24 March

Logistics

Say something if you can't hear me

Final assessment info to come by Friday

Feedback on week 6 assignment by Friday

Computer project part A due 3 April

Let me know of any dificulties – especially setting up

Plan for this week

Will return to anomalous diffusion of Friday

& part B of computer project

Today complete quantum gases (fermion case)

Maybe look ahead to systems of interacting objects

Recap – Any questions?

Quantum gases as application of <u>grand-canonical ensemble</u>

Work with fixed temperature (T) and chemical potential μ

to hide role of heat-bath and particle reservoir

Internal energy and particle number can fluctuate

$$\langle E \rangle = -T^2 \frac{\partial}{\partial T}\left(\frac{\Omega}{T}\right) + \mu \langle N \rangle = \Omega + T \cdot S + \mu \langle N \rangle$$

entropy $S = \frac{-\partial \Omega}{\partial T}$

$$\langle N \rangle = -\frac{\partial \Omega}{\partial \mu}$$

$$\Omega(T,\mu) = -T \ln Z_g(T,\mu) = -T \ln\left[\sum_{i=1}^{M} \exp(-\beta E_i + \beta\mu N_i)\right] \qquad \beta = \frac{1}{T}$$

grand potential — partion function — micro-states

Quantum gases

Countable discrete energy levels

Sum over microstates → sum over occupation numbers n_ℓ
For each energy level E_ℓ

Bose statistics: $n_\ell = 0, 1, 2, \dots$
Any number of "bosons" in each individual state

Fermi statistics: $n_\ell = 0, 1$
At most one "Fermion" in each individual state

Both become classical in appropriate high-temperature limit
$T \to \infty$ and $\mu \to -\infty$ such that $-\mu \gg T \gg E_\ell$
(Many more energy levels than particles
→ good approximation to sum over all energies each particle can have)

Photon gas: "Ultra-relativistically" gas of bosons

$$\hookrightarrow E_{ph} = \hbar\omega = \hbar c p = \frac{2\pi\hbar c}{\lambda}$$

momentum, wavelength

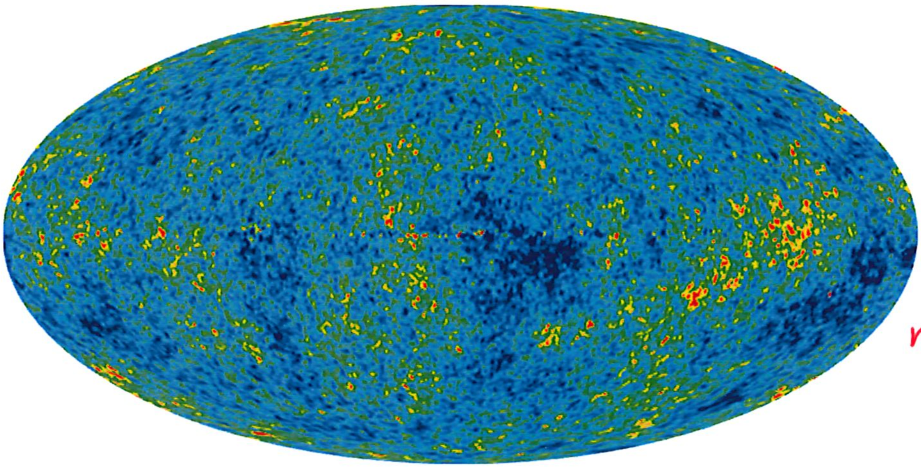
$$\langle E \rangle = \int P(\omega)\, \omega \qquad P(\omega) = \frac{\hbar V}{c^3 \pi^2} \frac{\omega^3}{\exp(\hbar\omega/T) - 1}$$

Planck spectrum

$P(\omega)$ is good mathematical model based on non-interacting gas
for physical systems from sun & stars
to "background" microwaves filling empty space

Full sky subtracting sun, stars, galaxies

Spectrum of the night sky (not from the stars): The Cosmic Microwave Background temperature fluctuations from the 7-year Wilkinson Microwave Anisotropy Probe data seen over the full sky.

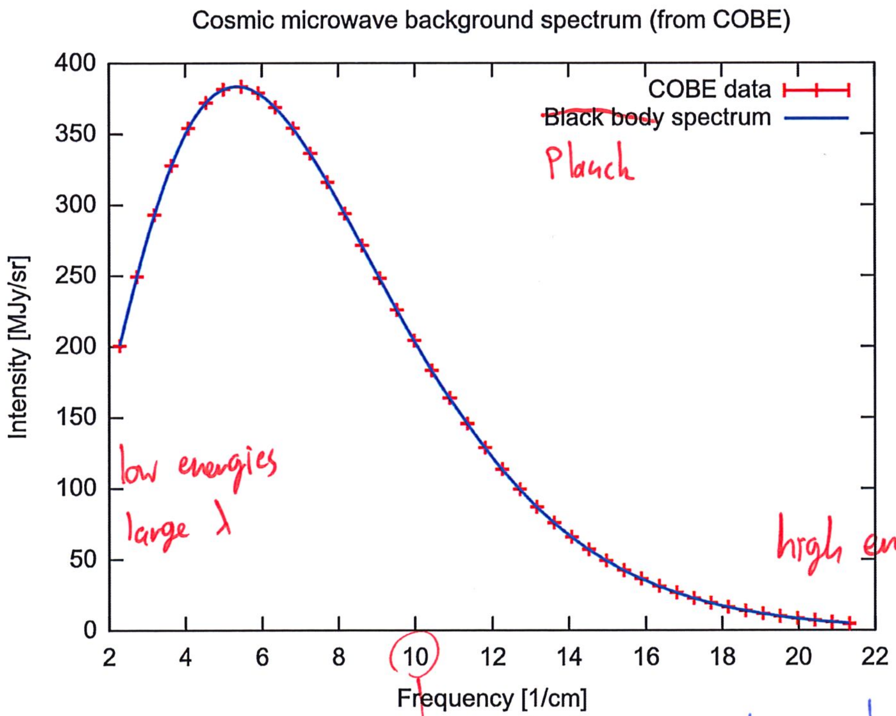


temperature of empty space

$T \approx 2.7\,K$

red - blue : ~~[illegible]~~

$\Delta T = 0.0002\,K$



~~$\lambda \approx 100{,}000\,\mu m$~~

$10\,\frac{1}{cm} = \frac{1}{0.1\,cm} = \frac{1}{\lambda}$

$\lambda = 0.1\,cm = 1{,}000\,\mu m$

Conclusion: Non-interacting Planck distribution of photon gas good mathematical model for real physical systems

8.2 Quantum gas of fermions

still grand-canonical

Let us consider a non-relativistic gas of fermions. We again adopt the experimental setup of a heatbath (temperature T) and particle reservoir (chemical potential μ).

still non-interacting

We already worked out the energy spectrum in section 5.1:

momentum, non-negative integers

$$E(p) = \frac{p^2}{2m}, \qquad p = |\vec{p}|, \qquad \vec{p} = \hbar \frac{\pi}{L} \vec{m}, \qquad \vec{m} \in \mathbb{N}^3 .$$

particle mass

We already calculated the statistics for systems of fremions (see (80)) and were able to reduce it to sum over the energy spectrum. We thus obtain:

$$-\frac{\Omega}{T} = \ln Z_{fermi} = \sum_{\vec{m}} \ln \left[1 + \exp\left(- \frac{\vec{p}^2}{2mT} + \frac{\mu}{T} \right) \right] .$$

$(-\vec{p})^2 = (\vec{p})^2$

We assume sufficiently large volumes so that we can replace:

$$\sum_{m=0}^{\infty} \quad \to \quad \frac{1}{2} \sum_{m=-\infty}^{\infty} \quad \to \quad \frac{1}{2} \int_{-\infty}^{\infty} dm .$$

$$dm_i = \frac{L}{\hbar \pi} dp_i$$

$$\left(\frac{1}{2}\right)^3 \int dm_1\, dm_2\, dm_3 = \left(\frac{L}{2\pi\hbar}\right)^3 \int d^3p = \frac{V\, 4\pi}{(2\pi\hbar)^3} \int_0^\infty dp\, p^2$$

We finally observe:

$$\ln Z_{fermi} = \frac{V}{2\pi^2 \hbar^3} \int_0^\infty dp\, p^2 \ln \left[1 + \exp\left(- \frac{E(p) - \mu}{T} \right) \right] . \tag{85}$$

A new quantum phenomenon comes to light if we study the particle number:

$$-\frac{\partial \Omega}{\partial \mu} = \langle N \rangle = T \frac{\partial \ln Z_{fermi}}{\partial \mu} = \frac{V}{2\pi^2 \hbar^3} \int_0^\infty dp\, p^2 \frac{1}{\exp\left(\frac{E(p)-\mu}{T}\right) + 1} \tag{86}$$

$$\langle N \rangle = \frac{V}{2\pi^2 \hbar} \int_0^\infty dp\, p^2\, n(p)$$

$\downarrow$

$n(E)$ via $E = \frac{p^2}{2m}$

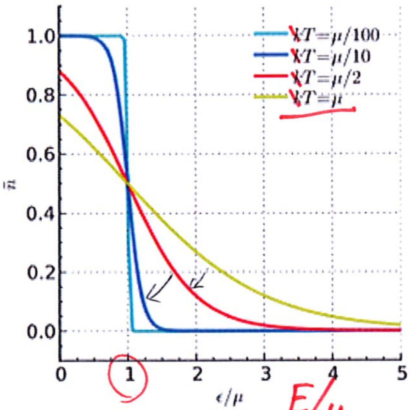
Let us study the so-called Fermi[13] function

$$n(E) = \frac{1}{\exp\{\frac{E-\mu}{T}\}+1} . \qquad E = \frac{p^2}{2m}$$

$T = \frac{\mu}{x}$

$\exp\left(\frac{E-\mu}{T}\right) = \exp\left[x\left(\frac{E}{\mu}-1\right)\right]$

n



E/μ

E/μ passing through 1

change sign $\exp(\pm x)$

Larger x → smaller $T = \frac{\mu}{x}$

sharper change

low-T $n_e = 1$ $\exp(-x) \ll 1$

high-T $n_e = 0$ $\exp(x) \gg 1$

$\mu \to -\infty$

For large temperatures, we enter the classical regime, and we have done the calculation in section 5.1. Let us focus on the cold regime, where we can approximate the Fermi function by a step function: quantum

$$n(E) \approx \begin{cases} 1 & \text{for} \quad E < \mu \\ 0 & \text{else} \end{cases} . \qquad \int_0^\infty dp\, p^2\, n(p) = \int_0^{\sqrt{2m\mu}} dp\, p^2$$

It means that we can cut integrals such as (86) when $E(p)$ reaches μ. It is therefore convenient to switch from the momentum variable p to the energy variable E by substitution:

$$E = \frac{p^2}{2m}, \qquad p = \sqrt{2m\,E}\,, \qquad dp = \sqrt{\frac{m}{2E}}\, dE\,.$$

This, we find from (86):

$$\langle N \rangle = \frac{V}{2\pi^2\hbar^3}\int_0^{\sqrt{2m\mu}} dp\, p^2 = \langle N \rangle \approx \frac{V\,m^{3/2}}{\sqrt{2}\,\pi^2\hbar^3}\int_0^\mu dE\,\sqrt{E} = \frac{\sqrt{2}\,V\,m^{3/2}}{3\,\pi^2\hbar^3}\,\mu^{3/2}\,. \tag{87}$$

[13]Enrico Fermi 1901 – 1954), was an Italian–American physicist and the creator of the world's first nuclear reactor, the Chicago Pile-1.

$$\langle N \rangle \propto \int^{\sqrt{\mu}} dp_1 \int^{\sqrt{\mu}} dp_2 \int^{\sqrt{\mu}} dp_3 = \mu^{3/2}$$

This is the desired relation between particle number and chemical potential. This relation does not depend on the temperature T because we are basically looking at the leading order of the low temperatuer expansion. Higher orders in the temperature can be systematically taken into account. This can be found in the literature under the name *Sommerfeld*[14] *expansion.*

$\langle N \rangle \propto \mu^{3/2}$

$T = 0$

Along the same lines, we can calculate the internal energy: Trich: $\sum_{l=1}^{L} E_l n_l = E_i$ vs. $\sum_{l=1}^{L} n_l = N_i$

$$\langle E \rangle = \frac{V}{2\pi^2\hbar^3}\int_0^\infty dp\, p^2 \frac{E(p)}{\exp\left(\frac{E(p)-\mu}{T}\right)+1} = \frac{V\, m^{3/2}}{\sqrt{2}\pi^2\hbar^3}\int_0^\infty dE\, E\sqrt{E}\, n(E)$$

step func.

$$\approx \frac{V\, m^{3/2}}{\sqrt{2}\pi^2\hbar^3}\int_0^\mu dE\,\sqrt{E}\, E = \frac{\sqrt{2}\, V\, m^{3/2}}{5\,\pi^2\hbar^3}\,\mu^{5/2} = \frac{3}{5}\,\mu\,\langle N \rangle\,. \tag{88}$$

$\langle E \rangle \sim \mu \langle N \rangle$

We make a very important observation:

Key observation: although the temperature vanishes, the thermal energy $\langle E \rangle$ is different from zero. (positive)

INTERPRETATION:

Ground state with $E_0 = 0$ can hold only one Fermion!
Then only one in next-lowest-energy state
and so on, will all states "filled", $n_l = 1$
up to $E_{max} = \mu$
(Fermi energy)

[14] Arnold Johannes Wilhelm Sommerfeld, 1868 – 1951, was a German theoretical physicist who pioneered developments in atomic and quantum physics.

Equation of state for grand-canonical ensemble

A surprise is waiting for us if we look at the pressure (52): pg. 72

$$p = -\frac{\partial \langle E \rangle}{\partial V}\Big|_{S,N}. \qquad (89)$$

fix particle #

The derivative has to be taken at constant entropy S, and we need to handle S first:

$$S = \frac{\partial}{\partial T}\left(\ln Z_{fermi}\right). = -\frac{\partial \Omega}{\partial T} = +\frac{\partial}{\partial T}(+T \ln Z_g)$$

Let us consider the function

$$\ln\left[1 + \exp\left(-\frac{E-\mu}{T}\right)\right]$$

for small temperatures T:

INTERPRETATION:

All occupied energy levels have $E \le \mu$

So $-\frac{E-\mu}{T} = \frac{\mu - E}{T} \gg 1, \quad \exp\left(\frac{\mu-E}{T}\right) \gg 1$

$$\ln\Big[\underbrace{1}_{\text{negligible}} + \exp\left(\frac{\mu-E}{T}\right)\Big] \approx \ln\left(\exp\left(\frac{\mu-E}{T}\right)\right) = \frac{\mu-E}{T}$$

$$\ln Z_{fermi} = \frac{V m^{3/2}}{\sqrt{2}\,\pi^2 \hbar^3}\int_0^{\mu} dE\,\sqrt{E}\,\ln\left[1 + \exp\left(-\frac{E-\mu}{T}\right)\right]$$

Hence, we find for (85):

$$\ln Z_{fermi} = \frac{V m^{3/2}}{\pi^2 \hbar^3}\int_0^{\mu} dE\,\sqrt{E}\,\frac{\mu - E(p)}{T}$$

$T \ln Z_{fermi} = \text{const. in } T$

This implies that, whatever $E(p)$ is that $T\ \ln Z_{fermi}$ is independent of T and, thus, the entropy vanishes.

$$S = \frac{\partial}{\partial T}\left(T \ln Z_{fermi}\right) = 0$$

INTERPRETATION:

$S = \ln M = 0$ $\qquad$ $M = \exp(S) = 1$

↳ # of micro-states

Only a single micro-state for sufficiently low T

All energy levels with $E_\ell \leq E_F = \mu$ filled, $n_\ell = 1$

We can make μ the subject of the equation (87) and insert this into the equation (88) for the thermal energy.

$$\langle N \rangle = \frac{\sqrt{2}\, V\, m^{3/2}}{3\pi^2 \hbar^3} \mu^{3/2} = C V \mu^{3/2}$$

$$\mu = (CV)^{-2/3} \langle N \rangle^{2/3}$$

$$\langle E \rangle \;=\; \frac{2}{5} \langle N \rangle^{5/3} \frac{\hbar^2}{m} V^{-2/3} \,.$$

We now can use equation (89) to calculate the pressure (Note that $\langle N \rangle$ is treated as a constant, and the entropy S is also constant, namely zero):

$$-\frac{\partial \langle E \rangle}{\partial V}\bigg|_{S,N} = p \;=\; \frac{\cancel{4}}{15} \frac{\hbar^2}{m} \rho^{5/3} \,, \qquad \rho := \frac{\langle N \rangle}{V} \quad \text{(density)} \,.$$

"degeneracy pressure"

The intersting observation is that the pressure *does not vanish* at zero temperature. It is a pure quantum effect that keeps up the pressure.

$p > 0 \quad T = 0$

At high temperature, we recover the ideal (classical) gas with the equation of state:

$$pV \;=\; \langle N \rangle T \,, \qquad p \;=\; \rho\, T \,.$$

We thus have qualitatively the following function $p(T)$:

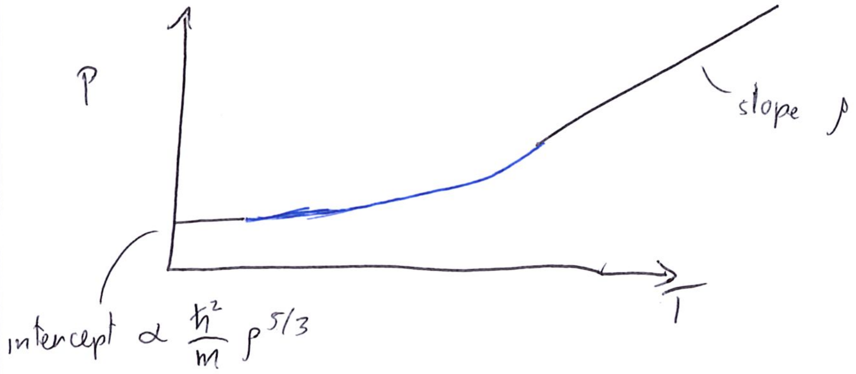
$$\langle E \rangle = \frac{3}{5} \mu \langle N \rangle = \frac{3}{5 C^{2/3}} V^{-2/3} \langle N \rangle^{5/3} = \frac{3}{5} \left(\frac{3\pi^2}{\sqrt{2}} \right)^{2/3} \frac{\hbar^2}{m} \langle N \rangle^{5/3} V^{-2/3}$$

$$p = \frac{-\partial \langle E \rangle}{\partial V}\bigg|_{S,N} = \frac{2}{5 C^{2/3}} \left(\frac{\langle N \rangle}{V} \right)^{5/3} = \frac{2}{5} \left(\frac{3\pi^2}{\sqrt{2}} \right)^{2/3} \frac{\hbar^2}{m} \rho^{5/3}$$

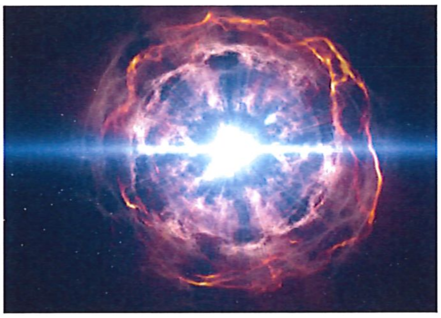
$$p = \frac{2}{5 C^{2/3}} \left(\frac{\langle N \rangle}{V} \right)^{2/3} \left(\frac{\langle N \rangle}{V} \right) = \frac{2}{5} \mu \frac{\langle N \rangle}{V}$$

$$pV = \frac{2}{5} \mu \langle N \rangle$$

INTERPRETATION:



This explains a cosmic phenomenon - the supernova explosion of stars:



Degeneracy pressure of inert core
balance gravitational "weight"
of very dense star

Huge amount of matter
can pile up ...
until it all collapses
(Chandrasekhar limit)

Implosion → very quickly increase in pressure and temperature
→ huge pressure
→ explosion

9 Phase transitions

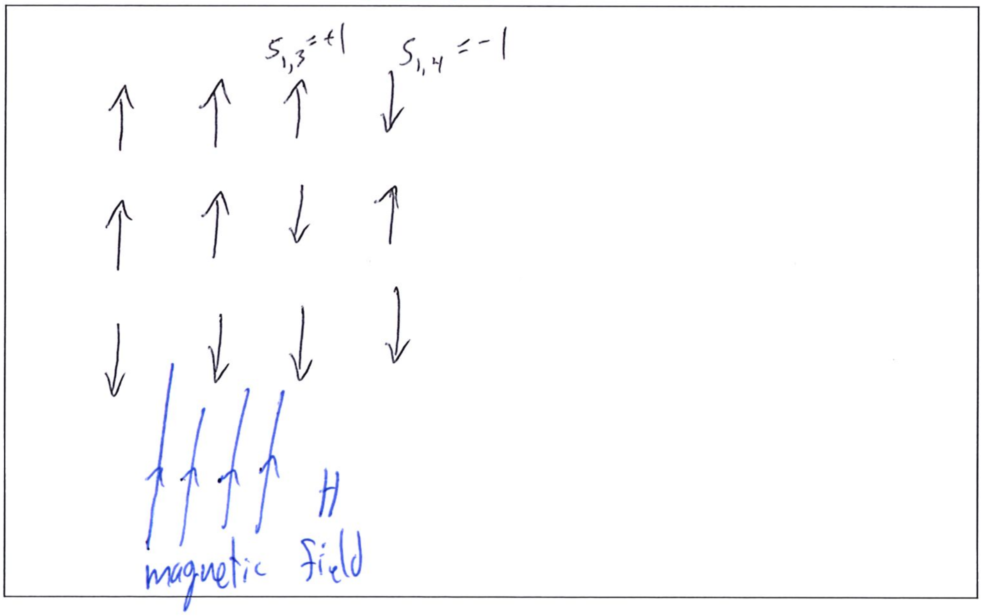
Phase transitions are a spectacular phenomenon in statistical physics. They describe e.g. the phenomenal transition from a liquid to a solid at freezing point, but also more elusive phenomena such as the transition form a quark gluon plasma to protons and neutrons in the Early Universe roughly one millionth of a second after the Big Bang. What does it take to describe such a drastic change in the properties of matter?

insulator
↓
conductor

A second question, which we going to study, is: what is actually the fundamental difference between matter in either phase? For example, what is the difference between ice and water? After all, both substances are made out of the same constituents namely H_2O molecules.

9.1 Interacting theories

Key ingredient, and in many cases a sufficient ingredient, is some (e.g. short range) interaction between the degrees of freedom of our statistical ensemble. We will address both questions above by means of the now familiar spin model: degrees of freedom are the spins $s_i \in \{-1, +1\}$, where i labels the postion of the spin in e.g. a spin chain or a lattice:



Once we know the energy E of the spin system, we can start to do statistics and e.g. expose the system of spins to a heatbath with temperature T. We have previously studied spins interacting with an external magnetic field H:

$$E = H \sum_i s_i \qquad \text{(non-interacting)} .$$

Sum over energies of each spin

What qualifies this spin system as *non-interacting*?

Defintion: ΔE_i is the change of the total energy E of a statistical system if *only* the state of the ith degree of freedom is changed. If ΔE_i is independent of all degrees of freedom $k \neq i$, the statistical system is called *non-interacting*.

Let us check whether the above spin model satisfies this condition:

$$E_{\text{before}} = H \sum_k s_k = H \Big(\cancel{\sum_{k \neq i} s_k} + s_i \Big)$$

$$E_{\text{after}} = H \Big(\cancel{\sum_{k \neq i} s_k} - s_i \Big)$$

$$\Delta E_i = E_{\text{after}} - E_{\text{before}} = -2 H s_i$$

The above property has far reaching mathematical consequences, namely the possibility to calculate the partition function in closed form (see also (32)):

$E_i = H s_i \qquad Z_1 = \exp(-\beta E)$

$$Z_{dist} = \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} \exp\left[-\beta \sum_i s_i\right]$$

$$= \left(\sum_{s_1=\pm 1} \exp(-\beta H s_1)\right) \times \cdots \times \left(\sum_{s_N=\pm 1} \exp(-\beta H s_N)\right)$$

$$= \left(e^{-\beta H} + e^{\beta H}\right) \times \cdots \times \left(e^{-\beta H} + e^{\beta H}\right)$$

$$= \left(e^{-\beta H} + e^{\beta H}\right)^N$$

How strenuous would be the calculation if we would *not* have the factorisation property? In the case of N spins, we need to do the sum

$$\sum_{\{s_i\}} = \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} .$$

This sum has 2^N terms. This calculation gets quickly out of hands:

$$2^{100} \approx 1.26 \times 10^{30} , \qquad 2^{10,000} \approx 2.00 \times 10^{3010} .$$

The later sum is even out of reach of modern supercomputers.

Before we make the above spin system *interacting*, we introduce the lattice and related objects: *site, link, plaquette, and cube.*