Thermal distributions 5

The Fermi-Dirac distribution

Modern physics for engineers

David Miller

The Fermi-Dirac distribution

Because of Pauli exclusion

states for fermions, such as

a $\mathbf{k}$ state in a semiconductor band

or an orbital in an atom

can only be occupied by

one electron of a given spin

For such fermions of a given spin

we can derive a form for

their distribution with temperature

based on the Gibbs factor

The Fermi-Dirac distribution

Suppose system M is in a particular state

- for a fermion of a given spin

So, we only have two possibilities for N for this state

- Either $N = 1$, with an energy ε
  - or $N = 0$, with an energy 0

The Fermi-Dirac distribution

- The Gibbs factor gives relative probabilities
  - To get to absolute probability here
    - we divide by the sum of the relative probabilities
      - here, for the two different possibilities
- Then the absolute probabilities add up to one

Partition function

Such a sum of relative probabilities over all possible states

is known as a "partition function", often denoted by Z

For a single state for a fermion

the partition function is particularly simple

It just has two possible terms in it

For energy 0 and $N = 0$

the Gibbs factor is $\exp\left[\left(0 \times \mu_C - 0\right) / \tau\right] = 1$

and for energy ε and $N = 1$ it is $\exp\left[\left(1 \times \mu_C - \varepsilon\right) / \tau\right]$

So $Z = 1 + \exp\left[\dfrac{\left(\mu_C - \varepsilon\right)}{\tau}\right]$

The Fermi-Dirac distribution

To get the absolute probability

for occupation of this state of energy ε

we divide the relative probability of occupation

which is the Gibbs factor $\exp\left[\left(\mu_C - \varepsilon\right)/\tau\right]$

by the sum of these two relative probabilities

that is, by the partition function Z

So, the probability that this state is occupied is

$$P\left(N=1,\varepsilon\right) \equiv f\left(\varepsilon\right) = \frac{\exp\left[\left(\mu_C - \varepsilon\right)/\tau\right]}{1+\exp\left[\left(\mu_C - \varepsilon\right)/\tau\right]}$$

The Fermi-Dirac distribution

Multiplying the top and bottom lines of

$$P(N=1,\varepsilon) \equiv f(\varepsilon) = \frac{\exp\left[(\mu_C - \varepsilon)/\tau\right]}{1+\exp\left[(\mu_C - \varepsilon)/\tau\right]}$$

by $\exp\left[(\varepsilon - \mu_C)/\tau\right]$

gives the Fermi-Dirac distribution

$$f_{FD}(\varepsilon) = \frac{1}{\exp\left[(\varepsilon - \mu_C)/\tau\right]+1}$$

The Fermi-Dirac distribution

Conventionally, for electrons $f_{FD}(\varepsilon) = \dfrac{1}{\exp\left[(\varepsilon - \mu_C)/\tau\right] + 1}$

is written as

$$f_{FD}(E) = \frac{1}{\exp\left(\dfrac{E - E_F}{k_B T}\right) + 1}$$

The chemical potential for fermions

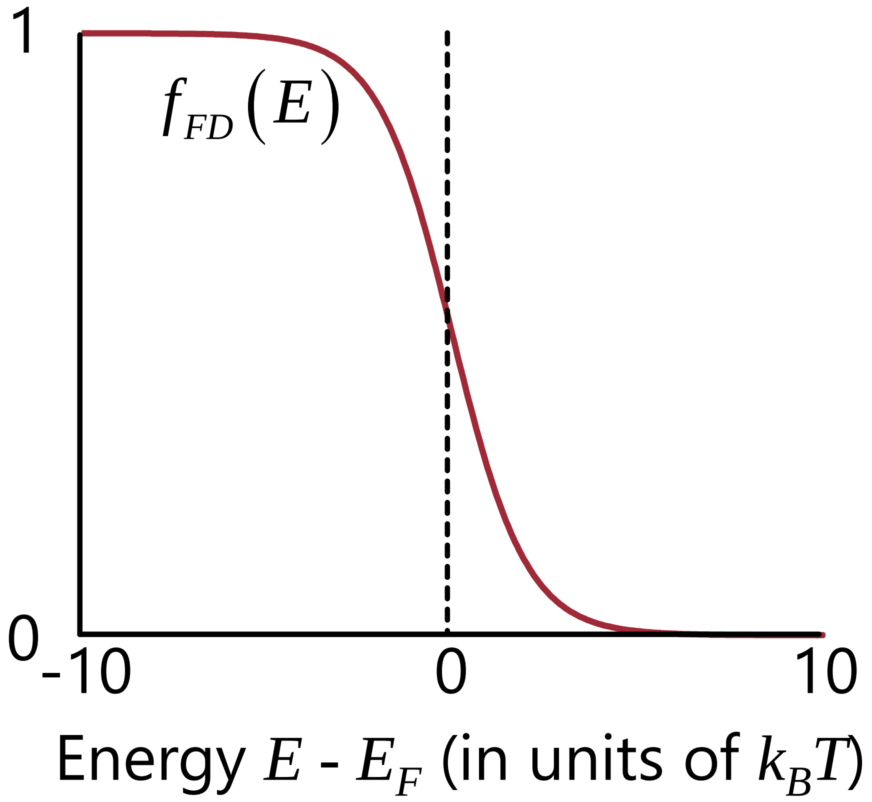
is conventionally called the Fermi energy

Note these are *exactly* the same concept, that is

$$E_F \equiv \mu_C$$

Fermi-Dirac distribution

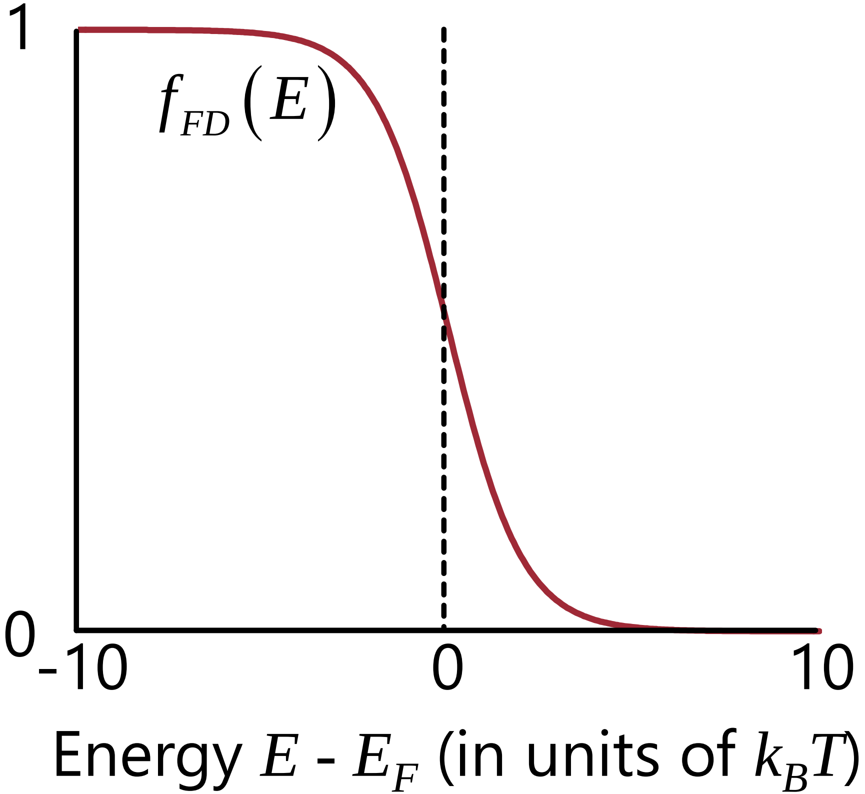
$$f_{FD}(E) = \frac{1}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1}$$



Fermi-Dirac distribution

For states of energies many $k_B T$ below the Fermi level

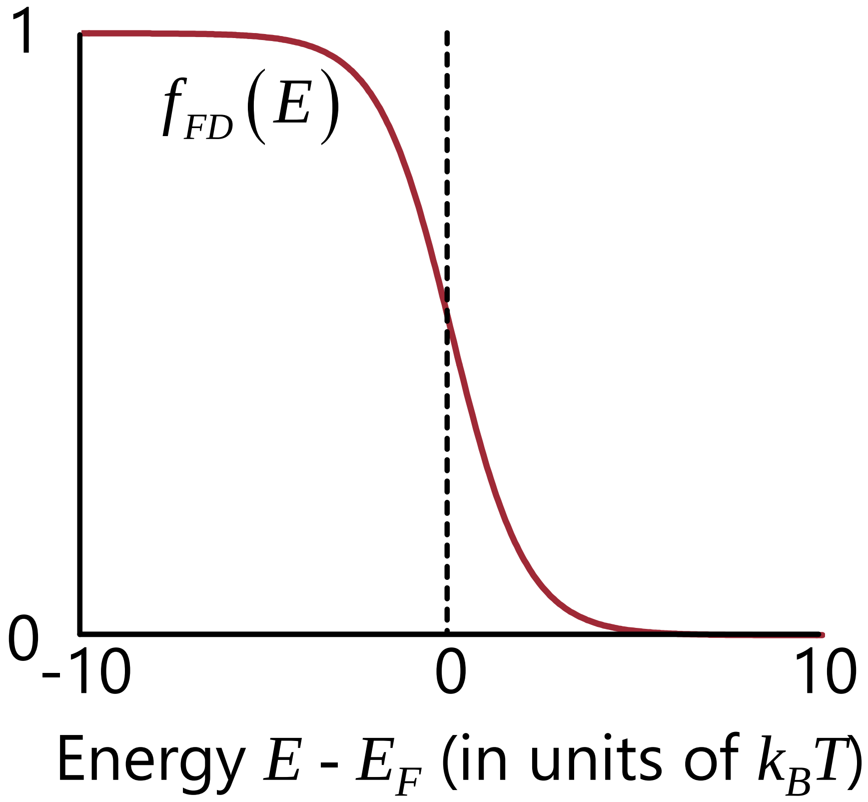
- the probability of occupation of any such state
  - gradually approaches 1
    - It cannot exceed 1
      - because we cannot have more than one electron in a state



Fermi-Dirac distribution

For a state of energy exactly equal to the Fermi level

- the probability of occupation is ½
  - which is sometimes used
    - as a practical definition of the Fermi level



Fermi-Dirac distribution

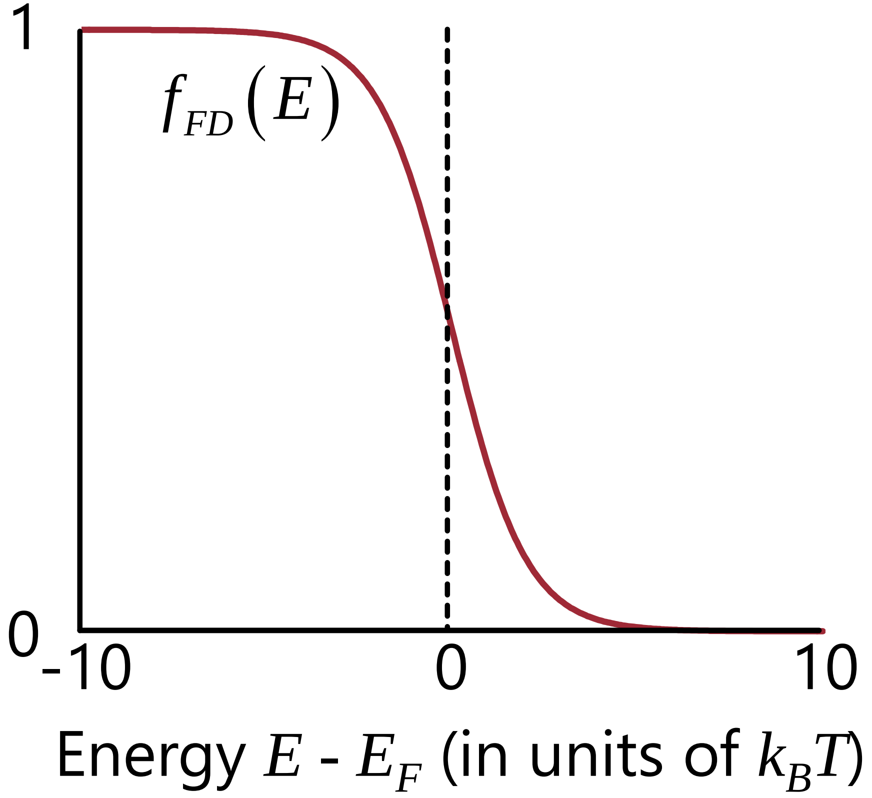
For states of energies many $k_B T$ above the Fermi level

the probability of occupation of any such state

gradually approaches 0

States within a few $k_B T$ of the Fermi level

have intermediate probabilities of occupation



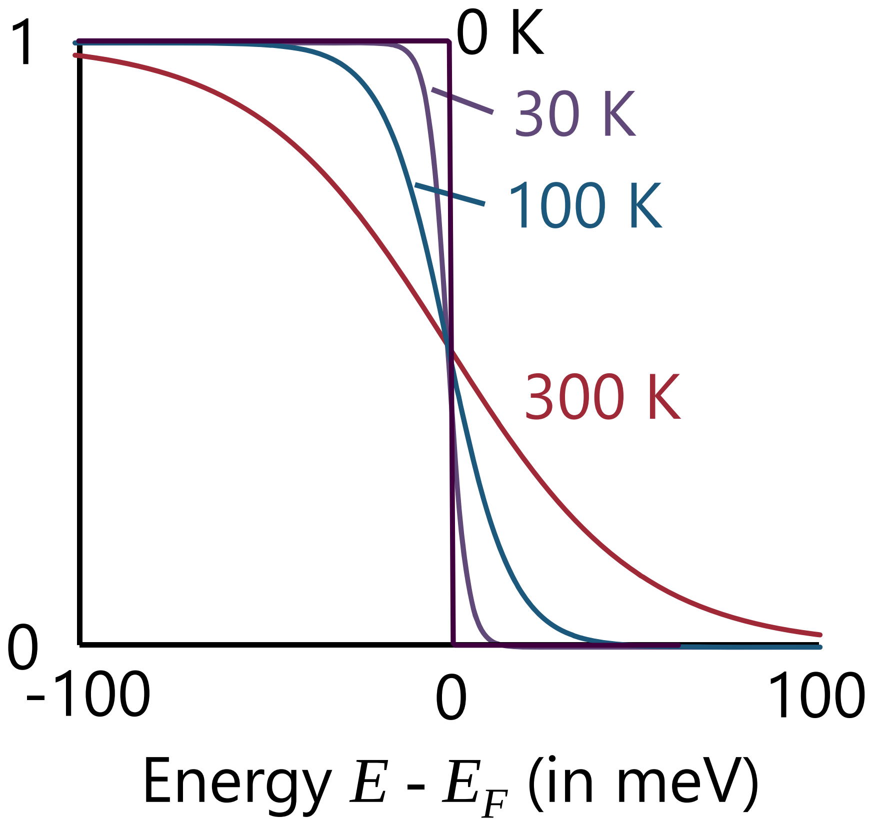
Fermi-Dirac distribution

At or close to absolute zero

- states below the Fermi level are essentially all occupied and
- states above the Fermi level are essentially all empty

With increasing temperature

- the curve "softens"
  - with a width of the "softening"
  - of the order of a few $k_B T$



Thermal distributions 5

The Bose-Einstein and Planck distributions

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Bose-Einstein distribution

- We can follow a similar argument for bosons
  - starting with the Gibbs factor
- The partition function is more complicated
  - because we are not restricted to just $N = 0$ or $N = 1$

Bose-Einstein distribution

The result is the Bose-Einstein distribution

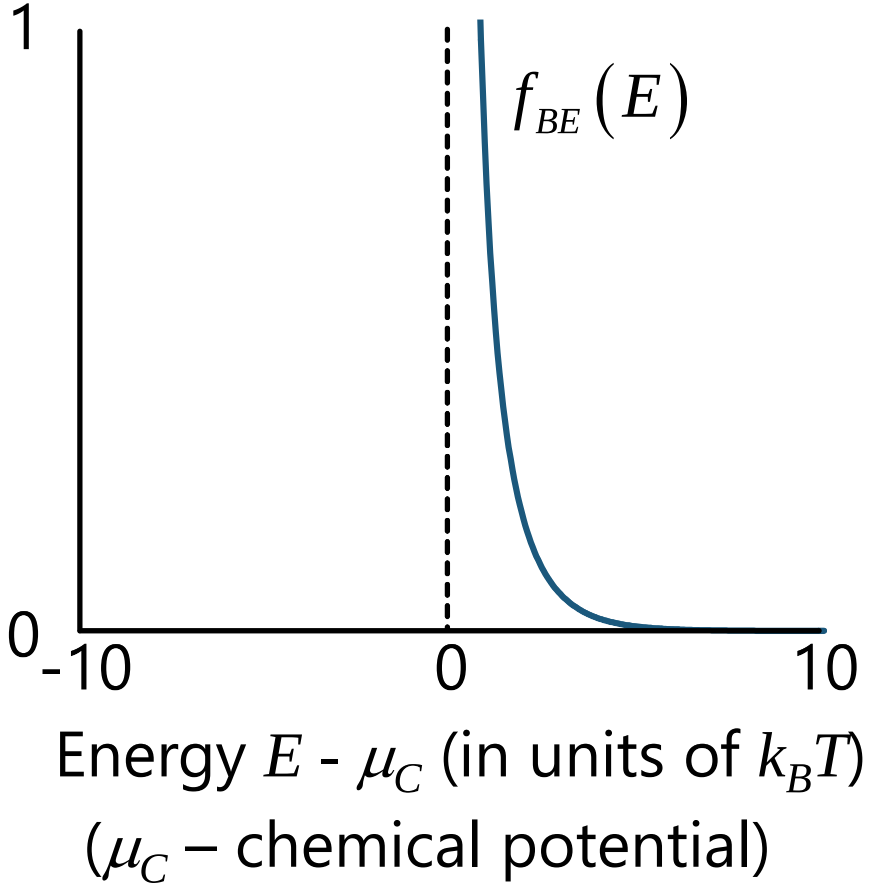
the expected number of bosons

in a boson mode of energy E per boson is

$$f_{BE}(E) = \frac{1}{\exp\left(\dfrac{E - \mu_C}{k_B T}\right) - 1}$$

Bose-Einstein distribution

$$f_{BE}(E) = \frac{1}{\exp\left(\frac{E - \mu_C}{k_B T}\right) - 1}$$



Bose-Einstein distribution

In its full form with the chemical potential

$$f_{BE}(E) = \frac{1}{\exp\left(\frac{E-\mu_C}{k_B T}\right) - 1}$$

In applications, the Bose-Einstein distribution

is used less often than the Fermi-Dirac distribution

Bose-Einstein distribution

- This is because most of the bosons in device applications
  - are photons, phonons, or similar quanta
    - associated with oscillations
- Unlike an atom, they have no excited states
  - This simplifies the resulting distribution

Bose-Einstein distribution

So

exchange of energy between the system and the reservoir

and

exchange of particles between the system and the reservoir

are the same physical process

Bose-Einstein distribution

So there is no need for two separate parameters

- temperature and chemical potential
  - to be matched to reach equilibrium

We only need one such parameter to equilibrate

- and by convention we use temperature

Planck distribution

Such bosons obey a simpler version of the Bose-Einstein distribution

- called the Planck distribution
  - Writing the energy for these bosons in the form $E = \hbar\omega$
    - where ω is mode's angular frequency
      - the Planck distribution is

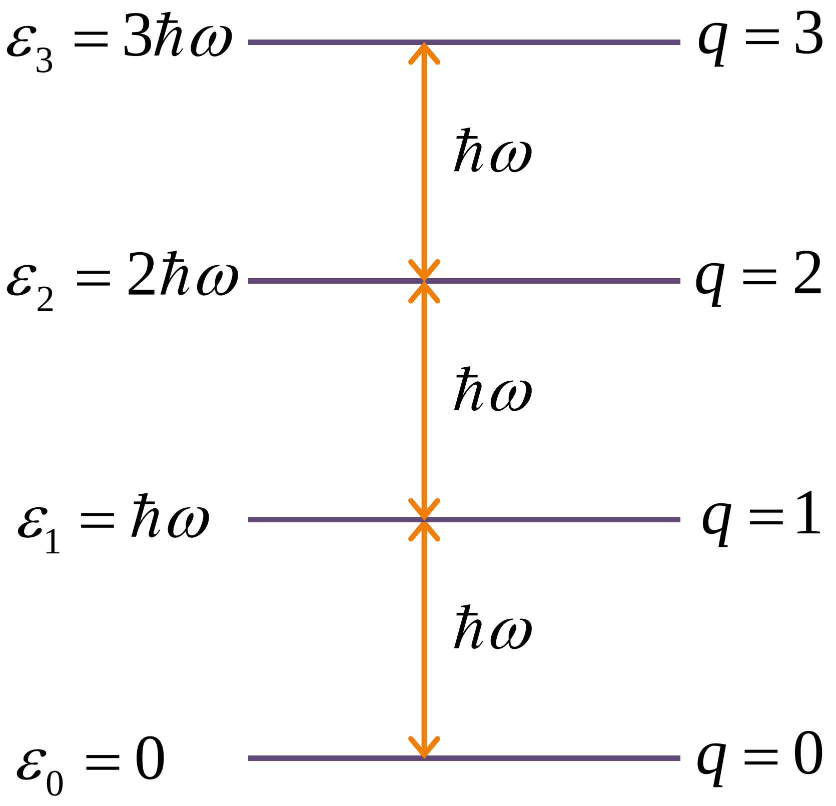
$$f_P(\hbar\omega) = \frac{1}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

It gives the number of such bosons per mode

Planck's distribution derivation

Planck's distribution

- Now consider a mode for light
  - e.g, a standing wave in a box
- We propose this mode of angular frequency ω
  - can be in one of several states
    - separated by an energy $\hbar\omega$
- The quanta of energy that separate the levels
  - can be described as photons
    - so q photons in the mode



Planck's distribution

The energy of such a mode can therefore be described as $\varepsilon_q = qh\nu \equiv q\hbar\omega$

- where q is zero or a positive integer
- possibly plus some overall additive constant
  - which will not matter in the end

We presume that, in equilibrium with a reservoir at temperature T

- the relative occupation probability of a state of energy ε_q compared to a state of energy 0
  - is given by the Boltzmann factor $\exp\left(-\varepsilon_q / k_B T\right)$

Planck's distribution

To get the absolute probability of finding the oscillator in the state of energy $\varepsilon_q = q\hbar\omega$

we need to normalize the relative probability $\exp\left(-\varepsilon_q / k_B T\right)$

by dividing by the sum (the partition function) Z

of all relative probabilities $Z = \sum_{q=0}^{\infty} \exp\left(-q\hbar\omega / k_B T\right)$

This sum is a geometric series

which sums to $Z = 1/\left[1 - \exp\left(-\hbar\omega / k_B T\right)\right]$

So the probability of finding the mode in the state with energy ε_q is

$$P(q) = \frac{\exp\left(-q\hbar\omega / k_B T\right)}{Z}$$

Planck's distribution

The average value of q for this mode

in thermal equilibrium at temperature T is therefore

$$\langle q \rangle = \sum_{q=0}^{\infty} q P(q) = \frac{1}{Z} \sum_{q=0}^{\infty} q \exp\left(-q\hbar\omega / k_B T\right)$$

Now we can use a mathematical trick, noting that

$$\sum_{q=0}^{\infty} q \exp\left(-qy\right) = -\frac{d}{dy}\left[\sum_{q=0}^{\infty} \exp\left(-qy\right)\right] = -\frac{d}{dy}\left[\frac{1}{1-\exp\left(-y\right)}\right] = \frac{\exp\left(-y\right)}{\left[1-\exp\left(-y\right)\right]^2}$$

So $\langle q \rangle = \dfrac{1}{Z} \dfrac{\exp\left(-\hbar\omega / k_B T\right)}{\left[1-\exp\left(-\hbar\omega / k_B T\right)\right]^2} = \dfrac{\exp\left(-\hbar\omega / k_B T\right)}{1-\exp\left(-\hbar\omega / k_B T\right)}$

Planck distribution

So, rearranging

- the average number of photons per mode
  - in thermal equilibrium at temperature T is
    - the Planck distribution

$$\langle q \rangle = \frac{1}{\exp\left(\hbar\omega / k_B T\right) - 1}$$

Planck distribution

We see that the Planck distribution is

$$\langle q \rangle = \frac{1}{\exp\left(\hbar\omega / k_B T\right) - 1}$$

is a Bose-Einstein distribution

with chemical potential of zero

Note incidentally that

$\langle q \rangle$ need not be an integer

Thermal distributions 5

The Maxwell-Boltzmann distribution

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Maxwell-Boltzmann distribution

For both the Fermi-Dirac $f_{FD}(E) = \dfrac{1}{\exp\left[\left(E-\mu_C\right)/k_B T\right]+1}$

and Bose-Einstein $f_{BE}(E) = \dfrac{1}{\exp\left[\left(E-\mu_C\right)/k_B T\right]-1}$

distributions

for $E-\mu_C \gg k_B T$

both of them tend to

$$f_{MB}(E) = A\exp\left(-\frac{E}{k_B T}\right)$$

where $A = \exp\left(\mu_C / k_B T\right)$

which is the Maxwell-Boltzmann distribution

Maxwell-Boltzmann distribution

This Maxwell-Boltzmann distribution

was originally derived for classical particles

which are presumed to be non-identical

and that full derivation is quite involved

In practice, in $f_{MB}(E) = A\exp(-E / k_B T)$

A is usually regarded as a number chosen

to give the correct total number of particles

though it can formally be related to chemical

potential through $A = \exp(\mu_C / k_B T)$

Thermal distributions

Non-identical particles

Maxwell-Boltzmann

$$f_{MB}(E) = \exp\left[-(E-\mu_C)/k_B T\right]$$

Identical bosons

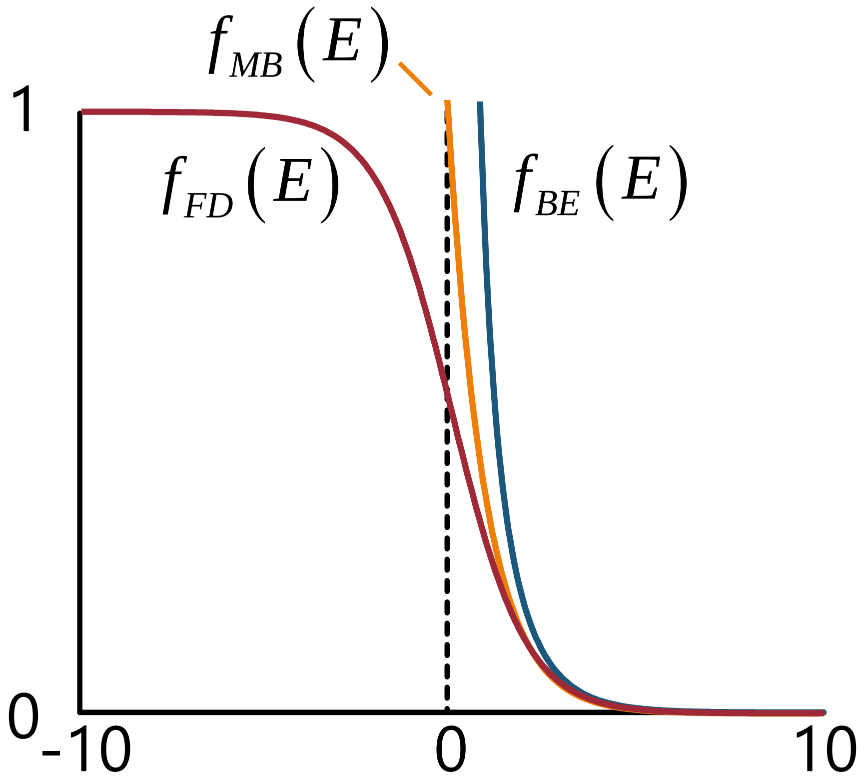
Bose-Einstein

$$f_{BE}(E) = \frac{1}{\exp\left[(E-\mu_C)/k_B T\right]-1}$$

Identical fermions

Fermi-Dirac

$$f_{FD}(E) = \frac{1}{\exp\left[(E-\mu_C)/k_B T\right]+1}$$



Energy E - μ_C (in units of k_BT)

(μ_C – chemical potential or Fermi energy)

Maxwell-Boltzmann limit

- We use the Maxwell-Boltzmann limit wherever possible
  - because its mathematics is much simpler
    - The full Fermi-Dirac distribution is difficult to integrate when counting particles, for example

Maxwell-Boltzmann limit

At high energies

- the Fermi-Dirac, Bose-Einstein and Maxwell-Boltzmann distributions
  - all are similar
    - because the probability of occupation is << 1
      - so issues of counting or forbidding multiple particles in a state do not arise

Thermal distributions

Identical bosons

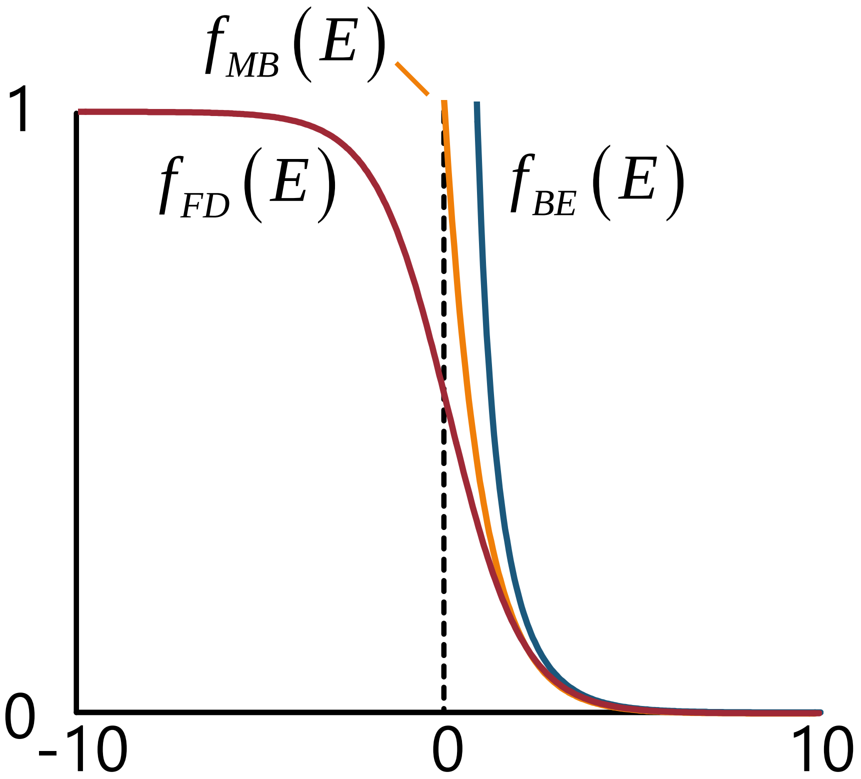
are more likely to be in the same mode

than are classical or non-identical particles

So the Bose-Einstein distribution

lies above

the Maxwell-Boltzmann distribution



Energy E - μ_C (in units of k_BT)

(μ_C – chemical potential or Fermi energy)

Thermal distributions

Identical fermions

are less likely to be in the same single-particle state

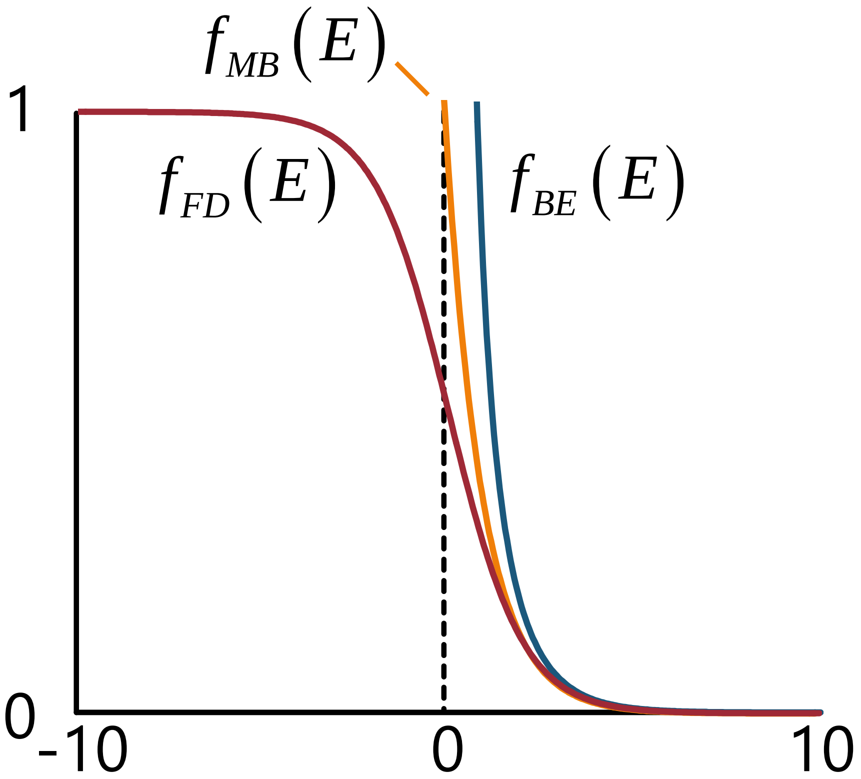
than are classical or non-identical particles

In fact, they never are in the same single-particle state

So the Fermi-Dirac distribution

lies below

the Maxwell-Boltzmann distribution



Energy E - μ_C (in units of k_BT)
(μ_C – chemical potential or Fermi energy)