Binary model systems
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1. Binary alloy system

We consider an alternate system – an alloy crystal with N distinct sites. A example is shown below. Each site is occupied by either an atom A or an atom B, without any vacant sites.

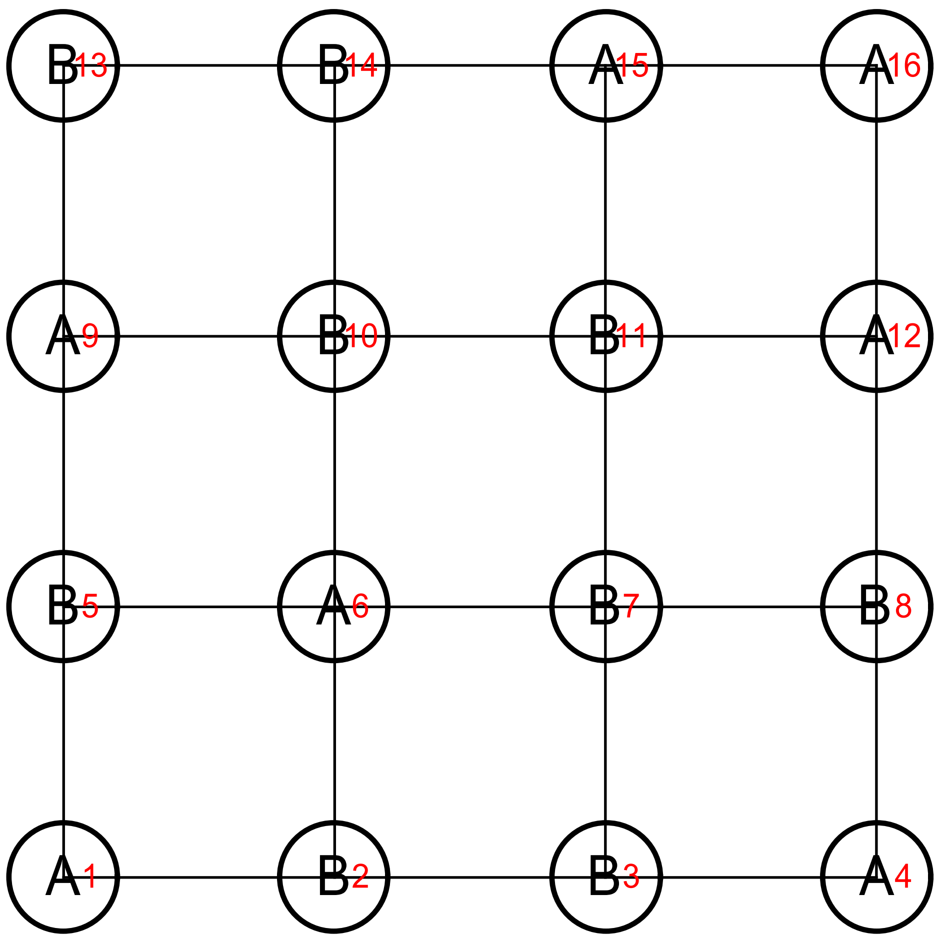


Fig. A binary alloy system of two chemical components A and B, whose atoms occupy distinct numbered sites. A and B are distributed on the lattice sites (1, 2, 3, …, 16).

Each site is occupied by either A or B atoms (1, 2, 3, 4, …, 12) such that

$$A_1 B_2 B_3 A_4 B_5 A_6 B_7 B_8 B_9 A_{10} A_{11} A_{12} B_{13} B_{14} A_{15} A_{16}$$

Every distinct state of a binary alloy system on *N* sites is contained in the symbolic product

$$(A_1 + B_1)(A_2 + B_2)(A_3 + B_3)......(A_N + B_N)$$

We consider the alloy system with the number of A atoms, $N_A = (1-x)N$, and the number of B atoms, $N_B = xN$, where

$$N_A + N_B = N$$

According to the polynomial theorem, the symbolic expression can be written as

$$(A+B)^N = \sum_{t=0}^{N} \frac{N!}{(N-t)!t!} A^{N-t} B^t$$

with

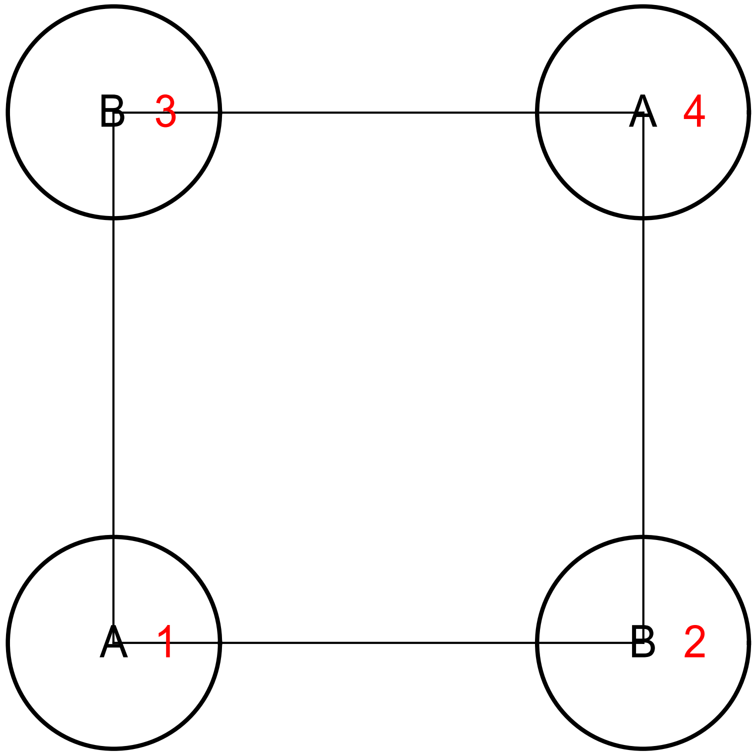
$$N_A = N - t = (1-x)N, \qquad N_B = t = Nx.$$

The co-efficient of $A^{N-t}B^t$ gives the number $g(N,t)$ of possible arrangements or states of $(N-t)$ atoms A and *t* atoms B on N sites;

$$g(N,t) = \binom{N}{t} = \frac{N!}{(N-t)!t!} = \frac{N!}{N_A! N_B!}$$

((**Simple case**)) $N = 4$.

We consider the simple case with 4 sites.



Every distinct state of a binary alloy system on 4 sites is contained in the symbolic product of 4 factors;

$$
\begin{aligned}
(A_1+B_1)(A_2+B_2)(A_3+B_3)(A_4+B_4) &= (A_1A_2+A_1B_2+B_1A_2+B_1B_2)(A_3A_4+A_3B_4+B_3A_4+B_3B_4)\\
&= A_1A_2A_3A_4+A_1A_2A_3B_4+A_1A_2B_3A_4+A_1A_2B_3B_4\\
&\quad +A_1B_2A_3A_4+A_1B_2A_3B_4+A_1B_2B_3A_4+A_1B_2B_3B_4\\
&\quad +B_1A_2A_3A_4+B_1A_2A_3B_4+B_1A_2B_3A_4+B_1A_2B_3B_4\\
&\quad +B_1B_2A_3A_4+B_1B_2A_3B_4+B_1B_2B_3A_4+B_1B_2B_3B_4\\
&= A_1A_2A_3A_4\\
&\quad +(A_1A_2A_3B_4+A_1A_2B_3A_4++A_1B_2A_3A_4++B_1A_2A_3A_4)\\
&\quad +(A_1A_2B_3B_4+A_1B_2A_3B_4+A_1B_2B_3A_4++B_1A_2A_3B_4+B_1A_2B_3A_4\\
&\quad +B_1B_2A_3A_4)+\\
&\quad +(B_1A_2B_3B_4+A_1B_2B_3B_4+B_1B_2A_3B_4+B_1B_2B_3A_4)\\
&\quad +B_1B_2B_3B_4
\end{aligned}
$$

The symbolic expression can be evaluated using the Mathematica. It is convenient for one to expand the following expression in the power of *a* and *b*.

$$(A_1a+B_1b)(A_2a+B_2b)(A_3a+B_3b)(A_4a+B_4b)$$

instead of $(A_1+B_1)(A_2+B_2)(A_3+B_3)(A_4+B_4)$

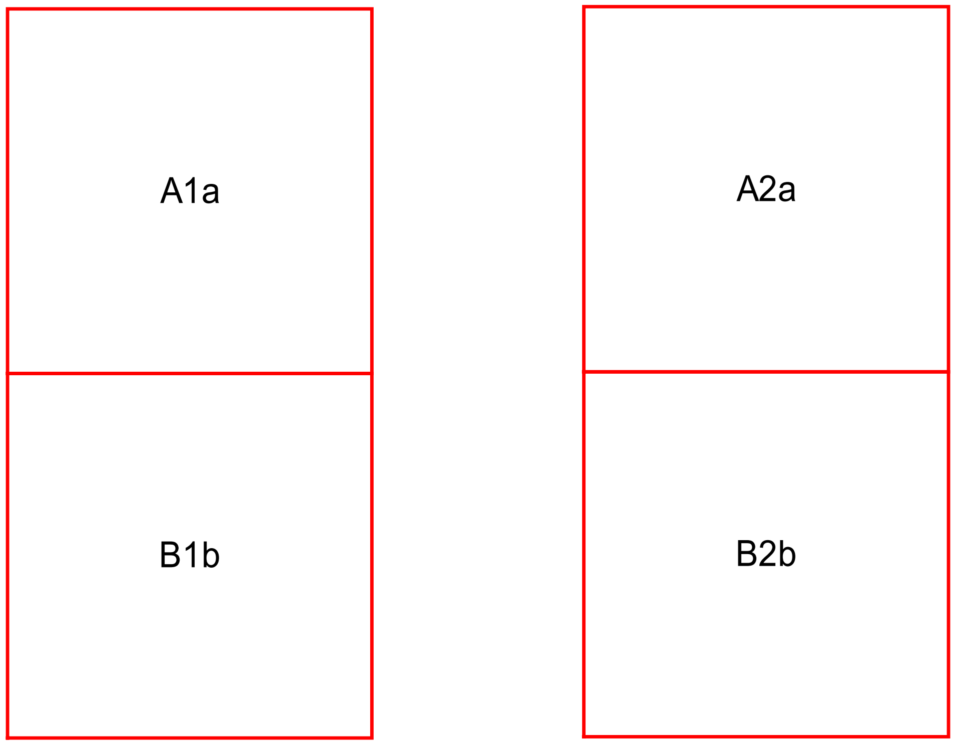


Fig. One of atoms of atom A and atom B stays at the site 1. One of atoms of atom A and atom B stays at the site 2.

((**Mathematica**))

```
Clear["Global`*"];
f1 = (A1 a + B1 b) (A2 a + B2 b) (A13 a + B3 b) (A4 a + B4 b) //
  Expand
```

a^4 A1 A13 A2 A4 + a^3 A13 A2 A4 b B1 +
a^3 A1 A13 A4 b B2 + a^2 A13 A4 b^2 B1 B2 +
a^3 A1 A2 A4 b B3 + a^2 A2 A4 b^2 B1 B3 + a^2 A1 A4 b^2 B2 B3 +
a A4 b^3 B1 B2 B3 + a^3 A1 A13 A2 b B4 + a^2 A13 A2 b^2 B1 B4 +
a^2 A1 A13 b^2 B2 B4 + a A13 b^3 B1 B2 B4 + a^2 A1 A2 b^2 B3 B4 +
a A2 b^3 B1 B3 B4 + a A1 b^3 B2 B3 B4 + b^4 B1 B2 B3 B4

```
Coefficient[f1, a^4]
```

A1 A13 A2 A4

```
Coefficient[f1, a^3 b]
```

A13 A2 A4 B1 + A1 A13 A4 B2 + A1 A2 A4 B3 + A1 A13 A2 B4

```
Coefficient[f1, a^2 b^2]
```

A13 A4 B1 B2 + A2 A4 B1 B3 + A1 A4 B2 B3 +
A13 A2 B1 B4 + A1 A13 B2 B4 + A1 A2 B3 B4

```
Coefficient[f1, a b^3]
```

A4 B1 B2 B3 + A13 B1 B2 B4 + A2 B1 B3 B4 + A1 B2 B3 B4

```
Coefficient[f1, b^4]
```

B1 B2 B3 B4

((**Mathematica**))

$$f2 = (a + b)^4 \; // \; \text{Expand}$$

$$a^4 + 4\, a^3\, b + 6\, a^2\, b^2 + 4\, a\, b^3 + b^4$$

So we get the way for each state

a^4	1	$\binom{4}{4}$
a^3b	4	$\binom{4}{3}$
a^2b^2	6	$\binom{4}{2}$
ab^3	4	$\binom{4}{1}$
b^4	1	$\binom{4}{0}$

2. Parking problem

We assume that there are N parking lots. For each site only one car can park. In other words, one car parks at the site, otherwise, no car is parking.

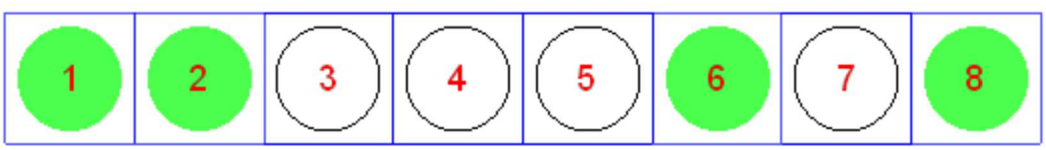
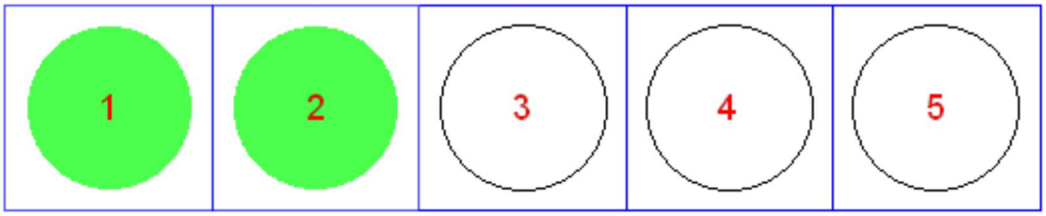


Fig. State of a parking lot with 8 numbered parking spaces. The green circles denote spaces occupied by a car; the open circles denote vacant spaces.

We consider the case of a parking lot with 5 numbered parking spaces.



There are 32 states. Every distinct state of the system is contained in a symbolic product of $N = 5$ factors;

[Pa(1)+Va(1)] [Pa(2)+Va(2)][Pa(3)+Va(3)] [Pa(4)+Va(4)] [Pa(5)+Va(5)]

where Pa(i) denotes that a car parks in the i site and Va(i) denotes that no car parks in the i site (vavant). These products can be expanded using the Mathematica below, leading to the 32 states.

We can also use

[Pa(1)x+Va(1)y] [Pa(2) x +Va(2) y][Pa(3) x +Va(3) y] [Pa(4) x +Va(4) y] [Pa(5) x +Va(5) y]

for the expansion of the powers of x and y.

((**Mathematica-1**))

```
Clear["Global`*"];
f1 = (Pa1 x + Va1 y) (Pa2 x + Va2 y) (Pa3 x + Va3 y)
   (Pa4 x + Va4 y) (Pa5 x + Va5 y) // Expand;
```

```
Coefficient[f1, x^5]
```

Pa1 Pa2 Pa3 Pa4 Pa5

```
Coefficient[f1, x^4 y]
```

Pa2 Pa3 Pa4 Pa5 Va1 + Pa1 Pa3 Pa4 Pa5 Va2 +
 Pa1 Pa2 Pa4 Pa5 Va3 + Pa1 Pa2 Pa3 Pa5 Va4 + Pa1 Pa2 Pa3 Pa4 Va5

```
Coefficient[f1, x^3 y^2]
```

Pa3 Pa4 Pa5 Va1 Va2 + Pa2 Pa4 Pa5 Va1 Va3 +
 Pa1 Pa4 Pa5 Va2 Va3 + Pa2 Pa3 Pa5 Va1 Va4 +
 Pa1 Pa3 Pa5 Va2 Va4 + Pa1 Pa2 Pa5 Va3 Va4 +
 Pa2 Pa3 Pa4 Va1 Va5 + Pa1 Pa3 Pa4 Va2 Va5 +
 Pa1 Pa2 Pa4 Va3 Va5 + Pa1 Pa2 Pa3 Va4 Va5

```
Coefficient[f1, x^2 y^3]
```

Pa4 Pa5 Va1 Va2 Va3 + Pa3 Pa5 Va1 Va2 Va4 +
Pa2 Pa5 Va1 Va3 Va4 + Pa1 Pa5 Va2 Va3 Va4 +
Pa3 Pa4 Va1 Va2 Va5 + Pa2 Pa4 Va1 Va3 Va5 +
Pa1 Pa4 Va2 Va3 Va5 + Pa2 Pa3 Va1 Va4 Va5 +
Pa1 Pa3 Va2 Va4 Va5 + Pa1 Pa2 Va3 Va4 Va5

```
Coefficient[f1, x^1 y^4]
```

Pa5 Va1 Va2 Va3 Va4 + Pa4 Va1 Va2 Va3 Va5 +
Pa3 Va1 Va2 Va4 Va5 + Pa2 Va1 Va3 Va4 Va5 + Pa1 Va2 Va3 Va4 Va5

```
Coefficient[f1, y^5]
```

Va1 Va2 Va3 Va4 Va5

We may drop the site labels when we are interested only in how many of the cars in the parking lot. In this case, the product become

$$(x+y)^5 = x^5 + 5x^4y + 10x^3y^2 + 10x^2y^3 + 5xy^4 + y^5$$

where x = Pa and Va = y. So we get the way for each state

x^5	1	$\binom{5}{5}$
x^4y	5	$\binom{5}{4}$
x^3y^2	10	$\binom{5}{3}$
x^2y^3	10	$\binom{5}{2}$
xy^4	5	$\binom{5}{1}$

y^5	1	$\binom{5}{0}$

(see the Pascal triangle)