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 $\boldsymbol{k}'$ and $\boldsymbol{G}$ with both indices running from $-\infty$ to $+\infty$. If, for the sake of simplicity, we consider a one-dimensional case (i.e. $\boldsymbol{k}'$ now denotes just *one* component) we have for the double sum

$$\Sigma\Sigma \;=\; \Sigma_{k'}\,\Sigma_G\, C_{k'} \cdot V_G \cdot \exp(i \cdot [k' + G]) \cdot r)$$

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

+	+	+
+ $C_4 \cdot V_7 \cdot \exp(i(4 + 7))$ +	$C_4 \cdot V_8 \cdot \exp(i(4 + 8))$ +	$C_4 \cdot V_9 \cdot \exp(i(4 + 9))$ +
+	+	+
+ $C_5 \cdot V_7 \cdot \exp(i(5 + 7))$ +	$C_5 \cdot V_8 \cdot \exp(i(5 + 8))$ +	$C_5 \cdot V_9 \cdot \exp(i(5 + 9))$ +
+	+	+

- 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 $\boldsymbol{k}$. The sum over a diagonal now means summing over all contributions where $\boldsymbol{k}' + \boldsymbol{G} = \text{const} = \boldsymbol{k}$
- We thus can rewrite the double sum by adding up all the diagonals with fixed exponents and obtain the expression used before:

$$\Sigma_{k'}\,\Sigma_G\, C_{k'} \cdot V_G \cdot \exp\,(i \cdot [k' + G] \cdot r) \;=\; \Sigma_{k-G}\Sigma_G\, C_{k-G} \cdot V_G \cdot \exp\,(ikr)$$