CHE502 Chemical and Statistical Thermodynamics
Topic 5
The basic concepts of statistical mechanics (thermodynamics)

URL: `http://theo.ism.u-bordeaux.fr/PBopp/vistec.2020.2021`

Note: This is an approximation, even though it is almost always made

$$\psi^{\text{system}} = \text{combination of molecular } \psi^{\text{molec}}$$

$$\psi^{\text{molec}} = \text{combination of } \psi^{\text{elec}}, \psi^{\text{vib}}, \psi^{\text{rot}}, \psi^{\text{trans}}, \ldots$$

So we 'build' our total states as combinations of the states of the subsystems
(like a LEGO)
the subsystems are assumed to be independent of each other (which does not always work)
(*eg ortho- and para hydrogen problem*)

In statistical mechanics, 'state' (like eg in 'sum of states') refers to the big ψ^{system}

which has an incredible number of variables, and of quantum numbers

This clearly need to be simplified

In most textbooks you will find a rather mathematical derivation of the (canonical) 'partition function', based on classical mechanics, and following to a large extent Ludwig Boltzmann's (1844-1906) original thinking.
(Boltzmann did not know about quantum mechanics, unfortunately! so he could not use the concept of 'state' as we do here)

If you have not studied this approach before, you do not need to try to understand it now.
A less exact, but more intuitive approach, using the notion of 'state' from quantum mechanics, will be sufficient for us.

We will use the lecture notes from last year and discuss
`http://theo.ism.u-bordeaux.fr/PBopp/vistec.2019.1/lecture.all.part1.pdf`
page 97-107 background, motivation
page 108-114 basic ideas, concepts
page 115 overview of possibilities
page 116-129 a couple of equations
page 130-133 equilibria, example $H_2 + D_2 \rightleftarrows 2\,HD$
page 134-139 normal modes (If we have time, or we do it in CHE501)
page 140-141 toward che501

I have collected these page in http://theo.ism.u-bordeaux.fr/PBopp/vistec.2020.2021/collect.pdf