PH-107

Quantum Physics and Applications

Elements of Statistical Physics-I

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Statistical Physics

What is it and who needs it?

We now know how to deal with the dynamics of a **single particle,** both in the classical and the quantum world.

We use either Newton's laws (classical) or the TDSE/TISE (quantum) to understand the time-evolution of the state of the particle.

But, how good is this knowledge in a macroscopic world consisting of many particles (interacting simultaneously with each other)?

Statistical Physics

What is it and who needs it?

As a simple example, description of the motion of air molecules in a closed room needs tracking at least 10^{23} particles.

Attempt to describe the motion of each molecule will clearly exhaust the computational power of any conceivable machine, not to mention that of the investigator!

Therefore, we need a means to assess the **collective behavior** of a large system, without having to track the evolution of each particle in the system.

Statistical Physics

What is it and who needs it?

The purpose of **statistical physics** is exactly this:

To explain the macroscopic (or collective) properties (for example, energy, momentum etc.) or thermodynamic parameters (pressure, volume, temperature, magnetization etc.) of a large collection of particles.

Specifically, we are interested in determining the number of particles ***dN(E)*** in the system with energy between ***E*** and ***E+dE***.

Henceforth, the term we will use for the large collection of particles is **system**.

Statistical Physics

Number of particles between E and $E+dE$

Obviously, $dN(E)$ depends on the total number of particles in the system, N.

A little less obviously, $dN(E)$ depends on two other factors:

1. The number of available energy states within the interval E and $E+dE$.

2. The probability that a particle can actually occupy a particular state.

Statistical Physics

Number of particles between *E* and *E+dE*

We may write the number of available energy states within the interval ***E*** and ***E+dE*** in terms of the **density of states**, ***g(E)***.

And we write the probability of a particle occupying an available state in the interval ***E*** and ***E+dE*** in terms of the **probability distribution function**, ***f(E)***.

The product ***g(E)f(E)dE*** thus gives ***dN(E)***.

Statistical Physics

Closer look at *g(E)*: Example of many particles in a 3D infinite potential box

Assume that we have a **large number of electrons** (~Avogadro's Number, N_A), in a macroscopic 3D potential box (L = 0.1 m).

The available energy states (assuming no interaction between the electrons) are of the form:

$$E = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) = 3.76 \times 10^{-17}(n_x^2 + n_y^2 + n_z^2)\ \mathrm{eV}$$

Thus, the spacing between the energy states $\Delta E \sim 10^{-17}$ eV.

Statistical Physics

Closer look at *g(E)*: Example of many particles in a 3D infinite potential box

The available energy levels are thus very closely spaced, defining a **quasi-continuum** of states

This explains the use of a density-of-states (DOS) function, ***g(E)***.

But still, the number of states within a certain energy range is finite (though quite large).

Statistical Physics

Closer look at *f(E)*:

The need for ***f(E)***, or a probabilistic description of an ensemble arises because

(a) We have a (classical) uncertainty due to the fact that **we cannot determine** the state of every particle at all times.

(b) Additionally (for quantum mechanical particles), we have an inherent uncertainty of **each individual particle's** quantum state.

Statistical Physics

f(E): Dependence on Particle Characteristics

Accordingly, ***f(E)*** depends on the **identity of the particles** in the system

i.e., whether the particles are

Classical Particles: Distinguishable, which need not obey **Pauli's Exclusion Principle.**

Bosons (Quantum Particles): Indistinguishable, which do not obey Pauli's Exclusion Principle.

Fermions (Quantum Particles): Indistinguishable, which obey Pauli's Exclusion Principle.

We know that quantum particles, Bosons and Fermions, obey integer and half-integer spin statistics.

Are there particles, which obey fractional quantum statistics? What are they called?

Statistical Physics

Pauli's Exclusion Principle

Based on Empirical Evidence, i.e., The Periodic table of Elements:

It is impossible for two **electrons** in an atom or molecule to have the same values of the four quantum numbers: n *as* the principal quantum number, ℓ as the angular-momentum quantum number, m_ℓ as the magnetic quantum number, and m_s as the spin quantum number.

Statistical Physics

Pauli's Exclusion Principle

A More General Statement:

Two identical Fermions (particles with **half-integer spin,** of which electron is an example) cannot occupy the same quantum state simultaneously.

The principle does not apply to particles with **integer spin** (Bosons) so that any number of Bosons can occupy the same state.

Pauli's Exclusion Principle

A more rigorous statement:

The total wave function for two identical fermions is **antisymmetric** with respect to exchange of the particles.

This means that the wave function changes its sign if the space *and* spin co-ordinates of any two particles are interchanged.

If we consider a two-Fermion wave function (including spin) $\Psi(r_1\sigma_1, r_2\sigma_2)$ then

$$\Psi(r_1\sigma_1, r_2\sigma_2) = -\Psi(r_2\sigma_2, r_1\sigma_1)$$

Pauli's Exclusion Principle

A more rigorous statement:

The total wave function for two identical Bosons is **symmetric** with respect to exchange of the particles.

i.e., if we consider a two-Boson wave function (including spin) $\Psi(r_1\sigma_1, r_2\sigma_2)$ then

$$\Psi(r_1\sigma_1, r_2\sigma_2) = +\Psi(r_2\sigma_2, r_1\sigma_1)$$

We thus see, that the number of Quantum particles that can be placed in any state depends on the **spin degree of freedom** of the particles.

Statistical Physics

The calculation of *f(E)*

The purpose of the rest of the lecture(s) on this topic is the calculation of ***f(E)*** for classical particles (Maxwell-Boltzmann), Bosons (Bose-Einstein) and Fermions (Fermi-Dirac).

How do we calculate ***f(E)***?

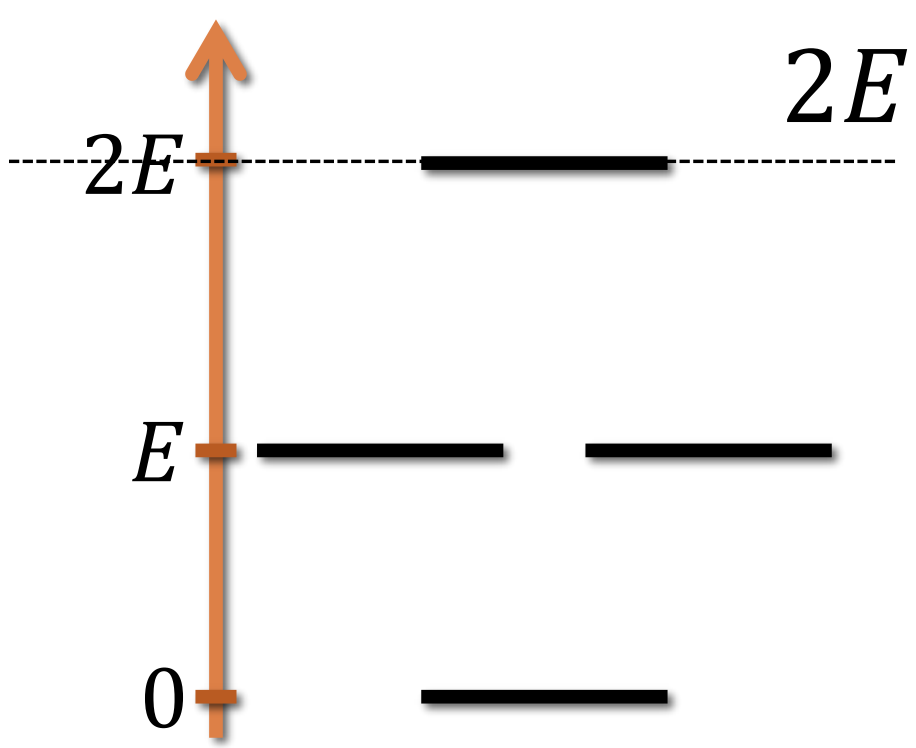
Let us analyze the question further: For a given fixed energy ***E*** of the system, how do I know what is ***dN(E)***, or (to start with) ***f(E)***?

Let's start answering this question with a simple example

Statistical Physics

2 particles occupying 3 states

Let's say that we have a system of **two particles** with total energy 2E. The energy states available to the system are 0, E, and 2E. The degeneracies of the states are 1,2, and 1, respectively.

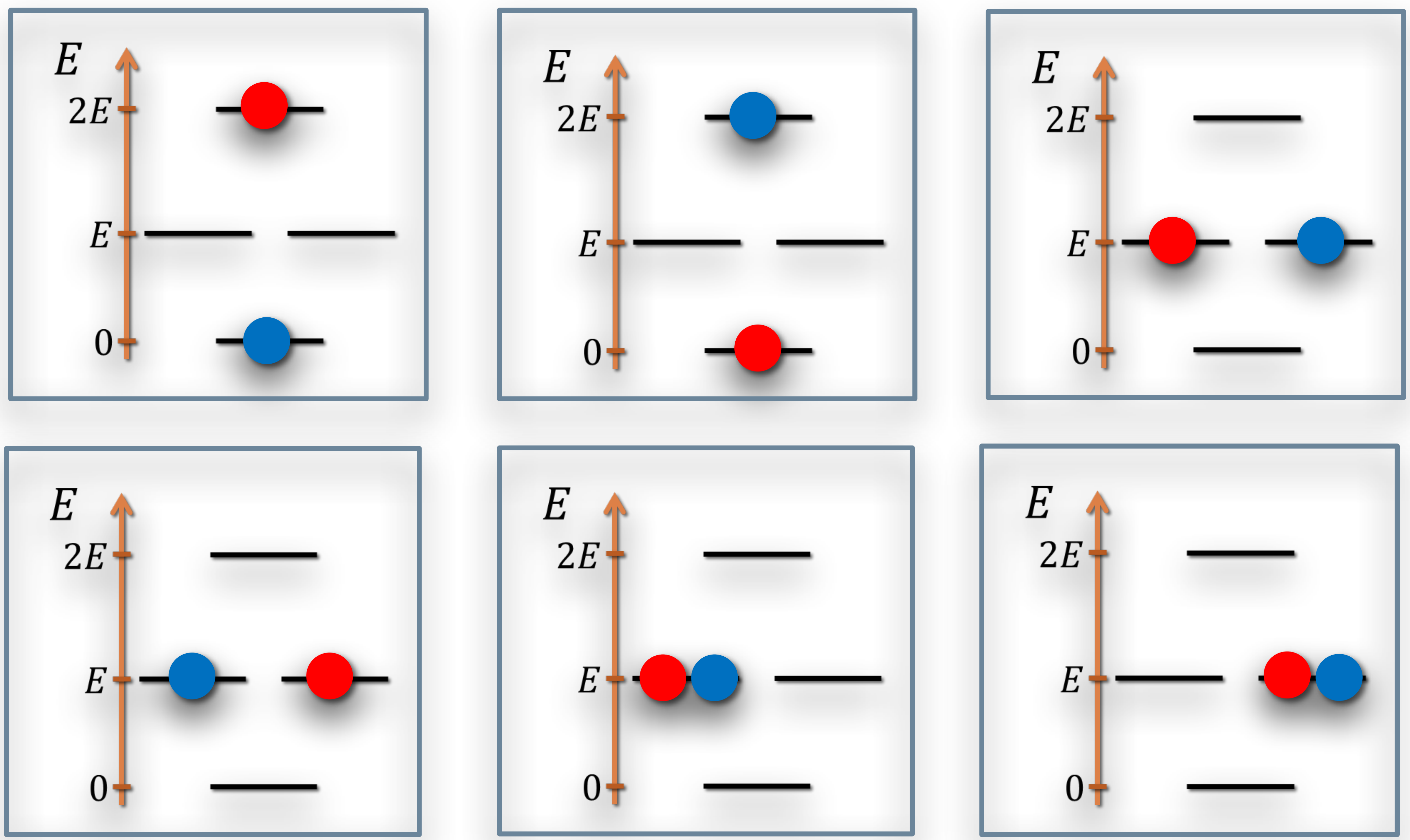


State Index (i)	State Energy	State degeneracy (g_i)
1	2E	1
2	E	2
3	0	1

Statistical Physics

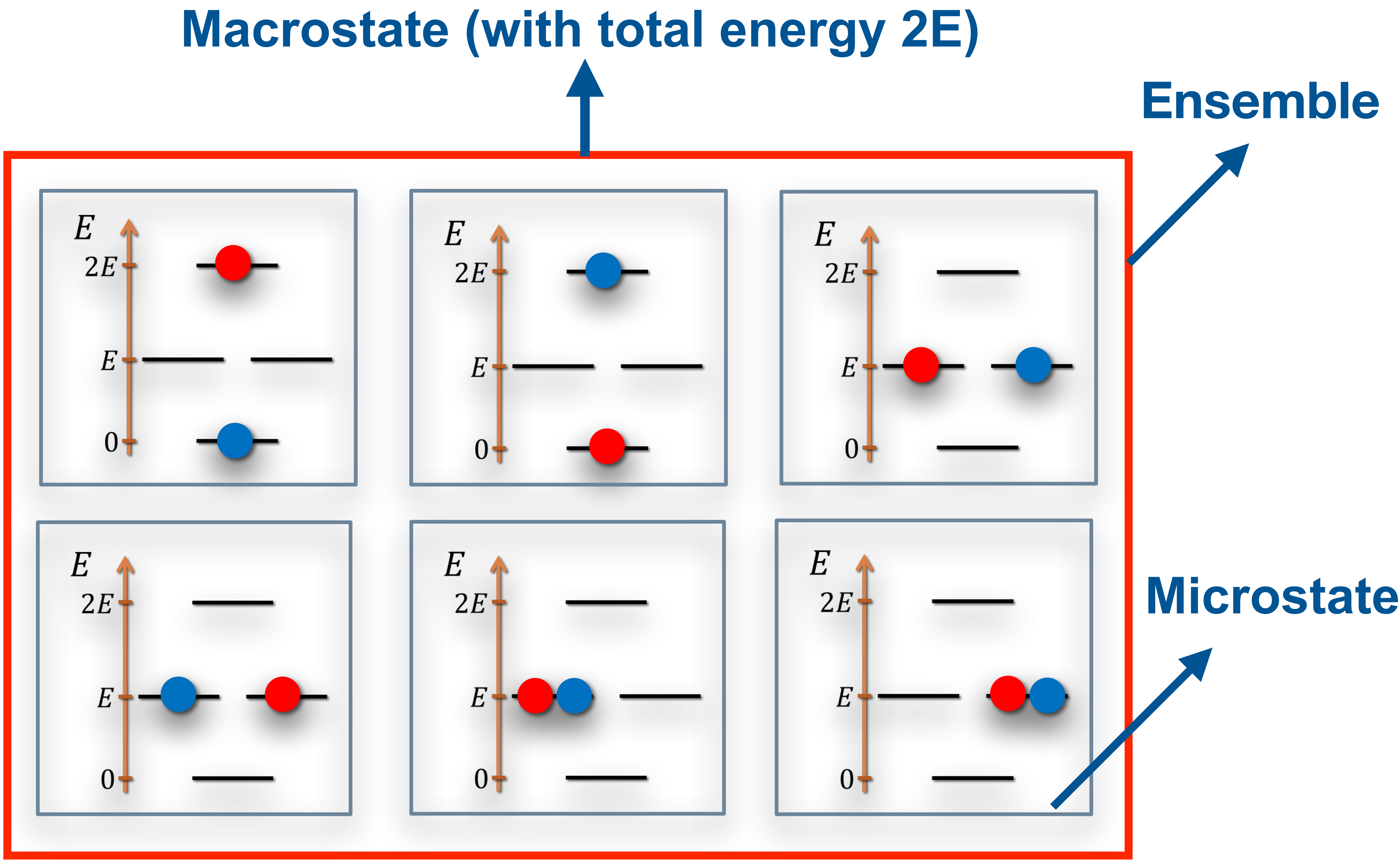
Different arrangements giving energy *E*

What are the different ways in which we get the total energy to be ***2E***?

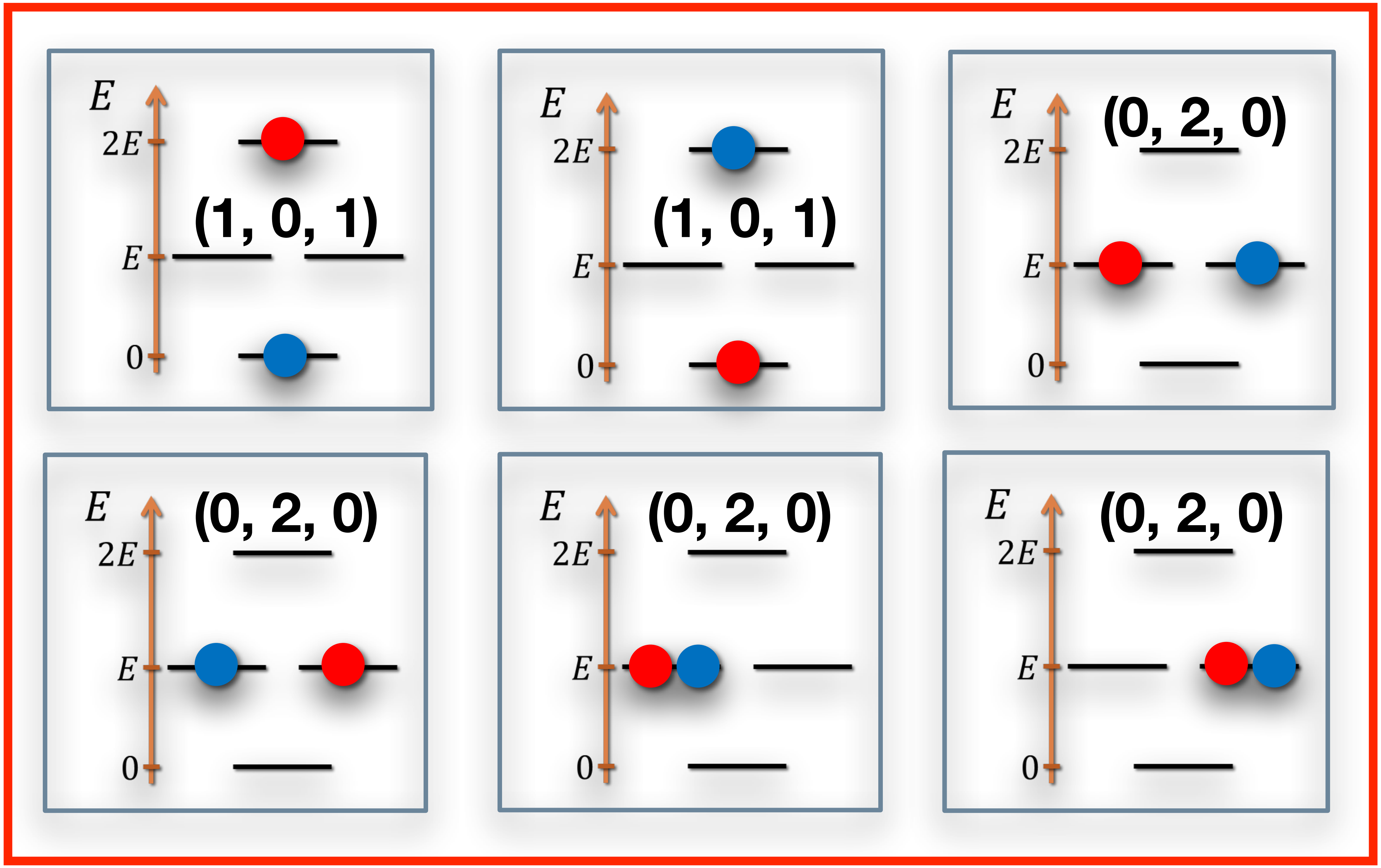


Statistical Physics

Microstates, ensemble, and the macrostate



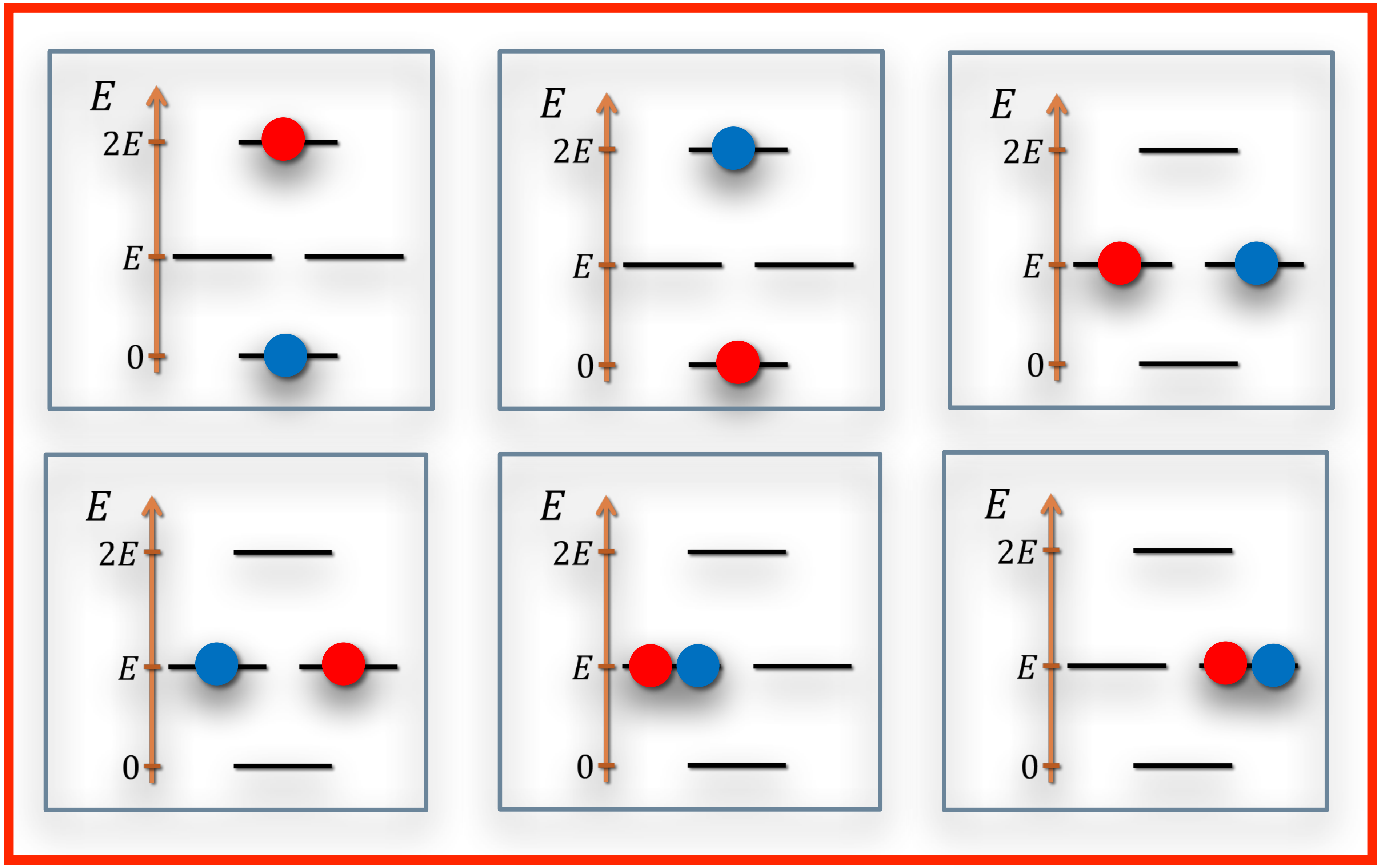
Configuration



The *apriori* probability of occupancy of all **microstates** is equal.

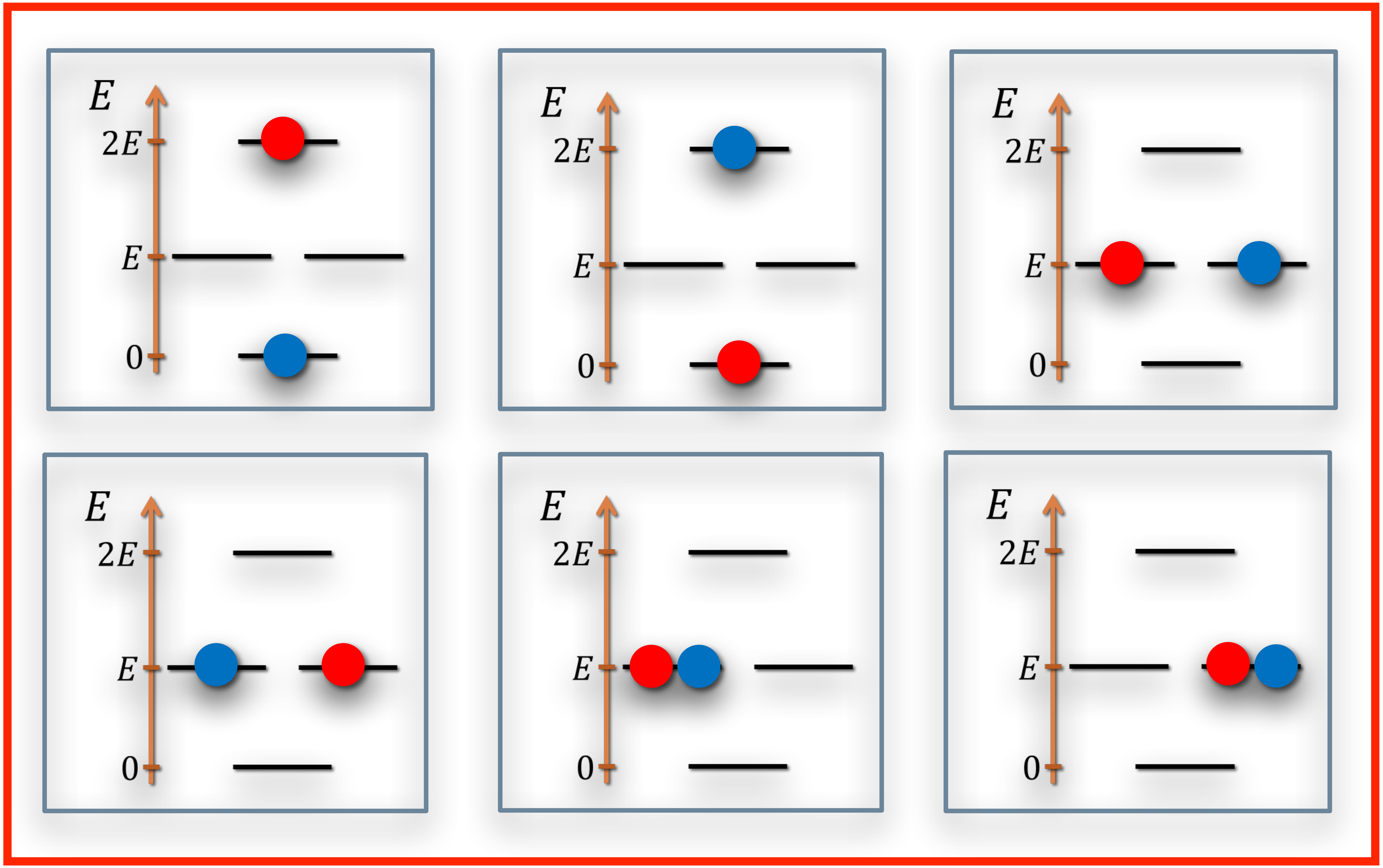
So, the (0,2,0) **configuration** is twice as probable as the (1,0,1).

Classical Particles

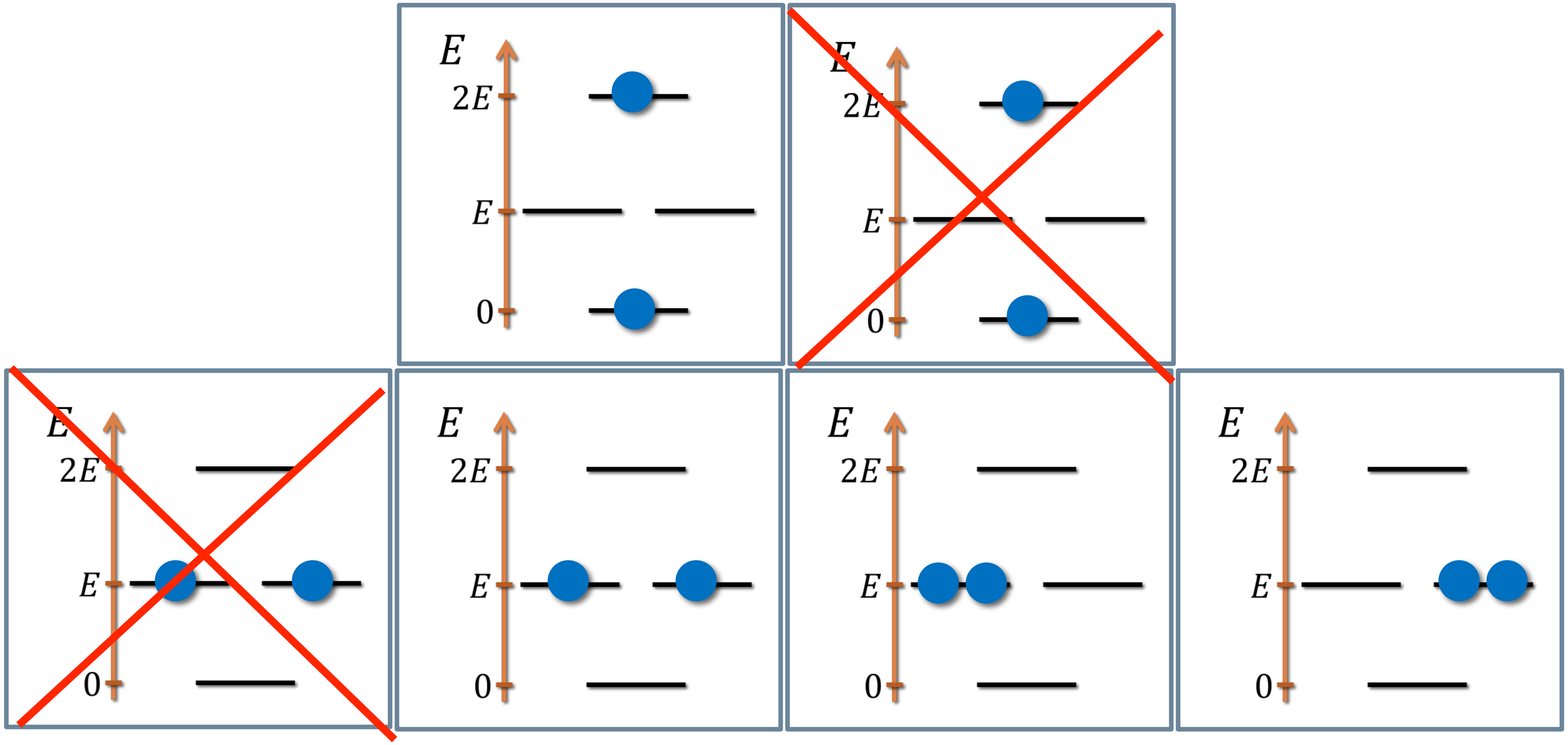


In this example, implicitly we assumed classical particles, which are distinguishable (red and blue) and which do not obey the Pauli's exclusion principle (microstate 5 and 6).

Bosons

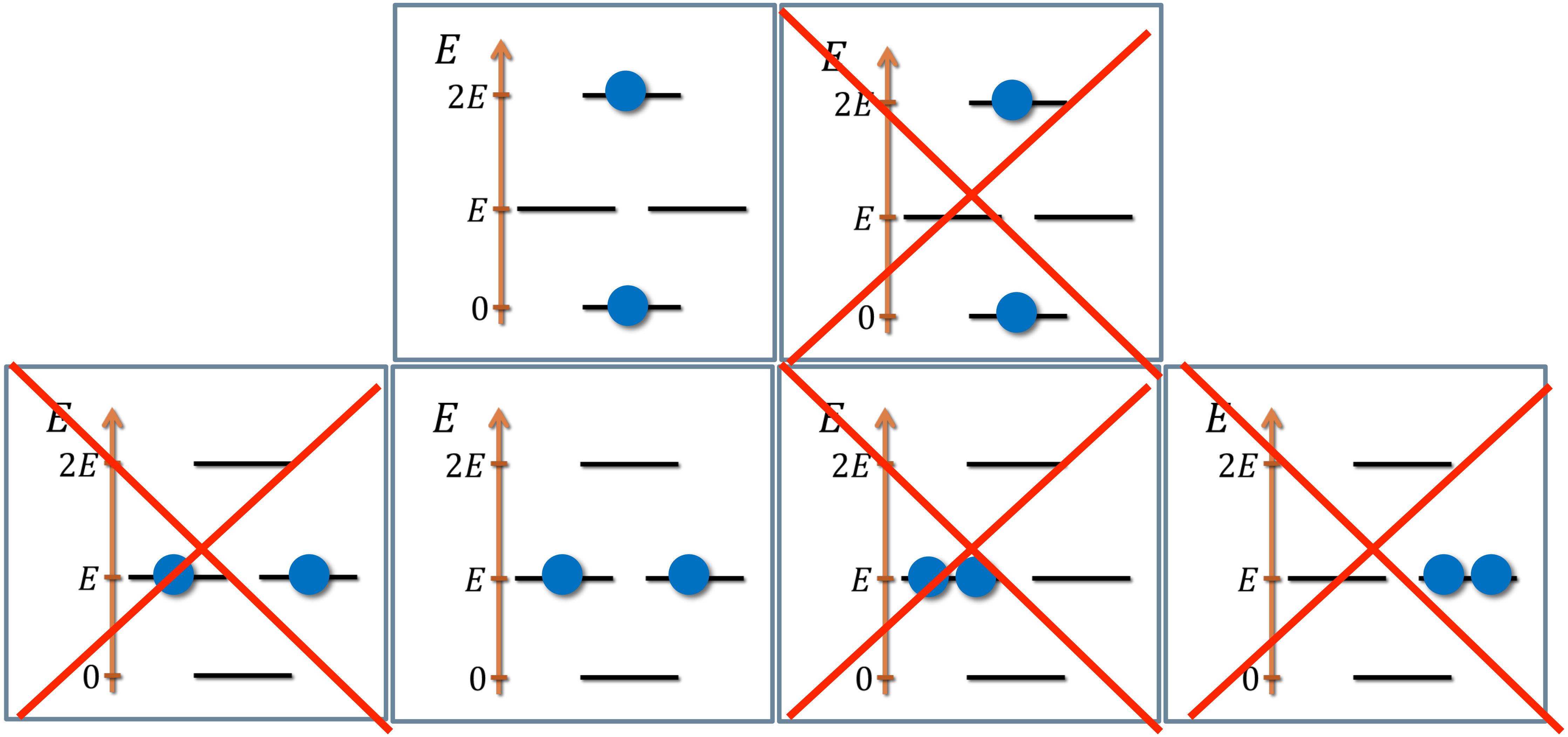


Bosons



The (0,2,0) configuration is thrice as probable as the (1,0,1).

Fermions



The (0,2,0) configuration is equally probable as the (1,0,1).

Statistical Physics

General problem (M-B, B-E, F-D)

Given a system with set of energy states E_i (0, E, 2E), each with degeneracy g_i (1, 2, 1)

with a fixed amount of energy, E(2E), and a fixed number of particles, N(2),

what is the most probable set of $N_i \equiv N(E_i)$ or most probable configuration?

In case of the classical particles, we found that the configuration $N_1 \equiv N(E_1) = N(2E) = 0$, $N_2 \equiv N(E_2) = N(E) = 2$ and $N_3 \equiv N(E_3) = N(0) = 0$ or (0,2,0) is the "more" probable one.

Statistical Physics

General problem (M-B, B-E, F-D)

$$\sum_{i=1}^{\infty} N_i = N$$

$$\sum_{i=1}^{\infty} E_i N_i = E$$

State Index (i)	State Energy (E_i)	State Degeneracy (g_i)	State Occupancy (N_i)
1	E_1	g_1	N_1
2	E_2	g_2	N_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$
i	E_i	g_i	N_i
$\vdots$	$\vdots$	$\vdots$	$\vdots$

Here we are generalizing the problem for a larger system. We are looking for $\{N_i\} \equiv (N_1, N_2, \ldots N_i \ldots)$

Equilibrium Configuration

The configuration for which the number or **multiplicity** of microstates is maximum corresponds to the most probable configuration.

This configuration is called the **equilibrium configuration**.

If the total energy E of the system is provided to the system as heat, so that it reaches an equilibrium temperature T, then this configuration is the most probable one at **thermal equilibrium** at temperature T**.**

Equilibrium Configuration

So the general problem we are trying to solve is, given a system with

$$\sum_{i=1}^{\infty} N_i = N$$

$$\sum_{i=1}^{\infty} E_i N_i = E$$

What is the configuration $\{N_i\} \equiv (N_1, N_2, \ldots N_i \ldots)$ for which the multiplicity $Q(\{N_i\})$ is maximum?

For this, we have to first learn how to calculate $Q(\{N_i\})$.

Recommended Readings

Statistical Physics, Chapter 10