(N-3)+N(N-1)(N-2)(N-3)(N-4)=$

$N(N-1)(N-2)(6+6N-18+N^2-7N+12)=N(N-1)(N-2)(N^2-N)=N^2(N-1)^2(N-2).$

H+K+L=0

$$\left(|E_H|^2-1\right)E_H E_K E_L = \frac{1}{N^{1/2}}\left(|E_H|^2-1\right)\left(|E_H|^2+|E_K|^2+|E_L|^2-2\right)$$

$$+\frac{N-2}{N^{3/2}}\left(|E_K|^2+|E_L|^2-2\right)$$

$$+\frac{N-3}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho}\exp 2\pi i\left(H\bullet r_\mu + K\bullet r_\nu + L\bullet r_\rho\right)$$

$$+\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho}\exp 2\pi i\left(H\bullet r_\mu - K\bullet r_\nu + (K-H)\bullet r_\rho\right)$$

$$+\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho}\exp 2\pi i\left(H\bullet r_\mu - L\bullet r_\nu + (L-H)\bullet r_\rho\right)$$

$$+\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho}\exp 2\pi i\left(2H\bullet r_\mu + K\bullet r_\nu + (L-H)\bullet r_\rho\right)$$

$$+\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho}\exp 2\pi i\left(2H\bullet r_\mu + L\bullet r_\nu + (K-H)- r_\rho\right)$$

$$+\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\exp 2\pi i\left(H\bullet (r_\mu - r_\nu) + K\bullet (r_\rho - r_\sigma)\right)$$

$$+\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\exp 2\pi i\left(H\bullet (r_\mu - r_\nu) + L\bullet (r_\rho - r_\sigma)\right)$$

$$+\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\exp 2\pi i\left(H\bullet (r_\mu + r_\nu) + K\bullet r_\rho + (L-H)\bullet r_\sigma\right)$$

$$+\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\exp 2\pi i\left(H\bullet (r_\mu + r_\nu) + L\bullet r_\rho + (K-H)\bullet r_\sigma\right)$$

$$+\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\exp 2\pi i\left(-H\bullet r_\mu+2H\bullet r_\nu+K\bullet r_\rho+L\bullet r_\sigma\right)$$

$$+\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho\neq\sigma\neq\tau}\exp 2\pi i\left(H\bullet(r_\mu-r_\nu)+H\bullet r_\rho+K\bullet r_\sigma+L\bullet r_\tau\right)$$

(18)

$$\left|E_H\right|^2-1=\frac{1}{N}\sum_{\mu\neq\nu}\exp 2\pi i H\bullet\left(r_\mu-r_\nu\right) \qquad N(N-1) \qquad (19)$$

$$\left|E_K\right|^2-1=\frac{1}{N}\sum_{\rho\neq\sigma}\exp 2\pi i K\bullet\left(r_\rho-r_\sigma\right) \qquad N(N-1) \qquad (20)$$

$$\left(\left|E_H\right|^2-1\right)\left(\left|E_K\right|^2-1\right)=\frac{1}{N^2}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\exp 2\pi i\left(H\bullet(r_\mu-r_\nu)+K\bullet(r_\rho-r_\sigma)\right) \quad N^2(N-1)^2 \quad (21)$$

$\mu=\rho$, $\nu=\sigma$

$$=\frac{1}{N^2}\sum_{\rho\neq\sigma}\exp 2\pi i\left((H+K)\bullet(r_\rho-r_\sigma)\right) \qquad N(N-1)$$

$\mu=\sigma$, $\nu=\rho$

$$+\frac{1}{N^2}\sum_{\rho\neq\sigma}\exp 2\pi i\left((H-K)\bullet(r_\sigma-r_\rho)\right) \qquad N(N-1)$$

$\mu=\rho$

$$+\frac{1}{N^2}\sum_{\rho\neq\nu\neq\sigma}\exp 2\pi i\left((H+K)\bullet r_\rho-H\bullet r_\nu-K\bullet r_\sigma\right) \qquad N(N-1)(N-2)$$

$\mu=\sigma$

$$+\frac{1}{N^2}\sum_{\sigma\neq\nu\neq\rho}\exp 2\pi i\left((H-K)\bullet r_\sigma-H\bullet r_\nu+K\bullet r_\rho\right) \qquad N(N-1)(N-2)$$

$\nu=\rho$

$$+\frac{1}{N^2}\sum_{\rho\neq\mu\neq\sigma}\exp 2\pi i\left((-H+K)\bullet r_\rho+H\bullet r_\mu-K\bullet r_\sigma\right) \qquad N(N-1)(N-2)$$

$\nu=\sigma$

$$+\frac{1}{N^2}\sum_{\sigma\neq\mu\neq\rho}\exp 2\pi i\left(-(H+K)\bullet r_\sigma+H\bullet r_\mu+K\bullet r_\rho\right) \qquad N(N-1)(N-2)$$

$$+\frac{1}{N^2}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\exp 2\pi i\big(H\bullet(r_\mu - r_\nu)+K\bullet(r_\rho - r_\sigma)\big) \qquad N(N-1)(N-2)(N-3)$$

(22)

Counting check: 2N(N-1)+4N(N-1)(N-2)+N(N-1)(N-2)(N-3)=

$N(N-1)(2+4N-8+N^2-5N+6)=N(N-1)(N^2-N)=N^2(N-1)^2$.

$$\left(|E_H|^2-1\right)\left(|E_K|^2-1\right)=\frac{1}{N}\left(|E_{H+K}|^2+|E_{H-K}|^2-2\right)$$

$$+\frac{1}{N^2}\sum_{\mu\neq\nu\neq\rho}\exp 2\pi i\big(-H\bullet r_\mu - K\bullet r_\nu + (H+K)\bullet r_\rho\big)$$

$$+\frac{1}{N^2}\sum_{\mu\neq\nu\neq\rho}\exp 2\pi i\big(-H\bullet r_\mu + K\bullet r_\nu + (H-K)\bullet r_\rho\big)$$

$$+\frac{1}{N^2}\sum_{\mu\neq\nu\neq\rho}\exp 2\pi i\big(H\bullet r_\mu - K\bullet r_\nu + (-H+K)\bullet r_\rho\big)$$

$$+\frac{1}{N^2}\sum_{\mu\neq\nu\neq\rho}\exp 2\pi i\big(H\bullet r_\mu + K\bullet r_\nu - (H+K)\bullet r_\rho\big)$$

$$+\frac{1}{N^2}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\exp 2\pi i\big(H\bullet(r_\mu - r_\nu)+K\bullet(r_\rho - r_\sigma)\big) \qquad (23)$$

$$\left(|E_H|^2 - 1\right)\left(|E_K|^2 - 1\right) = \frac{1}{N}\left(|E_{H+K}|^2 + |E_{H-K}|^2 - 2\right)$$

$$+ \frac{2}{N^2}\sum_{\mu \neq \nu \neq \rho} \cos 2\pi\left(H \bullet r_\mu + K \bullet r_\nu - (H+K) \bullet r_\rho\right)$$

$$+ \frac{2}{N^2}\sum_{\mu \neq \nu \neq \rho} \cos 2\pi\left(-H \bullet r_\mu + K \bullet r_\nu + (H-K) \bullet r_\rho\right)$$

$$+ \frac{1}{N^2}\sum_{\mu \neq \nu \neq \rho \neq \sigma} \cos 2\pi\left(H \bullet (r_\mu - r_\nu) + K \bullet (r_\rho - r_\sigma\right) \qquad (24)$$

H+K+L=0

Denote by S_3 summation over the three even permutations of H, K, L.

From (24)

$$\left(|E_H|^2-1\right)\left(|E_K|^2-1\right)+\left(|E_K|^2-1\right)\left(|E_L|^2-1\right)+\left(|E_L|^2-1\right)\left(|E_H|^2-1\right)=$$

$$\frac{1}{N}\left(|E_H|^2+|E_K|^2+|E_L|^2+|E_{H-K}|^2+|E_{K-L}|^2+|E_{L-H}|^2-6\right)$$

$$+\frac{6}{N^2}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(H\bullet r_\mu+K\bullet r_\nu+L\bullet r_\rho\right)$$

$$+S_3\bullet\frac{2}{N^2}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(-H\bullet r_\mu+K\bullet r_\nu+(H-K)\bullet r_\rho\right)$$

← N=3 cutoff

$$+S_3\bullet\frac{1}{N^2}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\cos 2\pi\left(H\bullet(r_\mu-r_\nu)+K\bullet(r_\rho-r_\sigma)\right) \qquad (25)$$

H+K+L=0

From (24)

$$\left(|E_H|^2-1\right)\left(|E_{K-L}|^2-1\right)=\frac{1}{N}\left(|E_{2L}|^2+|E_{2H}|^2-2\right)$$

$$+\frac{2}{N^2}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(H\bullet r_\mu+(K-L)\bullet r_\nu+2L\bullet r_\rho\right)$$

$$+\frac{2}{N^2}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(-H\bullet r_\mu+(K-L)\bullet r_\nu-2K\bullet r_\rho\right)$$

$$+\frac{1}{N^2}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\cos 2\pi\left(H\bullet(r_\mu-r_\nu)+(K-L)\bullet(r_\rho-r_\sigma)\right) \qquad (26)$$

H+K+L=0

$$\left(\left|E_H\right|^2-1\right)\left(\left|E_{K-L}\right|^2-1\right)+\left(\left|E_K\right|^2-1\right)\left(\left|E_{L-H}\right|^2-1\right)+\left(\left|E_L\right|^2-1\right)\left(\left|E_{H-K}\right|^2-1\right)=$$

$$\frac{2}{N}\left(\left|E_{2H}\right|^2+\left|E_{2K}\right|^2+\left|E_{2L}\right|^2-3\right)$$

$$+S_3\bullet\frac{2}{N^2}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(H\bullet r_\mu+(K-L)\bullet r_\nu+2L\bullet r_\rho\right)$$

$$+S_3\bullet\frac{2}{N^2}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(H\bullet r_\mu+(L-K)\bullet r_\rho+2K\bullet r_\rho\right)$$

← N=3 cutoff

$$+S_3\bullet\frac{1}{N^2}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\cos 2\pi\left(H\bullet(r_\mu-r_\nu)+(K-L)\bullet(r_\rho-r_\sigma)\right) \qquad (27)$$

H+K+L=0

Refer to (18).

$$\left(|E_H|^2+|E_K|^2+|E_L|^2-3\right)|E_H E_K E_L|\cos(\phi_H+\phi_K+\phi_L)=$$

$$\frac{1}{N^{1/2}}\left(|E_H|^2+|E_K|^2+|E_L|^2-3\right)\left(|E_H|^2+|E_K|^2+|E_L|^2-2\right)$$

$$+\frac{2(N-2)}{N^{3/2}}\left(|E_H|^2+|E_K|^2+|E_L|^2-3\right)$$

$$+\frac{3(N-3)}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(H\bullet r_\mu+K\bullet r_\nu+L\bullet r_\rho\right)$$

$$+S_3\bullet\frac{2}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(H\bullet r_\mu-K\bullet r_\nu+(K-H)\bullet r_\rho\right)$$

$$+S_3\bullet\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(H\bullet r_\mu+2L\bullet r_\nu+(K-L)\bullet r_\rho\right)$$

$$+S_3\bullet\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(H\bullet r_\mu+2K\bullet r_\nu+(L-K)\bullet r_\rho\right)$$

← N=3 cutoff

$$+S_3\bullet\frac{2}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\cos 2\pi\left(H\bullet(r_\mu-r_\nu)+K\bullet(r_\rho-r_\sigma)\right)$$

$$+S_3\bullet\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\cos 2\pi\left(H\bullet(r_\mu+r_\nu)+K\bullet r_\rho+(L-H)\bullet r_\sigma\right)$$

$$+S_3\bullet\frac{1}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho\neq\sigma}\cos 2\pi\left(H\bullet(r_\mu+r_\nu)+L\bullet r_\rho+(K-H)\bullet r_\sigma\right)$$

$$+S_3 \bullet \frac{1}{N^{5/2}} \sum_{\mu \neq \nu \neq \rho \neq \sigma} \cos 2\pi\left(-H \bullet r_\mu + 2H \bullet r_\nu + K \bullet r_\rho + L \bullet r_\sigma\right)$$

$\leftarrow$ N=4 cutoff

$$+S_3 \bullet \frac{1}{N^{5/2}} \sum_{\mu \neq \nu \neq \rho \neq \sigma \neq \tau} \cos 2\pi\left(H \bullet (r_\mu - r_\nu) + H \bullet r_\rho + K \bullet r_\sigma + L \bullet r_\tau\right) \qquad (28)$$

N=1, 2, or 3

H+K+L=0

$$2\times(28)-\frac{1}{N^{1/2}}\times(27)-\frac{2}{N^{1/2}}(25):$$

$$2\left(|E_H|^2+|E_K|^2+|E_L|^2-3\right)|E_H E_K E_L|\cos(\phi_H+\phi_K+\phi_L)$$

$$-\frac{1}{N^{1/2}}\left\{\left(|E_H|^2-1\right)\left(|E_{K-L}|^2-1\right)+\left(|E_K|^2-1\right)\left(|E_{L-H}|^2-1\right)+\left(|E_L|^2-1\right)\left(|E_{H-K}|^2-1\right)\right\}$$

$$-\frac{2}{N^{1/2}}\left\{\left(|E_H|^2-1\right)\left(|E_K|^2-1\right)+\left(|E_K|^2-1\right)\left(|E_L|^2-1\right)+\left(|E_L|^2-1\right)\left(|E_{H-K}|^2-1\right)\right\}=$$

$$\frac{2}{N^{1/2}}\left(|E_H|^2+|E_K|^2+|E_L|^2-3\right)\left(|E_H|^2+|E_K|^2+|E_L|^2-2\right)$$

$$+\frac{4(N-2)}{N^{3/2}}\left(|E_H|^2+|E_K|^2+|E_L|^2-3\right)$$

$$+\frac{6(N-3)}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(H\bullet r_\mu+K\bullet r_\nu+L\bullet r_\rho\right)$$

$$-\frac{2}{N^{3/2}}\left(|E_{2H}|^2+|E_{2K}|^2+|E_{2L}|^2-3\right)$$

$$-\frac{2}{N^{3/2}}\left(|E_H|^2+|E_K|^2+|E_L|^2+|E_{H-K}|^2+|E_{K-L}|^2+|E_{L-H}|^2-6\right)$$

$$-\frac{12}{N^{5/2}}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(H\bullet r_\mu+K\bullet r_\nu+L\bullet r_\rho\right) \quad (29)$$

H+K+L=0

Refer to (12) to infer

$$\frac{1}{N^{3/2}}\sum_{\mu\neq\nu\neq\rho}\cos 2\pi\left(H\bullet r_\mu + K\bullet r_\nu + L\bullet_\rho\right)=$$

$$\left|E_H E_K E_L\right|\cos\left(\phi_H+\phi_K+\phi_L\right)-\frac{1}{N^{1/2}}\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2-2\right) \qquad (30)$$

N=3

H+K+L=0

Substitute from (30) into (29):

$$\left\{2\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2-3\right)+4\right\}\left|E_H E_K E_L\right|\cos\left(\phi_H+\phi_K+\phi_L\right)=$$

$$+\frac{4}{\sqrt{3}}\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2-2\right)$$

$$+\frac{1}{\sqrt{3}}\left\{\left(\left|E_H\right|^2-1\right)\left(\left|E_{K-L}\right|^2-1\right)+\left(\left|E_K\right|^2-1\right)\left(\left|E_{L-H}\right|^2-1\right)+\left(\left|E_L\right|^2-1\right)\left(\left|E_{H-K}\right|^2-1\right)\right\}$$

$$+\frac{2}{\sqrt{3}}\left\{\left(\left|E_H\right|^2-1\right)\left(\left|E_K\right|^2-1\right)+\left(\left|E_K\right|^2-1\right)\left(\left|E_L\right|^2-1\right)+\left(\left|E_L\right|^2-1\right)\left(\left|E_H\right|^2-1\right)\right\}$$

$$+\frac{2}{\sqrt{3}}\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2-3\right)\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2-2\right)$$

$$+\frac{4}{3\sqrt{3}}\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2-3\right)$$

$$-\frac{2}{3\sqrt{3}}\left(\left|E_{2H}\right|^2+\left|E_{2K}\right|^2+\left|E_{2L}\right|^2-3\right)$$

$$-\frac{2}{3\sqrt{3}}\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2+\left|E_{H-K}\right|^2+\left|E_{K-L}\right|^2+\left|E_{L-H}\right|^2-6\right) \qquad (31)$$

N=3

H+K+L=0

or, finally,

$$
\begin{aligned}
&6\sqrt{3}\left(|E_H|^2+|E_K|^2+|E_L|^2-1\right)|E_H E_K E_L|\cos(\phi_H+\phi_K+\phi_L)= \\
&6\left(|E_H|^4+|E_K|^4+|E_L|^4\right) \\
&+18\left(|E_H E_K|^2+|E_K E_L|^2+|E_L E_H|^2\right) \\
&+3\left(|E_H E_{K-L}|^2+|E_K E_{L-H}|^2+|E_L E_{H-K}|^2\right) \\
&-31\left(|E_H|^2+|E_K|^2+|E_L|^2\right) \\
&-2\left(|E_{2H}|^2+|E_{2K}|^2+|E_{2L}|^2\right) \\
&-5\left(|E_{H-K}|^2+|E_{K-L}|^2+|E_{L-H}|^2\right) \qquad (32) \\
&+45
\end{aligned}
$$

$$H + K + L = 0, \qquad N = 3$$

$\text{Cos}(\phi_H + \phi_K + \phi_L)$ is the Root of a Linear Equation with Coefficients that are Polynomials in Nine Magnitudes |E|.

N=3, H+K+L=0

In general

$$E_H = \frac{1}{\sqrt{N}} \sum_{\mu=1}^{N} \exp 2\pi i H \bullet r_\mu$$

$$E_H = |E_H| \exp i\phi_H$$

$$\sum_{\mu<\nu}^{3} \cos 2\pi H \bullet (r_\mu - r_\nu) = \frac{3}{2}\left(|E_H|^2 - 1\right)$$

Proof:

$$E_H = \frac{1}{\sqrt{3}} \sum_{\mu=1}^{3} \exp 2\pi i H \bullet r_\mu$$

$$E_H^* = \frac{1}{\sqrt{3}} \sum_{\nu=1}^{3} \exp - 2\pi i H \bullet r_\nu$$

$$|E_H|^2 = \frac{1}{3} \sum_{\mu,\nu \atop 1}^{3} \exp 2\pi i H \bullet (r_\mu - r_\nu)$$

$$= \frac{1}{3}\left\{3 + \sum_{\mu,\nu \atop 1}^{3} \cos 2\pi H \bullet (r_\mu - r_\nu)\right\}$$

$$|E_H|^2 - 1 = \frac{2}{3} \sum_{\mu<\nu \atop 1}^{3} \cos 2\pi H \bullet (r_\mu - r_\nu)$$

I.A. The General Case

$$\sum_{\substack{\mu<\nu \\ 1}}^{N} \cos 2\pi \mathbf{H} \bullet (\mathbf{r}_\mu - \mathbf{r}_\nu) = \frac{N}{2}\left(|E_H|^2 - 1\right) \qquad \tfrac{1}{2}N(N-1) \text{ terms}$$

H+K+L=0

II.

$$\sum_{\substack{\mu\neq\nu\neq\rho \\ 1}}^{N} \cos 2\pi(\mathbf{H}\bullet \mathbf{r}_\mu + \mathbf{K}\bullet \mathbf{r}_\nu + \mathbf{L}\bullet \mathbf{r}_\rho) =$$

$$N\sqrt{N}|E_H E_K E_L|\cos(\phi_H + \phi_K + \phi_L) - N\left(|E_H|^2 + |E_K|^2 + |E_L|^2 - 2\right)$$

$$\sum_{\substack{\mu\neq\nu\neq\rho \\ 1}}^{N} \sin 2\pi(\mathbf{H}\bullet \mathbf{r}_\mu + \mathbf{K}\bullet \mathbf{r}_\nu + \mathbf{L}\bullet \mathbf{r}_\rho) = N\sqrt{N}|E_H E_K E_L|\sin(\phi_H + \phi_K + \phi_L)$$

N(N-1)(N-2) terms

II.A. The Case N=3

$$\cos 2\pi(\mathbf{H}\bullet \mathbf{r}_1 + \mathbf{K}\bullet \mathbf{r}_2 + \mathbf{L}\bullet \mathbf{r}_3) + \cos 2\pi(\mathbf{H}\bullet \mathbf{r}_1 + \mathbf{K}\bullet \mathbf{r}_3 + \mathbf{L}\bullet \mathbf{r}_2) + \cos 2\pi(\mathbf{H}\bullet \mathbf{r}_2 + \mathbf{K}\bullet \mathbf{r}_1 + \mathbf{L}\bullet \mathbf{r}_3)$$
$$+ \cos 2\pi(\mathbf{H}\bullet \mathbf{r}_2 + \mathbf{K}\bullet \mathbf{r}_3 + \mathbf{L}\bullet \mathbf{r}_1) + \cos 2\pi(\mathbf{H}\bullet \mathbf{r}_3 + \mathbf{K}\bullet \mathbf{r}_1 + \mathbf{L}\bullet \mathbf{r}_2) + \cos 2\pi(\mathbf{H}\bullet \mathbf{r}_3 + \mathbf{K}\bullet \mathbf{r}_2 + \mathbf{L}\bullet \mathbf{r}_1) =$$
$$3\sqrt{3}|E_H E_K E_L|\cos(\phi_H + \phi_K + \phi_L) - 3\left(|E_H|^2 + |E_K|^2 + |E_L|^2 - 2\right)$$

$$\sin 2\pi(\mathbf{H}\bullet \mathbf{r}_1 + \mathbf{K}\bullet \mathbf{r}_2 + \mathbf{L}\bullet \mathbf{r}_3) + \sin 2\pi(\mathbf{H}\bullet \mathbf{r}_1 + \mathbf{K}\bullet \mathbf{r}_3 + \mathbf{L}\bullet \mathbf{r}_2) + \sin 2\pi(\mathbf{H}\bullet \mathbf{r}_2 + \mathbf{K}\bullet \mathbf{r}_1 + \mathbf{L}\bullet \mathbf{r}_3)$$
$$+ \sin 2\pi(\mathbf{H}\bullet \mathbf{r}_2 + \mathbf{K}\bullet \mathbf{r}_3 + \mathbf{L}\bullet \mathbf{r}_1) + \sin 2\pi(\mathbf{H}\bullet \mathbf{r}_3 + \mathbf{K}\bullet \mathbf{r}_1 + \mathbf{L}\bullet \mathbf{r}_2) + \sin 2\pi(\mathbf{H}\bullet \mathbf{r}_3 + \mathbf{K}\bullet \mathbf{r}_2 + \mathbf{L}\bullet \mathbf{r}_1) =$$
$$3\sqrt{3}|E_H E_K E_L|\sin(\phi_H + \phi_K + \phi_L).$$

N=3, H+K+L=0

III.

$$|E_H E_K E_{H-K}|\cos(\phi_{-H} + \phi_K + \phi_{H-K}) = -|E_H E_K E_L|\cos(\phi_H + \phi_K + \phi_L)$$

$$+\frac{\sqrt{3}}{6}\left(3|E_H E_K|^2 + |E_H|^2 + |E_K|^2 + |E_L|^2 + |E_{H-K}|^2 - 3\right)$$

$$|E_K E_L E_{K-L}|\cos(\phi_{-K} + \phi_L + \phi_{K-L}) = -|E_H E_K E_L|\cos(\phi_H + \phi_K + \phi_L)$$

$$+\frac{\sqrt{3}}{6}\left(3|E_K E_L|^2 + |E_H|^2 + |E_K|^2 + |E_L|^2 + |E_{K-L}|^2 - 3\right)$$

$$|E_L E_H E_{L-H}|\cos(\phi_{-L} + \phi_H + \phi_{L-H}) = -|E_H E_K E_L|\cos(\phi_H + \phi_K + \phi_L)$$

$$+\frac{\sqrt{3}}{6}\left(3|E_L E_H|^2 + |E_H|^2 + |E_K|^2 + |E_L|^2 + |E_{L-H}|^2 - 3\right)$$

Proof: $$\frac{3}{2}\left(|E_H|^2-1\right)=\cos 2\pi H\bullet(r_1-r_2)+\cos 2\pi H\bullet(r_1-r_3)+\cos 2\pi H\bullet(r_2-r_3) \qquad \text{(I)}$$

$$\frac{3}{2}\left(|E_K|^2-1\right)=\cos 2\pi K\bullet(r_1-r_2)+\cos 2\pi K\bullet(r_1-r_3)+\cos 2\pi K\bullet(r_2-r_3) \qquad \text{(I)}$$

$$\frac{9}{4}\left(|E_H|^2-1\right)\left(|E_K|^2-1\right)=\frac{1}{2}\cos 2\pi L\bullet(r_1-r_2)+\ldots \quad 3\ \text{terms}$$

$$+\frac{1}{2}\cos 2\pi(H-K)\bullet(r_1-r_2)+\ldots \quad 3\ \text{terms}$$

$$+\frac{1}{2}\cos 2\pi\left(H\bullet r_1+K\bullet r_2+L\bullet r_3\right)+\ldots \quad 6\ \text{terms}$$

$$+\frac{1}{2}\cos 2\pi\left(-H\bullet r_1+K\bullet r_2+(H-K)\bullet r_3\right)+\ldots \quad 6\ \text{terms}$$

$$=\frac{3}{4}\left(|E_L|^2-1\right)+\frac{3}{4}\left(|E_{H-K}|^2-1\right) \qquad \text{(I)}$$

$$+\frac{3\sqrt{3}}{2}|E_HE_KE_L|\cos(\phi_H+\phi_K+\phi_L)-\frac{3}{2}\left(|E_H|^2+|E_K|^2+|E_L|^2-2\right) \qquad \text{(II)}$$

$$+\frac{3\sqrt{3}}{2}|E_HE_KE_{H-K}|\cos(\phi_{-H}+\phi_K+\phi_{H-K})-\frac{3}{2}\left(|E_H|^2+|E_K|^2+|E_{H-K}|^2-2\right) \qquad \text{(II)}$$

Simplify.

N=3, H+K+L=0

IV.

$$\left|E_{H-K}E_{K-L}E_{L-H}\right|\cos\left(\phi_{H-K}+\phi_{K-L}+\phi_{L-H}\right)=$$

$$-3\left|E_H E_K E_L\right|\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2-2\right)\cos\left(\phi_H+\phi_K+\phi_L\right)+$$

$$\frac{\sqrt{3}}{6}\left\{9\left|E_H E_K E_L\right|^2+3\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2\right)^2-12\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2\right)\right.$$

$$\left.+\left(\left|E_{H-K}\right|^2+\left|E_{K-L}\right|^2+\left|E_{L-H}\right|^2\right)+9\right\}$$

Proof: From II.

$$3\sqrt{3}|E_H E_K E_L|\cos(\phi_H + \phi_K + \phi_L) - 3\left(|E_H|^2 + |E_K|^2 + |E_L|^2 - 2\right) = \cos 2\pi(H \bullet r_1 + K \bullet r_2 + L \bullet r_3) + \ldots 6 \text{ terms}$$

$$3\sqrt{3}|E_H E_K E_L|\sin(\phi_H + \phi_K + \phi_L) = \sin 2\pi(H \bullet r_1 + K \bullet r_2 + L \bullet r_3) + \ldots 6 \text{ terms}$$

Square and add

$$27|E_H E_K E_L|^2 - 18\sqrt{3}|E_H E_K E_L|\left(|E_H|^2 + |E_K|^2 + |E_L|^2 - 2\right)\cos(\phi_H + \phi_K + \phi_L) +$$

$$9\left(|E_H|^2 + |E_K|^2 + |E_L|^2 - 2\right)^2 = 6 + 2\{\cos 2\pi(H - K) \bullet (r_1 - r_2) + \ldots 3 \text{ terms}\} +$$

$$2\{\cos 2\pi(K - L) \bullet (r_1 - r_2) + \ldots 3 \text{ terms}\} + 2\{\cos 2\pi(L - H) \bullet (r_1 - r_2) + \ldots 3 \text{ terms}\}$$

$$+2\{\cos 2\pi((H - K) \bullet r_1 + (K - L) \bullet r_2 + (L - H) \bullet r_3) + \ldots 6 \text{ terms}\} =$$

$$6 + 3\left(|E_{H-K}|^2 - 1\right) + 3\left(|E_{K-L}|^2 - 1\right) + 3\left(|E_{L-H}|^2 - 1\right) + 6\sqrt{3}|E_{H-K} E_{K-L} E_{L-H}|\cos(\phi_{H-K} + \phi_{K-L} + \phi_{L-H})$$

$$-6\left(|E_{H-K}|^2 + |E_{K-L}|^2 + |E_{L-H}|^2 - 2\right) \qquad \text{I. \& II.}$$

$$6\sqrt{3}|E_{H-K} E_{K-L} E_{L-H}|\cos(\phi_{H-K} + \phi_{K-L} + \phi_{L-H}) = -18\sqrt{3}|E_H E_K E_L|\left(|E_H|^2 + |E_K|^2 + |E_L|^2 - 2\right) \times$$

$$\cos(\phi_H + \phi_K + \phi_L) + 27|E_H E_K E_L|^2 + 9\left(|E_H|^2 + |E_K|^2 + |E_L|^2\right)^2 - 36\left(|E_H|^2 + |E_K|^2 + |E_L|^2\right) + 36 - 9$$

$$+3\left(|E_{H-K}|^2 + |E_{K-L}|^2 + |E_{L-H}|^2\right)$$

Simplify.

N=3

V.

$$\left|E_H{}^2 E_{2H}\right|\cos(2\phi_H - \phi_{2H}) = \frac{\sqrt{3}}{6}\left(3\left|E_H\right|^4 - 4\left|E_H\right|^2 + \left|E_{2H}\right|^2\right)$$

Substitute $K = -H,\ \ L = 0,\ \ E_0 = \sqrt{3},\ \ \phi_0 = 0$ in III.

$$\left|E_H{}^2 E_{2H}\right|\cos(2\phi_H - \phi_{2H}) = -\sqrt{3}\left|E_H\right|^2 + \frac{\sqrt{3}}{6}\left(3\left|E_H\right|^4 + 2\left|E_H\right|^2 + 3 + \left|E_{2H}\right|^2 - 3\right)$$

$$= \frac{\sqrt{3}}{6}\left(3\left|E_H\right|^4 - 4\left|E_H\right|^2 + \left|E_{2H}\right|^2\right)3$$

N=3, H+K+L=0

VI.

$$|E_H E_K E_L|\left(|E_H|^2+|E_K|^2+|E_L|^2-1\right)\cos(\phi_H+\phi_K+\phi_L)=$$

$$\frac{\sqrt{3}}{18}\Big\{6\left(|E_H|^4+|E_K|^4+|E_L|^4\right)+18\left(|E_H E_K|^2+|E_K E_L|^2+|E_L E_H|^2\right)$$

$$+3\left(|E_H E_{K-L}|^2+|E_K E_{L-H}|^2+|E_L E_{H-K}|^2\right)$$

$$-31\left(|E_H|^2+|E_K|^2+|E_L|^2\right)-2\left(|E_{2H}|^2+|E_{2K}|^2+|E_{2L}|^2\right)$$

$$-5\left(|E_{H-K}|^2+|E_{K-L}|^2+|E_{L-H}|^2\right)+45\Big\}$$

Proof:

$$\frac{3}{2}\left(|E_H|^2-1\right)=\cos 2\pi H\bullet(r_1-r_2)+\cos 2\pi H\bullet(r_1-r_3)+\cos 2\pi H\bullet(r_2-r_3)$$

$$\frac{3}{2}\left(|E_K|^2-1\right)=\cos 2\pi K\bullet(r_1-r_2)+\cos 2\pi K\bullet(r_1-r_3)+\cos 2\pi K\bullet(r_2-r_3)$$

$$\frac{3}{2}\left(|E_L|^2-1\right)=\cos 2\pi L\bullet(r_1-r_2)+\cos 2\pi L\bullet(r_1-r_3)+\cos 2\pi L\bullet(r_2-r_3)$$

$$\frac{27}{8}\left(|E_H|^2-1\right)\left(|E_K|^2-1\right)\left(|E_L|^2-1\right)=$$

N=3, H+K+L=0

In the following $+ \ldots + \circlearrowright\circlearrowleft 6$ means the 6 permutations of r_1, r_2, r_3;

$+ \ldots + \circlearrowright 3$ means the 3 even permutations of H, K, L

$$\cos 2\pi H \bullet (r_1 - r_2) \cos 2\pi K \bullet (r_1 - r_2) \cos 2\pi L \bullet (r_1 - r_2) +$$

$$\cos 2\pi H \bullet (r_1 - r_3) \cos 2\pi K \bullet (r_1 - r_3) \cos 2\pi L \bullet (r_1 - r_3) +$$

$$\cos 2\pi H \bullet (r_2 - r_3) \cos 2\pi K \bullet (r_2 - r_3) \cos 2\pi L \bullet (r_2 - r_3) +$$

$$\left\{\cos 2\pi H \bullet (r_1 - r_2) \cos 2\pi K \bullet (r_1 - r_2) \cos 2\pi L \bullet (r_1 - r_3) + \ldots + \circlearrowright\circlearrowleft 6\right\} +$$

$$\left\{\cos 2\pi K \bullet (r_1 - r_2) \cos 2\pi L \bullet (r_1 - r_2) \cos 2\pi H \bullet (r_1 - r_3) + \ldots + \circlearrowright\circlearrowleft 6\right\} +$$

$$\left\{\cos 2\pi L \bullet (r_1 - r_2) \cos 2\pi H \bullet (r_1 - r_2) \cos 2\pi K \bullet (r_1 - r_3) + \ldots + \circlearrowright\circlearrowleft 6\right\} +$$

$$\cos 2\pi H \bullet (r_1 - r_2) \cos 2\pi K \bullet (r_1 - r_3) \cos 2\pi L \bullet (r_2 - r_3) + \ldots + \circlearrowright\circlearrowleft 6 =$$

$$\frac{3}{4} + \frac{1}{4}\left\{\cos 4\pi H \bullet (r_1 - r_2) + \ldots + \circlearrowright 3\right\} +$$

$$\frac{1}{4}\left\{\cos 4\pi H \bullet (r_1 - r_3) + \ldots + \circlearrowright 3\right\} +$$

$$\frac{1}{4}\left\{\cos 4\pi H \bullet (r_2 - r_3) + \ldots + \circlearrowright 3\right\} +$$

$$\frac{2}{4}\left\{\cos 2\pi H \bullet (r_1 - r_2) + ... + \circlearrowright 3\right\} +$$

$$\frac{2}{4}\left\{\cos 2\pi H \bullet (r_1 - r_3) + ... + \circlearrowright 3\right\} +$$

$$\frac{2}{4}\left\{\cos 2\pi H \bullet (r_2 - r_3) + ... + \circlearrowright 3\right\} +$$

$$+\frac{1}{4}\left\{\left(\cos 2\pi\left(2H \bullet r_1 - H \bullet r_2 - H \bullet r_3\right) + ... + \circlearrowright 3\right) + ... + \circlearrowright\circlearrowleft 6\right\} +$$

$$+\frac{1}{4}\left\{\left(\cos 2\pi\left(H \bullet r_1 + (K - L) \bullet r_2 + 2L \bullet r_3\right) + ... + \circlearrowright 3\right) + ... + \circlearrowright\circlearrowleft 6\right\} +$$

$$+\frac{1}{4}\left\{\left(\cos 2\pi\left(-H \bullet r_1 + (K - L) \bullet r_2 - 2K \bullet r_3\right) + ... + \circlearrowright 3\right) + ... + \circlearrowright\circlearrowleft 6\right\} +$$

$$+\frac{1}{4}\left\{\left(\cos 2\pi\left(-H \bullet r_1 + K \bullet r_2 + (H - K) \bullet r_3\right) + ... + \circlearrowright 3\right) + ... + \circlearrowright\circlearrowleft 6\right\} +$$

$$+\frac{1}{4}\left\{\cos 2\pi\left((H - K) \bullet r_1 + (K - L) \bullet r_2 + (L - H) \bullet r_3\right) + ... + \circlearrowright\circlearrowleft 6\right\}$$

N=3, H+K+L=0

$$9\left(|E_H|^2-1\right)\left(|E_K|^2-1\right)\left(|E_L|^2-1\right)=$$

$$2+\left(|E_{2H}|^2+|E_{2K}|^2+|E_{2L}|^2-3\right)+2\left(|E_H|^2+|E_K|^2+|E_L|^2-3\right)$$

$$+2\sqrt{3}\left|E_H{}^2E_{2H}\right|\cos\left(2\phi_H-\phi_{2H}\right)-2\left(2|E_H|^2+|E_{2H}|^2-2\right)$$

$$+2\sqrt{3}\left|E_K{}^2E_{2K}\right|\cos\left(2\phi_K-\phi_{2K}\right)-2\left(2|E_K|^2+|E_{2K}|^2-2\right)$$

$$+2\sqrt{3}\left|E_L{}^2E_{2L}\right|\cos\left(2\phi_L-\phi_{2L}\right)-2\left(2|E_L|^2+|E_{2L}|^2-2\right)$$

$$+2\sqrt{3}\left|E_HE_{K-L}E_{2L}\right|\cos\left(\phi_H+\phi_{K-L}+\phi_{2L}\right)-2\left(|E_H|^2+|E_{K-L}|^2+|E_{2L}|^2-2\right)$$

$$+2\sqrt{3}\left|E_KE_{L-H}E_{2H}\right|\cos\left(\phi_K+\phi_{L-H}+\phi_{2H}\right)-2\left(|E_K|^2+|E_{L-H}|^2+|E_{2H}|^2-2\right)$$

$$+2\sqrt{3}\left|E_LE_{H-K}E_{2K}\right|\cos\left(\phi_L+\phi_{H-K}+\phi_{2K}\right)-2\left(|E_L|^2+|E_{H-K}|^2+|E_{2K}|^2-2\right)$$

$$+2\sqrt{3}\left|E_HE_{K-L}E_{2K}\right|\cos\left(\phi_{-H}+\phi_{K-L}+\phi_{2K}\right)-2\left(|E_H|^2+|E_{K-L}|^2+|E_{2K}|^2-2\right)$$

$$+2\sqrt{3}\left|E_KE_{L-H}E_{2L}\right|\cos\left(\phi_{-K}+\phi_{L-H}+\phi_{2L}\right)-2\left(|E_K|^2+|E_{L-H}|^2+|E_{2L}|^2-2\right)$$

$$+2\sqrt{3}\left|E_LE_{H-K}E_{2H}\right|\cos\left(\phi_{-L}+\phi_{H-K}+\phi_{2H}\right)-2\left(|E_L|^2+|E_{H-K}|^2+|E_{2H}|^2-2\right)$$

$$+2\sqrt{3}\left|E_H E_K E_{H-K}\right|\cos\left(\phi_{-H}+\phi_K+\phi_{H-K}\right)-2\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_{H-K}\right|^2-2\right)$$

$$+2\sqrt{3}\left|E_K E_L E_{K-L}\right|\cos\left(\phi_{-K}+\phi_L+\phi_{K-L}\right)-2\left(\left|E_K\right|^2+\left|E_L\right|^2+\left|E_{K-L}\right|^2-2\right)$$

$$+2\sqrt{3}\left|E_L E_H E_{L-H}\right|\cos\left(\phi_{-L}+\phi_H+\phi_{L-H}\right)-2\left(\left|E_L\right|^2+\left|E_H\right|^2+\left|E_{L-H}\right|^2-2\right)$$

$$+2\sqrt{3}\left|E_{H-K} E_{K-L} E_{L-H}\right|\cos\left(\phi_{H-K}+\phi_{K-L}+\phi_{L-H}\right)-2\left(\left|E_{H-K}\right|^2+\left|E_{K-L}\right|^2+\left|E_{L-H}\right|^2-2\right)$$

N=3, H+K+L=0

$$9\left(|E_H|^2-1\right)\left(|E_K|^2-1\right)\left(|E_L|^2-1\right)=$$

$$2+\left(|E_{2H}|^2+|E_{2K}|^2+|E_{2L}|^2-3\right)+2\left(|E_H|^2+|E_K|^2+|E_L|^2-3\right)$$

$$+\left(3|E_H|^4-4|E_H|^2+|E_{2H}|^2\right)-2\left(2|E_H|^2+|E_{2H}|^2-2\right)$$

$$+\left(3|E_K|^4-4|E_K|^2+|E_{2K}|^2\right)-2\left(2|E_K|^2+|E_{2K}|^2-2\right)$$

$$+\left(3|E_L|^4-4|E_L|^2+|E_{2L}|^2\right)-2\left(2|E_L|^2+|E_{2L}|^2-2\right)$$

$$+\left(3|E_H E_{K-L}|^2+|E_H|^2+|E_{K-L}|^2+|E_{2L}|^2+|E_{2K}|^2-3\right)$$

$$-2\left(2|E_H|^2+2|E_{K-L}|^2+|E_{2K}|^2+|E_{2L}|^2-4\right)$$

$$+\left(3|E_K E_{L-H}|^2+|E_K|^2+|E_{L-H}|^2+|E_{2H}|^2+|E_{2L}|^2-3\right)$$

$$-2\left(2|E_K|^2+2|E_{L-H}|^2+|E_{2L}|^2+|E_{2H}|^2-4\right)$$

$$+\left(3|E_L E_{H-K}|^2+|E_L|^2+|E_{H-K}|^2+|E_{2K}|^2+|E_{2H}|^2-3\right)$$

$$-2\left(2|E_L|^2+2|E_{H-K}|^2+|E_{2H}|^2+|E_{2K}|^2-4\right)$$

$$-2\sqrt{3}|E_H E_K E_L|\cos(\phi_H + \phi_K + \phi_L) + \left(3|E_H E_K|^2 + |E_H|^2 + |E_K|^2 + |E_L|^2 + |E_{H-K}|^2 - 3\right)$$

$$-2\left(|E_H|^2 + |E_K|^2 + |E_{H-K}|^2 - 2\right)$$

$$-2\sqrt{3}|E_H E_K E_L|\cos(\phi_H + \phi_K + \phi_L) + \left(3|E_K E_L|^2 + |E_H|^2 + |E_K|^2 + |E_L|^2 + |E_{K-L}|^2 - 3\right)$$

$$-2\left(|E_K|^2 + |E_L|^2 + |E_{K-L}|^2 - 2\right)$$

$$-2\sqrt{3}|E_H E_K E_L|\cos(\phi_H + \phi_K + \phi_L) + \left(3|E_L E_H|^2 + |E_H|^2 + |E_K|^2 + |E_L|^2 + |E_{L-H}|^2 - 3\right)$$

$$-2\left(|E_L|^2 + |E_H|^2 + |E_{L-H}|^2 - 2\right)$$

$$-6\sqrt{3}|E_H E_K E_L|\left(|E_H|^2 + |E_K|^2 + |E_L|^2 - 2\right)\cos(\phi_H + \phi_K + \phi_L) + 9|E_H E_K E_L|^2$$

$$+3\left(|E_H|^2 + |E_K|^2 + |E_L|^2\right)^2 - 12\left(|E_H|^2 + |E_K|^2 + |E_L|^2\right) + \left(|E_{H-K}|^2 + |E_{K-L}|^2 + |E_{L-H}|^2\right)$$

$$+9 - 2\left(|E_{H-K}|^2 + |E_{K-L}|^2 + |E_{L-H}|^2 - 2\right)$$

N=3, H+K+L=0

$$6\sqrt{3}\left|E_H E_K E_L\right|\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2-1\right)\cos\left(\phi_H+\phi_K+\phi_L\right)=$$

$$-9\left|E_H E_K E_L\right|^2+9\left(\left|E_H E_K\right|^2+\left|E_K E_L\right|^2+\left|E_L E_H\right|^2-\left|E_H\right|^2-\left|E_K\right|^2-\left|E_L\right|^2+1\right)$$

$$+2+\left(\left|E_{2H}\right|^2+\left|E_{2K}\right|^2+\left|E_{2L}\right|^2\right)-3+2\left(\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2\right)-6$$

$$+3\left|E_H\right|^4-4\left|E_H\right|^2+\left|E_{2H}\right|^2-4\left|E_H\right|^2-2\left|E_{2H}\right|^2+4$$

$$+3\left|E_K\right|^4-4\left|E_K\right|^2+\left|E_{2K}\right|^2-4\left|E_K\right|^2-2\left|E_{2K}\right|^2+4$$

$$+3\left|E_L\right|^4-4\left|E_L\right|^2+\left|E_{2L}\right|^2-4\left|E_L\right|^2-2\left|E_{2L}\right|^2+4$$

$$+3\left|E_H E_{K-L}\right|^2+\left|E_H\right|^2+\left|E_{K-L}\right|^2+\left|E_{2L}\right|^2+\left|E_{2K}\right|^2-3-4\left|E_H\right|^2$$

$$-4\left|E_{K-L}\right|^2-2\left|E_{2K}\right|^2-2\left|E_{2L}\right|^2+8$$

$$+3\left|E_K E_{L-H}\right|^2+\left|E_K\right|^2+\left|E_{L-H}\right|^2+\left|E_{2H}\right|^2+\left|E_{2L}\right|^2-3-4\left|E_K\right|^2$$

$$-4\left|E_{L-H}\right|^2-2\left|E_{2L}\right|^2-2\left|E_{2H}\right|^2+8$$

$$+3\left|E_L E_{H-K}\right|^2+\left|E_L\right|^2+\left|E_{H-K}\right|^2+\left|E_{2K}\right|^2+\left|E_{2H}\right|^2-3-4\left|E_L\right|^2$$

$$-4\left|E_{H-K}\right|^2-2\left|E_{2H}\right|^2-2\left|E_{2K}\right|^2+8$$

$$+3\left|E_H E_K\right|^2+\left|E_H\right|^2+\left|E_K\right|^2+\left|E_L\right|^2+\left|E_{H-K}\right|^2-3-2\left|E_H\right|^2-2\left|E_K\right|^2-2\left|E_{H-K}\right|^2+4$$

$$+3\left|E_K E_L\right|^2 + \left|E_H\right|^2 + \left|E_K\right|^2 + \left|E_L\right|^2 + \left|E_{K-L}\right|^2 - 3 - 2\left|E_K\right|^2 - 2\left|E_L\right|^2 - 2\left|E_{K-L}\right|^2 + 4$$

$$+3\left|E_L E_H\right|^2 + \left|E_H\right|^2 + \left|E_K\right|^2 + \left|E_L\right|^2 + \left|E_{L-H}\right|^2 - 3 - 2\left|E_L\right|^2 - 2\left|E_H\right|^2 - 2\left|E_{L-H}\right|^2 + 4$$

$$+9\left|E_H E_K E_L\right|^2 + 3\left(\left|E_H\right|^4 + \left|E_K\right|^4 + \left|E_L\right|^4 + 2\left|E_H E_K\right|^2 + 2\left|E_K E_L\right|^2 + \left|E_L E_H\right|^2\right)$$

$$-12\left(\left|E_H\right|^2 + \left|E_K\right|^2 + \left|E_L\right|^2\right) + \left(\left|E_{H-K}\right|^2 + \left|E_{K-L}\right|^2 + \left|E_{L-H}\right|^2\right) + 9$$

$$-2\left(\left|E_{H-K}\right|^2 + \left|E_{K-L}\right|^2 + \left|E_{L-H}\right|^2\right)$$

N=3, H+K+L=0

$$6\sqrt{3}\left|E_H E_K E_L\right|\left(\left|E_H\right|^2 + \left|E_K\right|^2 + \left|E_L\right|^2 - 1\right)\cos\left(\phi_H + \phi_K + \phi_L\right) =$$

$$6\left(\left|E_H\right|^4 + \left|E_K\right|^4 + \left|E_L\right|^4\right) + 18\left(\left|E_H E_K\right|^2 + \left|E_K E_L\right|^2 + \left|E_L E_H\right|^2\right)$$

$$+3\left(\left|E_H E_{K-L}\right|^2 + \left|E_K E_{L-H}\right|^2 + \left|E_L E_{H-K}\right|^2\right) - 31\left(\left|E_H\right|^2 + \left|E_K\right|^2 + \left|E_L\right|^2\right)$$

$$-2\left(\left|E_{2H}\right|^2 + \left|E_{2K}\right|^2 + \left|E_{2L}\right|^2\right) - 5\left(\left|E_{H-K}\right|^2 + \left|E_{K-L}\right|^2 + \left|E_{L-H}\right|^2\right) + 45$$

N=2

$$\sqrt{2}\left|E_H E_K E_L\right|\cos\left(\phi_H + \phi_K + \phi_L\right) = \left|E_H\right|^2 + \left|E_K\right|^2 + \left|E_L\right|^2 - 2\cos\left(\phi_H + \phi_K + \phi_L\right) = \pm 1$$

N=1

$$\cos\left(\phi_H + \phi_K + \phi_L\right) = +1$$

$$D = |E|^2 - 1$$

H+K+L=0

N=1, $$|E|^2 = 1$$

$$\cos(\phi_H + \phi_K + \phi_L) = 1$$

N=2, $$\cos(\phi_H + \phi_K + \phi_L) = \pm 1$$

$$\sqrt{2}|E_H E_K E_L| \cos(\phi_H + \phi_K + \phi_L) = D_H + D_K + D_L + 1$$

N=3,

$$6\sqrt{3}|E_H E_K E_L|(D_H + D_K + D_L + 2)\cos(\phi_H + \phi_K + \phi_L) =$$

$$6(D_H{}^2 + D_K{}^2 + D_L{}^2) + 18(D_H D_K + D_K D_L + D_L D_H)$$

$$+3(D_H D_{K-L} + D_K D_{L-H} + D_L D_{H-K})$$

$$+20(D_H + D_K + D_L) - 2(D_{2H} + D_{2K} + D_{2L})$$

$$-2(D_{H-K} + D_{K-L} + D_{L-H}) + 12$$

In equivalent notations for $N=3$, since $\mathbf{h}+\mathbf{k}+\mathbf{l}=0$, $\mathbf{l}=-(\mathbf{h}+\mathbf{k})$, and $|E_{-\mathbf{h}}|=|E_{+\mathbf{h}}|$,

$$\begin{aligned}
6\sqrt{3}\,|E_{\mathbf{h}}E_{\mathbf{k}}E_{\mathbf{l}}|\left(|E_{\mathbf{h}}|^2+|E_{\mathbf{k}}|^2+|E_{\mathbf{l}}|^2-1\right)\cos(\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}) = {}&\\
6\left(|E_{\mathbf{h}}|^4+|E_{\mathbf{k}}|^4+|E_{\mathbf{l}}|^4\right)&\\
+18\left(|E_{\mathbf{h}}E_{\mathbf{k}}|^2+|E_{\mathbf{k}}E_{\mathbf{l}}|^2+|E_{\mathbf{l}}E_{\mathbf{h}}|^2\right)&\\
+3\left(|E_{\mathbf{h}}E_{\mathbf{k}-\mathbf{l}}|^2+|E_{\mathbf{k}}E_{\mathbf{l}-\mathbf{h}}|^2+|E_{\mathbf{l}}E_{\mathbf{h}-\mathbf{k}}|^2\right)&\\
-31\left(|E_{\mathbf{h}}|^2+|E_{\mathbf{k}}|^2+|E_{\mathbf{l}}|^2\right)&\\
-2\left(|E_{2\mathbf{h}}|^2+|E_{2\mathbf{k}}|^2+|E_{2\mathbf{l}}|^2\right)&\\
-5\left(|E_{\mathbf{h}-\mathbf{k}}|^2+|E_{\mathbf{k}-\mathbf{l}}|^2+|E_{\mathbf{l}-\mathbf{h}}|^2\right)+45\,,&\quad \text{if}\quad N=3 \quad\text{and}\quad \mathbf{h}+\mathbf{k}+\mathbf{l}=0\,,
\end{aligned}$$

$$\begin{aligned}
6\sqrt{3}\,|E_{\mathbf{h}}E_{\mathbf{k}}E_{-\mathbf{h}-\mathbf{k}}|\left(|E_{\mathbf{h}}|^2+|E_{\mathbf{k}}|^2+|E_{-\mathbf{h}-\mathbf{k}}|^2-1\right)\cos(\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h}-\mathbf{k}}) = {}&\\
6\left(|E_{\mathbf{h}}|^4+|E_{\mathbf{k}}|^4+|E_{-\mathbf{h}-\mathbf{k}}|^4\right)&\\
+18\left(|E_{\mathbf{h}}E_{\mathbf{k}}|^2+|E_{\mathbf{k}}E_{-\mathbf{h}-\mathbf{k}}|^2+|E_{-\mathbf{h}-\mathbf{k}}E_{\mathbf{h}}|^2\right)&\\
+3\left(|E_{\mathbf{h}}E_{\mathbf{h}+2\mathbf{k}}|^2+|E_{\mathbf{k}}E_{-2\mathbf{h}-\mathbf{k}}|^2+|E_{-\mathbf{h}-\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}|^2\right)&\\
-31\left(|E_{\mathbf{h}}|^2+|E_{\mathbf{k}}|^2+|E_{-\mathbf{h}-\mathbf{k}}|^2\right)&\\
-2\left(|E_{2\mathbf{h}}|^2+|E_{2\mathbf{k}}|^2+|E_{-2\mathbf{h}-2\mathbf{k}}|^2\right)&\\
-5\left(|E_{\mathbf{h}-\mathbf{k}}|^2+|E_{\mathbf{h}+2\mathbf{k}}|^2+|E_{-2\mathbf{h}-\mathbf{k}}|^2\right)+45\,,&
\end{aligned}$$

$$\begin{aligned}
6\sqrt{3}\,|E_{\mathbf{h}}E_{\mathbf{k}}E_{\mathbf{h}+\mathbf{k}}|\left(|E_{\mathbf{h}}|^2+|E_{\mathbf{k}}|^2+|E_{\mathbf{h}+\mathbf{k}}|^2-1\right)\cos(\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h}-\mathbf{k}}) = {}&\\
6\left(|E_{\mathbf{h}}|^4+|E_{\mathbf{k}}|^4+|E_{\mathbf{h}+\mathbf{k}}|^4\right)&\\
+18\left(|E_{\mathbf{h}}E_{\mathbf{k}}|^2+|E_{\mathbf{k}}E_{\mathbf{h}+\mathbf{k}}|^2+|E_{\mathbf{h}+\mathbf{k}}E_{\mathbf{h}}|^2\right)&\\
+3\left(|E_{\mathbf{h}}E_{\mathbf{h}+2\mathbf{k}}|^2+|E_{\mathbf{k}}E_{2\mathbf{h}+\mathbf{k}}|^2+|E_{\mathbf{h}+\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}|^2\right)&\\
-31\left(|E_{\mathbf{h}}|^2+|E_{\mathbf{k}}|^2+|E_{\mathbf{h}+\mathbf{k}}|^2\right)&\\
-2\left(|E_{2\mathbf{h}}|^2+|E_{2\mathbf{k}}|^2+|E_{2\mathbf{h}+2\mathbf{k}}|^2\right)&\\
-5\left(|E_{\mathbf{h}-\mathbf{k}}|^2+|E_{\mathbf{h}+2\mathbf{k}}|^2+|E_{2\mathbf{h}+\mathbf{k}}|^2\right)+45\,.&
\end{aligned}$$