Simplified analysis of phase transitions in thermodynamics

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- Talk available at: tinyurl.com/jay-umassd
- Example: Bose-Einstein condensation (and Ising model)
- Simplified analysis (iPAS)
  - insight without convoluted numerics
  - Possible to do at lower level courses
  - Analysis with Lambert W special function
  - Symbolic hands-on computation

Bose-Einstein condensation

The number of particles $N = \sum$ (BE dist) $\times$ (density of states), or

$$N = A\int_0^\infty f(p)dp,\ f(p) = \frac{p^2}{e^{(p^2-\mu)/kT}-1},\ A = \frac{4\pi V}{h^3}(2m)^{3/2}$$

The key to understanding BEC is the relationship between μ vs T.

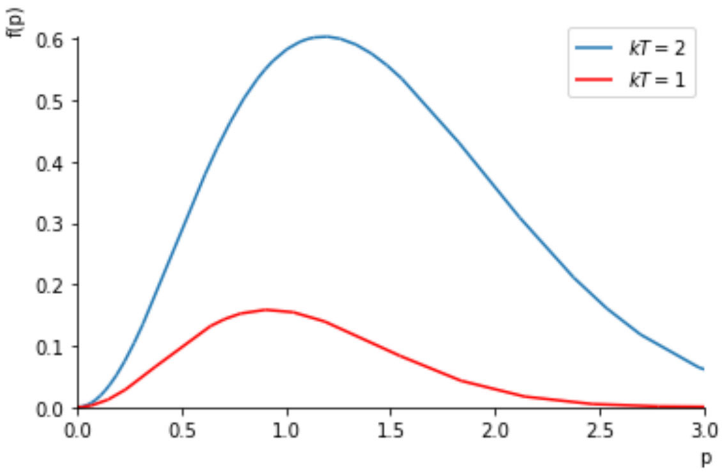
Use `sympy` , the symbolic lib, to examine the integrand,

In [1]:
```
from sympy import *
init_printing()    # pretty math symbols
%matplotlib inline

p, kT, mu = symbols('p kT mu')
def f(p,kT,mu):
    return p**2/(exp((p**2-mu)/kT)-1)
```

The integrand at fixed μ and T

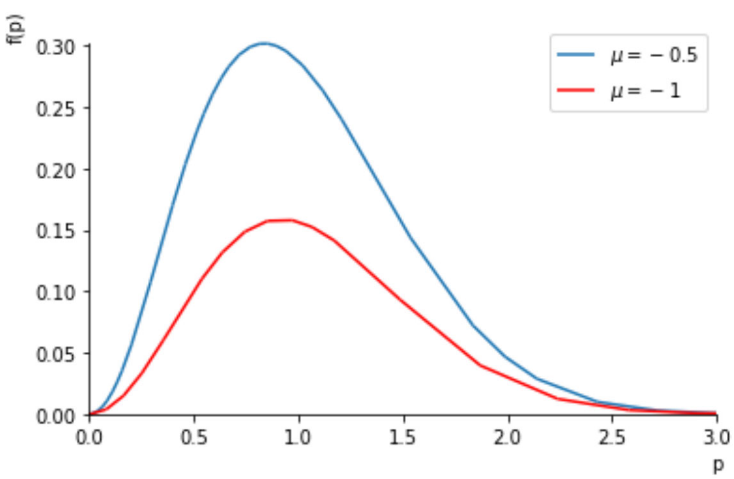
In [2]:
```
plt = plot(f(p,kT=2,mu=-1), f(p,kT=1,mu=-1), ### Fixed chem. pot.
        xlim=[0,3], legend=1, show=0)
plt[0].label='$kT=2$'; plt[1].line_color='red'; plt[1].label='$kT=1$'
plt.show()
```



At fixed μ,
$f(p)$ decreases as T decreases

At fixed T,
$f(p)$ increases as μ increases

In [3]:
```
plt = plot(f(p,kT=1,mu=-.5), f(p,kT=1,mu=-1), ### Fixed T
        xlim=[0,3], legend=1, show=0)
plt[0].label='$\mu=-0.5$'; plt[1].line_color='red'; plt[1].label='$\mu=-1$'
plt.show()
```



So, μ must increase when T decreases to conserve particle number N. Quantitatively, one must either do some numerical acrobatics; or some *simplification*. We choose the latter, semiquantitatively correct and suitable for lower level courses.
Assumption: The area is $\sim$ proportional to the height of the peak,

$$\int f(p)dp \sim C\ f(p_{max})$$

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This is justified because the width varies much slower than height (details in Am. J. Phys. 2019, accepted)

Effectively, $f_{max} \propto N$, some scaled particle number.
To find the maximum, set $df/dp = 0$,

In [4]:
```
dfdp = diff(f(p,kT,mu), p)   # derivative, f'(p)
dfdp
```

Out[4]:

$$\frac{2p}{e^{\frac{1}{kT}(-\mu+p^2)}-1} - \frac{2p^3 e^{\frac{1}{kT}(-\mu+p^2)}}{kT\left(e^{\frac{1}{kT}(-\mu+p^2)}-1\right)^2}$$

Solve for p_{max},

In [5]:
```
pmax = solve(dfdp, p) # find maximum
pmax
```

Out[5]:

$$\left[0,\quad \sqrt{kT}\sqrt{\operatorname{LambertW}\left(-e^{\frac{1}{kT}(-kT+\mu)}\right)+1},\quad -\sqrt{kT}\sqrt{\operatorname{LambertW}\left(-e^{-\frac{1}{kT}(kT-\mu)}\right)+1}\right]$$

Note the Lambert W function appears (more on it later).
To find $f_{max} = f(p_{max})$

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In [6]:
```
fmax=f(pmax[1],kT,mu)
fmax
```

Out[6]:

$$\frac{kT\left(\operatorname{LambertW}\left(-e^{\frac{1}{kT}(-kT+\mu)}\right)+1\right)}{e^{\frac{1}{kT}\left(kT\left(\operatorname{LambertW}\left(-e^{\frac{1}{kT}(-kT+\mu)}\right)+1\right)-\mu\right)}-1}$$

which simplifies to (`sympy` needs a bit help at times)

$$f_{max} = -kT\, W(-e^{\mu/kT-1}), \quad p_{max} = \left[kT\left(W(-e^{\mu/kT-1}\right)+1\right]^{1/2}$$

In [7]:
```
fmax = -kT*LambertW(-exp(mu/kT-1))
fmax
```

Out[7]:

$$-kT \operatorname{LambertW}\left(-e^{-1+\frac{\mu}{kT}}\right)$$

Recall f_{max} represents the area (or N)

Now as T decreases, μ must adjust such that $f_{max} = const$, say 1 (equiv $kT_c = 1$) for some fixed N. Solve $f_{max} - 1 = 0$ for μ

In [8]:
```
u = solve(fmax-1, mu)
u
```

Out[8]:

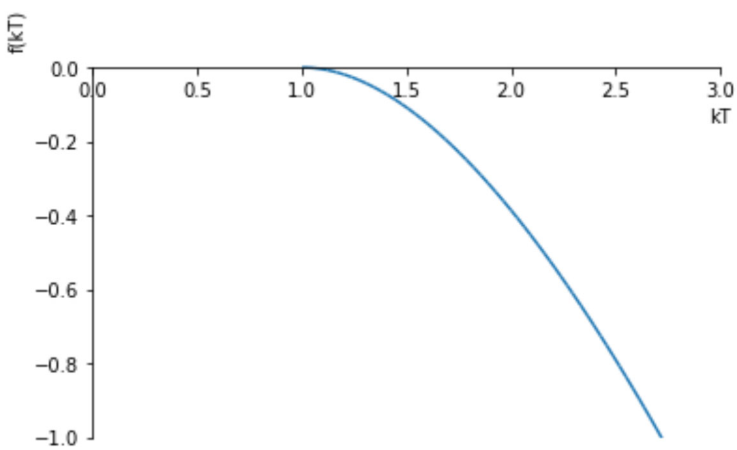
$$\left[kT\left(\log\left(\frac{e^{-\frac{1}{kT}}}{kT}\right)+1\right)\right]$$

or make it tidier, $\mu = \begin{cases} kT(1-\ln kT)-1, & (T > T_c) \\ 0, & (T \le T_c) \end{cases}$

Central closed-form result: how μ changes to keep N constant.

Relationship between μ and T, critical temperature at $kT = 1$

In [9]:
```
plot(u[0],  (kT,1,3), xlim=[0,3], ylim=[-1,.1]);
```



The maximum of μ is zero. What if T continues to decrease?

Because $\mu = 0$ after T_c, it can no longer compensate for the shrinking integral. Evidently, the "missing" particles fall into the ground state, the Bose-Einstein condensate, i.e., $N = N_{exci} + N_{grnd}$

T	$\frac{N_{exci}}{N}$	$\frac{N_{grnd}}{N}$
$T > T_c$	1	0
$T < T_c$	$\frac{T}{T_c}$	$1 - \frac{T}{T_c}$
$T \sim 0$	0	1

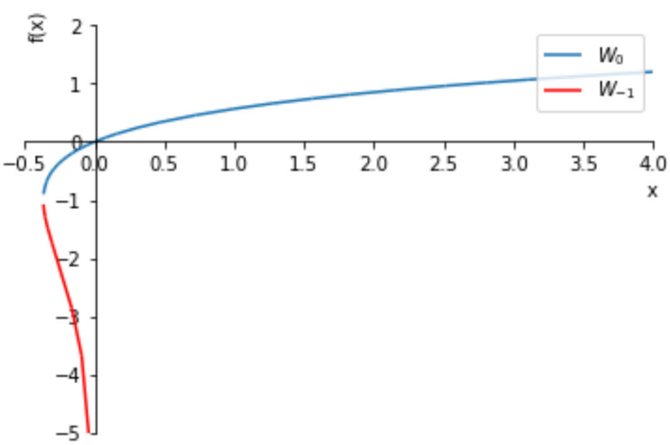
$$\frac{N_{exci}}{N} = \begin{cases} 1, & T > T_c, \\ \frac{T}{T_c}, & T \le T_c, \end{cases}, \quad \frac{N_{grnd}}{N} = \begin{cases} \sim 0, & T > T_c, \\ 1 - \frac{T}{T_c}, & T \le T_c. \end{cases}$$

T	N_{exci}/N	N_{grnd}/N
$T > T_c$	~ 1	~ 0
$T < T_c$	T/T_c	1-T/T_c

The Lambert W function: defined as the $W(x)$ satisfying $W(x)e^{W(x)} = x$

In [10]:
```
x = symbols('x')
W = LambertW    # shorthand

plt = plot(W(x,0), W(x,-1), xlim=[-.5,4], ylim=[-5,2], legend=1, show=0)
plt[0].label='$W_0$'; plt[1].line_color='red'; plt[1].label='$W_{-1}$'; plt.show()
```



In [11]:
```
diff(W(x),x)
```

Out[11]:

$$\frac{\text{LambertW}(x)}{x\left(\text{LambertW}(x) + 1\right)}$$

In [12]:
```
integrate(W(x),x)
```

Out[12]:

$$x\,\text{LambertW}(x) - x + \frac{x}{\text{LambertW}(x)}$$

Discussion

- Simplified analysis of BEC with the W function; Ising model may be solved similarly (AJP 2019 accepted)
- The W function recently used in CM, QM, thermo, chaos, helio- & astro-phys, eco-bio systems, supply-chain problems
- Potential application to yet unknown thermal problems due to FD and BE distributions involving $[\exp((E-\mu)/kT) \pm 1]^{-1}$
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