Mathematics Short Sum Up

Convert d-dimensional potential summations into a universal integral summation

$$G(\mathbf{L},\mathbf{v}) = D\int_0^\infty t^{C-1}(-\delta(\mathbf{v},B) + \sum_{\mathbf{k}\in\mathbb{Z}^d} e^{-A\pi\|\mathbf{Lk}+\mathbf{v}\|^2 t - \frac{B}{t}})dt, \tag{1}$$

with different constants A, B, C, D, then use integral split up

$$G(\mathbf{L},\mathbf{v}) = \int_0^1 \cdot\, dt + \int_1^\infty \cdot\, dt = G_{Fourier}(\mathbf{L},\mathbf{v}) + G_{direct}(\mathbf{L},\mathbf{v}), \tag{2}$$

where $G_{Fourier}$ denotes long-range term and G_{direct} denotes short-range term. Since convergence with t in $G_{Fourier}$ is slow, we do

$$t \to \frac{1}{t} \tag{3}$$

and Poisson summation

$$\sum_{\mathbf{k}\in\mathbb{Z}^d} e^{-2\pi i\mathbf{w}\cdot\mathbf{Lk} - \pi t\|\mathbf{Lk}+\mathbf{v}\|^2} = \frac{t^{-\frac{d}{2}} e^{2\pi i \mathbf{w}\cdot\mathbf{v}}}{\det\mathbf{L}} \sum_{\mathbf{k}\in\mathbb{Z}^d} e^{2\pi i\mathbf{L}'\mathbf{k}\cdot\mathbf{v} - \frac{\pi}{t}\|\mathbf{L}'\mathbf{k}+\mathbf{w}\|^2}. \tag{4}$$

We obtain

$$\begin{aligned} G_{Fourier}(\mathbf{L},\mathbf{v}) &= -\frac{D\delta(\mathbf{v},B)}{C} + \frac{\delta(B)}{\det\mathbf{L}}\frac{D}{(C-\frac{d}{2})A^{\frac{d}{2}}} \\ &+ \frac{1}{\det\mathbf{L}}\frac{D}{A^{\frac{d}{2}}} \sum_{\mathbf{k}\in\mathbb{Z}^d, \pi\|\mathbf{L}'\mathbf{k}\|^2/A+B>0} e^{2\pi i\mathbf{L}'\mathbf{k}\cdot\mathbf{v}} K_{C-\frac{d}{2}}(\frac{\pi\|\mathbf{L}'\mathbf{k}\|^2}{A} + B, 0) \end{aligned} \tag{5}$$

and

$$G_{direct}(\mathbf{L},\mathbf{v}) = D\delta(\mathbf{v})B^C(\Gamma(-C) - \Gamma(-C,B)) + D\sum_{\mathbf{k}\in\mathbb{Z}^d, \|\mathbf{Lk}+\mathbf{v}\|\neq 0} K_{-C}(A\pi\|\mathbf{Lk}+\mathbf{v}\|^2, B). \tag{6}$$

with incomplete Bessel function

$$K_\nu(x,y) = \int_1^\infty t^{-\nu-1} e^{-xt-y/t} dt. \tag{7}$$

We show that summation of incomplete Bessel functions

$$\sum_{\mathbf{k}\in\mathbb{Z}^d, \pi\alpha\|\mathbf{Lk}+\mathbf{v}\|^2+\gamma>0} K_\nu(\pi\alpha\|\mathbf{Lk}+\mathbf{v}\|^2 + \gamma, \beta), \tag{8}$$

with $\alpha > 0, \beta \geq 0, \gamma \geq 0$, is bound by the Gaussian Lattice Sum

$$E(\mathbf{L},\mathbf{v},\alpha) = \sum_{\mathbf{k}\in\mathbb{Z}^d} e^{-\pi\alpha\|\mathbf{Lk}+\mathbf{v}\|^2} < \frac{d}{2}\left(\frac{2}{\rho}\right)^d \Gamma\left(\frac{d}{2}, \left(\frac{\rho}{2}\right)^2\right). \tag{9}$$

where $\rho = \min\{\sqrt{\pi\alpha}\|\mathbf{Lk}\| \mid \mathbf{k}\in\mathbb{Z}^d, \mathbf{k}\neq\mathbf{0}\}$.