Merging particle species [tln92]

Here we investigate the circumstances under which two or more species of particles can be merged into a single species with equivalent combinatorics.[1]

Consider a system with M species of particles with given specifications:

$$W(\{N_m\}) = \prod_{m=1}^{M} \binom{d_m + N_m - 1}{N_m}, \quad d_m = A_m - \sum_{m'=1}^{M} g_{mm'}(N_{m'} - \delta_{mm'}).$$

If two species $m = 1, 2$ are to be merged into a new species $m = 0$, their specifications must satisfy, as necessary conditions, Anghel's rules:

$$A_1 + A_2 \doteq A_0, \tag{1}$$
$$g_{11} + g_{21} = g_{12} + g_{22} \doteq g_{00}, \tag{2}$$
$$g_{m1} = g_{m2} \doteq g_{m0}, \quad m = 3, \ldots, M, \tag{3}$$
$$g_{1m} + g_{2m} \doteq g_{0m}, \quad m = 3, \ldots, M. \tag{4}$$

These rules were derived in the context of a statistical mechanical analysis of macroscopic systems.

On the level the combinatorial analysis, rules (1) and (2) must be made more stringent for mergers in systems of any size.

The multiplicity expressions of the old and new sets of species must satisfy the relations

$$W(N_0, N_3, \ldots) = \sum_{N_1=0}^{N_0} W(N_1, N_0 - N_1, N_3, \ldots).$$

All binomial factors with $m \geq 3$ are identical if condition (3) is satisfied. We are thus left to prove the equation,

$$\binom{d_0 + N_0 - 1}{N_0} = \sum_{N_1=0}^{N_0} \binom{d_1 + N_1 - 1}{N_1} \binom{d_2 + N_0 - N_1 - 1}{N_0 - N_1} \tag{5}$$

with

$$d_0 + N_0 - 1 = D_0 + g_{00} - 1 - (g_{00} - 1)N_0, \tag{6}$$
$$d_1 + N_1 - 1 = D_1 + g_{11} - 1 - g_{12}N_0 + (g_{12} - g_{11} + 1)N_1, \tag{7}$$
$$d_2 + N_0 - N_1 - 1 = D_2 + g_{22} - 1 - g_{21}N_0 + (g_{21} - g_{22} + 1)(N_0 - N_1), \tag{8}$$
$$D_m \doteq A_m - \sum_{m'=3}^{M} g_{mm'}N_{m'}, \quad m = 0, 1, 2. \tag{9}$$

[1] Anghel 2007, 2010; Liu et al. 2012.

We note that $D_1 + D_2 = D_0$ if conditions (1) and (4) are satisfied. Next we enforce condition (2) by means of the parametrization,

$$
\begin{aligned}
g_{11} &= \frac{1}{2}g_{00} + u, \quad g_{12} = \frac{1}{2}g_{00} + v, \\
g_{21} &= \frac{1}{2}g_{00} - u, \quad g_{22} = \frac{1}{2}g_{00} - v.
\end{aligned} \tag{10}
$$

We have identified two scenarios in which (5) is proven to hold. Both necessitate a tightening of condition (2) and one requires that condition (1) be tightened as well.

- ▷ Type 1 mergers require that $u = v + 1$, thus eliminating the last term in both (7) and (8) and reducing (5) to the identity,

$$
\sum_{i=0}^{k} \binom{m}{i} \binom{n}{k-i} = \binom{m+n}{k}. \tag{11}
$$

- ▷ Type 2 mergers require that $u = v = 0$ and $A_1 = A_2$, implying $D_1 = D_2$ and reducing (5) to the identity

$$
\sum_{i=0}^{k} \binom{m+i}{i} \binom{m+k-i}{k-i} = \binom{2m+k+1}{k}. \tag{12}
$$

The amendments to rules (1)-(4) in more generic form thus read

$$
g_{11} = g_{12} \pm 1, \quad g_{22} = g_{21} \pm 1 \qquad : \text{ type 1,} \tag{13a}
$$

$$
g_{11} = g_{12} = g_{21} = g_{22}, \quad A_1 = A_2 \qquad : \text{ type 2.} \tag{13b}
$$

All mergers involving more than two species can be implemented sequentially, either as type-1 or type-2 mergers. The order in the sequence matters in most cases. Implementing one merger may be a precondition for another merger.

Anghel's rules are determinate when species are merged but some are indeterminate – even with amendments (13) – without implied assumptions or additional input when species are split.