

## Double Sums and Index Shuffling

### Basics

- Double sums over indexed parameters are usually bad enough, but doing arithmetic with the indices is often a bit mind boggling. Lets look at this in some detail:
- We have the double sum over  $\mathbf{K}$  and  $\mathbf{G}$  with both indices running from  $-\infty$  to  $+\infty$ . If, for the sake of simplicity, we consider a one-dimensional case (i.e.  $\mathbf{K}$  now denotes just *one* component) we have for the double sum

$$\Sigma \Sigma = \Sigma_{\mathbf{K}'} \Sigma_{\mathbf{G}} C_{\mathbf{K}'} \cdot V_{\mathbf{G}} \cdot \exp(i \cdot [\mathbf{K}' + \mathbf{G}] \cdot r)$$

- We can write this double sum as a matrix with, e.g., constant values of the  $C_{\mathbf{K}'}$  in a *row* and constant values of the  $V_{\mathbf{G}}$  in a *column*. Shown is the part with  $\mathbf{K}' = 4$  and  $\mathbf{K}' = 5$ , and likewise  $\mathbf{G} = 7, 8, 9$ .

$$\begin{array}{ccccc} & + & & + & & + \\ + & C_4 \cdot V_7 \cdot \exp(i(4 + 7)) & + & C_4 \cdot V_8 \cdot \exp(i(4 + 8)) & + & C_4 \cdot V_9 \cdot \exp(i(4 + 9)) & + \\ & + & & + & & + \\ + & C_5 \cdot V_7 \cdot \exp(i(5 + 7)) & + & C_5 \cdot V_8 \cdot \exp(i(5 + 8)) & + & C_5 \cdot V_9 \cdot \exp(i(5 + 9)) & + \\ & + & & + & & + \end{array}$$

- Doing the sum does not depend on which way we take through the matrix, as long as we do not drop any element.
- "Intuitively" one would tend to go *horizontally* and back and forth through all the terms, but we can just as well move *diagonally*, following the lines indicated by identical color.
- In this case, the exponent is constant, we can name it  $k$ . The sum over a diagonal now means summing over all contributions where  $\mathbf{K}' + \mathbf{G} = \text{const} = k$
- We thus can rewrite the double sum by adding up all the diagonals with fixed exponents and obtain the expression [used before](#):

$$\Sigma_{\mathbf{K}'} \Sigma_{\mathbf{G}} C_{\mathbf{K}'} \cdot V_{\mathbf{G}} \cdot \exp(i \cdot [\mathbf{K}' + \mathbf{G}] \cdot r) = \Sigma_{k - \mathbf{G}} \Sigma_{\mathbf{G}} C_{k - \mathbf{G}} \cdot V_{\mathbf{G}} \cdot \exp(i k r)$$