Quantum Field Theory for Many Particle Systems (nonrelativistic)

Applications in Statistical Mechanics

Harris, Chapters 8 and 9

Start with this non-relativistic Q.F.T.

$$H = H_0 + H_I$$

$$H_0 = \int d^3x \; \psi^\dagger(x) \left[\frac{-\hbar^2}{2m} \nabla^2 + V \right] \psi(x)$$

$$H_I = \int d^3x \, d^3x' \; \psi^\dagger(x) \psi^\dagger(x') \, v_2(x, x') \, \psi(x') \psi(x)$$

$$\left[\psi(x), \psi^\dagger(x') \right]_\pm = \delta^3(\vec{x} - \vec{x}')$$ fermions / bosons

Comments: In the Heisenberg picture $\Psi(\mathbf{x})$ also depends on t. Spin indices are suppressed.

Today, assume

$$V(\mathbf{x}) = 0$$

and

$$v_2(\mathbf{x},\mathbf{x}') = v_2(\,\mathbf{x} - \mathbf{x}'\,).$$

Expand the field in plane waves,

$$\psi(\vec{x}) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{x}}}{\sqrt{\Omega}} \, b_{\vec{k}}$$

using periodic boundary conditions for a finite volume ; $\Omega = L^3$. Then

$$H_0 = \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} b_k^\dagger b_k$$

$$H_I = \frac{1}{\Omega} \sum_{\vec{k}_1} \sum_{\vec{k}_2} \sum_{\vec{q}} \hat{v}(\vec{q}) \, b^\dagger_{k_1+q} \, b^\dagger_{k_2-q} \, b_{k_2} \, b_{k_1}$$

$$\hat{v}(\vec{q}) = \int d^3x \; v_2(\vec{x}) \, e^{-i\vec{q}\cdot\vec{x}}$$

<u>Weakly interacting spin = 0 bosons at temperature T</u>

Imagine the system in equilibrium with a heat bath at temperature T.

Let N(**k**) be the number of particles with momentum ħ**k** .

Understand the meaning of this quantity.

N(k) is not the quantum operator $b_{\mathbf{k}}^{\dagger}\, b_{\mathbf{k}}$.

N(k) here means

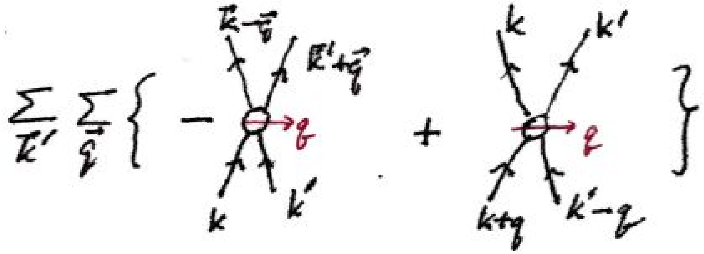
$$N(\mathbf{k}) = \sum_{\alpha} P(\alpha)\ \langle \alpha \,|\, b_{\mathbf{k}}^{\dagger}\, b_{\mathbf{k}} \,|\, \alpha \rangle$$

("density matrix")

Now consider a time interval δt . During that time the particles scatter from each other due to the 2-body interaction, v_2 .

Calculate δN(**k**).

Pictorial expression,

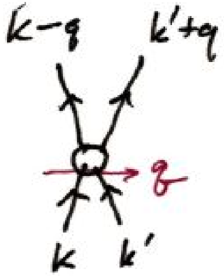


I.e., N(**k**) can change for two reasons: a particle in the state **k** can scatter out of this state; a particle not in the state **k** can scatter into this state.

First case; $\delta N(\mathbf{k}) < 0$:

$\mathbf{k} + \mathbf{k}' \rightarrow [\mathbf{k}+\mathbf{q}] + [\mathbf{k}'-\mathbf{q}]$

$\mathbf{k}_1 + \mathbf{k}_2 \rightarrow \mathbf{k}_3 + \mathbf{k}_4$



The transition rate can be calculated using perturbation theory for the interaction v_2 ;
by Fermi's Golden Rule,

$$dR = \frac{2\pi}{\hbar} \sum_f \left| \langle f | H_I | i \rangle \right|^2 \delta(E_f - E_i)$$

$$\langle f | H_I | i \rangle = \langle f | \sum_{k_1 k_2 q} \frac{\hat{v}(q)}{\Omega} b^+_{k_1+q} b^+_{k_2-q} b_{k_2} b_{k_1} | i \rangle$$

$\vec{k}_1, \vec{k}_2$ could be $\vec{k}, \vec{k}'$ or $\vec{k}', \vec{k}$

$$b_{\vec{k}} | i \rangle = \sqrt{N(\vec{k})}\, | i' \rangle$$

$$b_{\vec{k}'} | i' \rangle = \sqrt{N(\vec{k}')}\, | i'' \rangle$$

$$b^+_{k'-q} | i'' \rangle = \sqrt{N(k'-q)+1}\, | i''' \rangle$$

$$b^+_{k+q} | i''' \rangle = \sqrt{N(k+q)+1}\, | f \rangle$$

$$E_f - E_i = E_3 + E_4 - E_1 - E_2$$

$$\delta N^{(1)}(\vec{k}) = -\frac{2\pi}{\hbar}\sum_{k'}\sum_{q}\left|\frac{\hat{v}(\vec{q})}{\Omega}\right|^2 \delta(\varepsilon_3+\varepsilon_4-\varepsilon_1-\varepsilon_2)$$

$$2\, N(\vec{k})\, N(\vec{k}')\,[N(k'-q)+1]\,[N(k+q)+1] \quad \delta t$$

Similarly,

$$\delta N^{(2)}(\vec{k}) = +(\text{same})\ \delta(\varepsilon_1+\varepsilon_2-\varepsilon_3-\varepsilon_4)$$

$$2\,[N(k)+1]\,[N(k')+1]\, N(k+q)\, N(k'-q) \quad \delta t$$

Result : $\delta N(\mathbf{k}) / \delta t = R_1 + R_2$

Now, the *equilibrium state* has

$$\delta N(\mathbf{k}) / \delta t = 0 \,; \qquad \text{i.e., } R_2 = -R_1 \,.$$

The solution of this equation is

(homework)

$$N(\vec{k}) = \frac{1}{C e^{E(k)/KT} - 1} \qquad \text{(bosons)}$$

where $E(k) = \hbar^2 k^2 / 2m$;

(K=Boltzmann constant, T = temperature)

This expression is just the Bose-Einstein distribution function for non-interacting particles.

Now, C is a constant, i.e., independent of **k** .

So how do we determine C?

Let N_{tot} = the total number of particles.

Then $N_{tot} = \sum_{\mathbf{k}} N(\mathbf{k})$

That equation determines C.

Another notation is $C = e^{-\mu/KT}$ where μ = “the chemical potential”.

THE IDEAL BOSE-EINSTEIN GAS

Now it's time to take the limit $\Omega \to \infty$.

Periodic boundary conditions:

$\mathbf{k} = (2\pi / L)\, \mathbf{n}$ where $\mathbf{n}$ has integer components.

Then $\sum_{\mathbf{k}} \to \int (L / 2\pi)^3 \; d^3k$

Thus

$$N_{tot} = \frac{\Omega}{(2\pi)^3} \int \frac{d^3k}{C\, e^{E(k)/kT} - 1}$$

this assumes that there is no Bose-Einstein condensate.

$$N_{tot} = \frac{\Omega}{(2\pi)^3}\, 4\pi \int_0^\infty \frac{k^2 dk}{C\, e^{\hbar^2 k^2/2mkT} - 1}$$

Let $x = \frac{\hbar^2 k^2}{2mkT}$; $dx = \frac{\hbar^2 k\, dk}{mkT}$

$$N_{tot} = \frac{\Omega}{2\pi^2} \frac{mkT}{\hbar^2} \left(\frac{2mkT}{\hbar^2}\right)^{1/2} \int_0^\infty \frac{\sqrt{x}\, dx}{C\, e^x - 1}$$

Write $C = e^{x_0}$

$$N_{tot} = \frac{\Omega\sqrt{2}}{2\pi^2} \left(\frac{mkT}{\hbar^2}\right)^{3/2} f(x_0)$$

where $f(x_0) = \int_0^\infty \frac{\sqrt{x}\, dx}{e^{x_0} e^x - 1}$

Note: $C \geq 1$ and $x_0 \geq 0$.

Bose-Einstein condensation

Let's use specific parameter values.

These are the parameters for liquid helium-4.

(*Of course, liquid He-4 is not an ideal gas; but we're just choosing some interesting parameter values to see what we get.*)

$m = 4\,u = 4 \times 1.66 \times 10^{-27}$ kg

$$\rho = \begin{cases} 0.125 \text{ g/cc} & (\text{ b.p. at 1 atm}) \\ 0.145 \text{ g/cc} & (\text{ m.p. at 1 atm}) \end{cases}$$

$\nu = N_{tot} / \Omega = \rho / m$ (particle density)

Apply these numbers to the equations,

$$N_{tot} = \frac{\Omega \sqrt{2}}{2\pi^2} \left(\frac{mkT}{\hbar^2} \right)^{3/2} f(x_0)$$

where $f(x_0) = \int_0^\infty \frac{\sqrt{x}\, dx}{e^{x_0} e^{x} - 1}$

Note: $C \geq 1$ and $x_0 \geq 0$.

Assuming there is no condensate,

$$N_{tot} = \frac{\Omega\sqrt{2}}{2\pi^2}\left(\frac{mkT}{\hbar^2}\right)^{3/2} f(x_0)$$

where $f(x_0) = \int_0^\infty \frac{\sqrt{x}\,dx}{e^{x_0}e^{x}-1}$

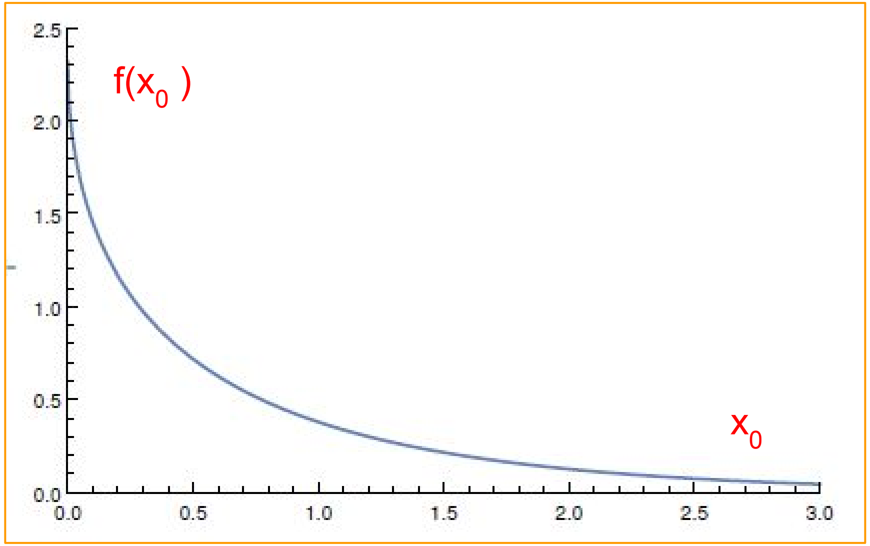
Now use Mathematica to analyze the equations.

```
f[x0_] := Integrate[Sqrt[x] / (Exp[x0 + x] - 1), {x, 0, Infinity}]

f[ξ]
```

$\frac{1}{2}\sqrt{\pi}\,\text{PolyLog}\left[\frac{3}{2}, e^{-\xi}\right]$

```
fPL[x0_] := Sqrt[Pi] / 2 * PolyLog[3 / 2, Exp[-x0]]
Plot[fPL[x0], {x0, 0, 3},
  PlotRange → {{0, 3}, {0, 2.5}}]
```




```
fPL[0]
SetPrecision[fPL[0.0], 5]
```

$\frac{1}{2}\sqrt{\pi}\,\text{Zeta}\left[\frac{3}{2}\right]$

2.3152

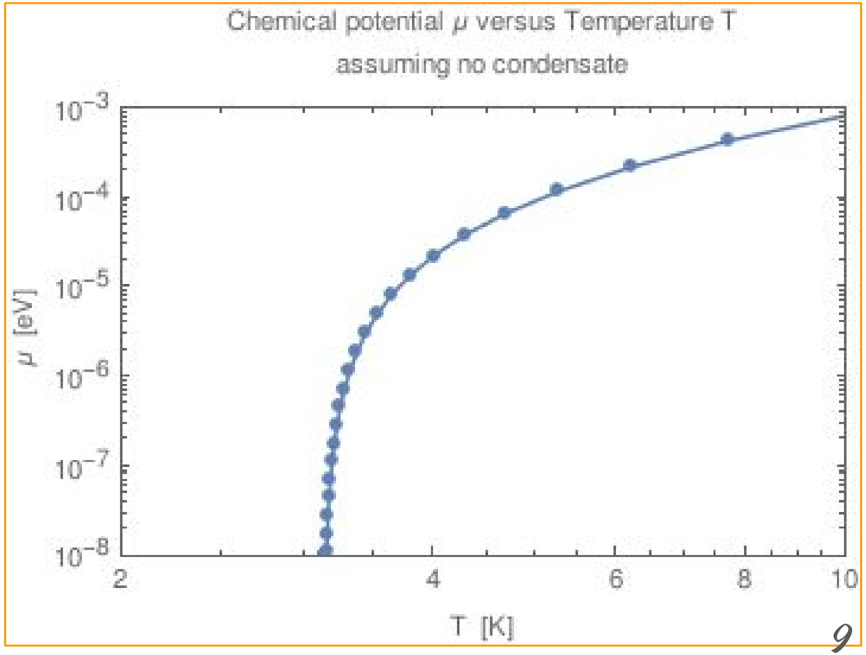
As T decreases, x_0 must decrease.

```
(* parameters  *)
mass  =4*1.66*^-27*Ukg;
(* density of liquid helium  = 0.125 g/cc at the b.p. *)
(* density of liquid helium  = 0.145 g/cc at the m .p. *)
rho = 0.145 * (1.0*^-3 *Ukg) / (0.01*Um ) ^3;
nu = rho / mass ;
hbar = 1.0546*^-34 *Ukg*Um ^2 / Us;
UeV = 1.602*^-19 *Ukg*Um ^2 / Us^2;
KB = 8.617*^-5 *UeV;

(* calculate temperature  *)
KT[x0_] := PowerExpand[
    Power[Sqrt[2]*Pi^2*nu/fPL[x0]*hbar^3/mass ^(3/2), 2/3]/UeV]
{"For x0 = 0.0001; KT in eV = ", KT[0.0001]}
{"For x0 = 0.0001; T in degK = ", degK = KT[0.0001]*UeV/KB}
```

```
tbl = {}
Do[
  x0v = 10^(-4 + 0.2*j);
  degK = KT[x0v] *UeV / KB;
  μ = KT[x0v] *x0v;
  tbl = Join[tbl, {{degK, μ}}],
  {j, 1, 40}]
tbl;
```

```
ListLogLogPlot[Re[tbl],
  Joined→True, Mesh→Full,
  PlotRange→{{2, 10}, {1.0*^-8, 1.0*^-3}},
  Frame →True,
  FrameTicks →{{2, 3, 4, 5, 6, 7, 8, 9, 10}, Automatic , None, None},
  FrameLabel →{"T  [K]", " μ  [eV]",
      "Chemical  potential μ versus Temperature  T
assuming  no condensate"}]
```



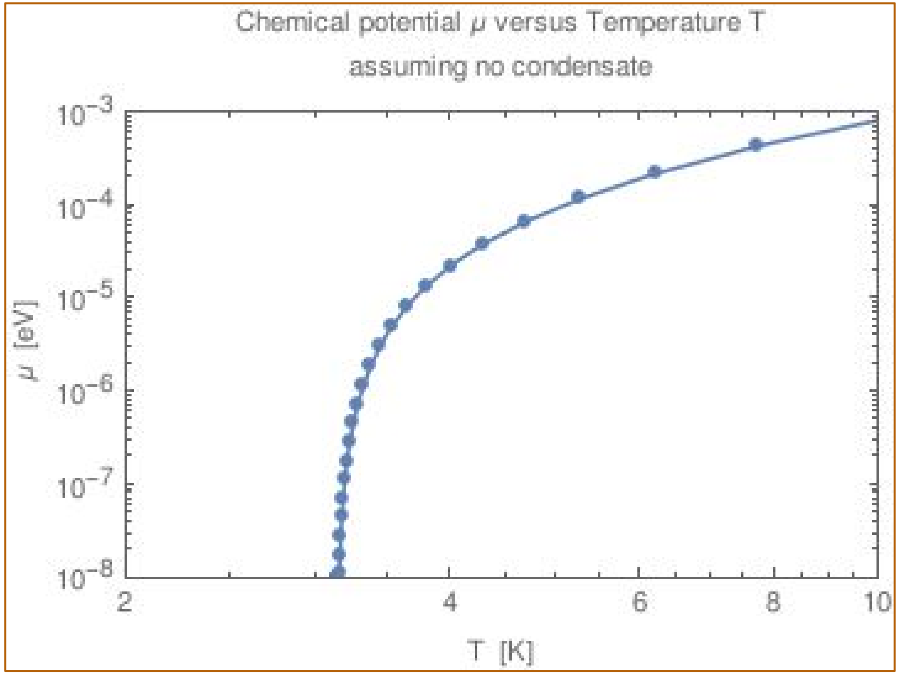
Something happens for $T \lesssim 3$ Kelvin.

Calculate the transition temperature accurately:

- $|\mu| = x_0\, KT(x_0) \longrightarrow 0$ as $x_0 \longrightarrow 0$
- $f(x_0) \longrightarrow 2.315$ as $x_0 \longrightarrow 0$
- $KT = \hbar^2/m \;\; [\sqrt{(2)}\, \pi^2\, \nu / f(x_0)\,]^{2/3}$

  $\longrightarrow$ 3.14 deg Kelvin as $x_0 \longrightarrow 0$

So… For $T < T_C$, there must be a Bose-Einstein condensate; i.e., a significant fraction (≡ F) of the particles are in the ground state
| **k = 0** >.
Then we need a different calculation for $T < T_C$.



For T < T_C we must have

$$N_{tot} = \underbrace{N(0)}_{F N_{tot}} + \frac{\Omega}{(2\pi)^3}\int \frac{d^3k}{C e^{E/kT} - 1}$$

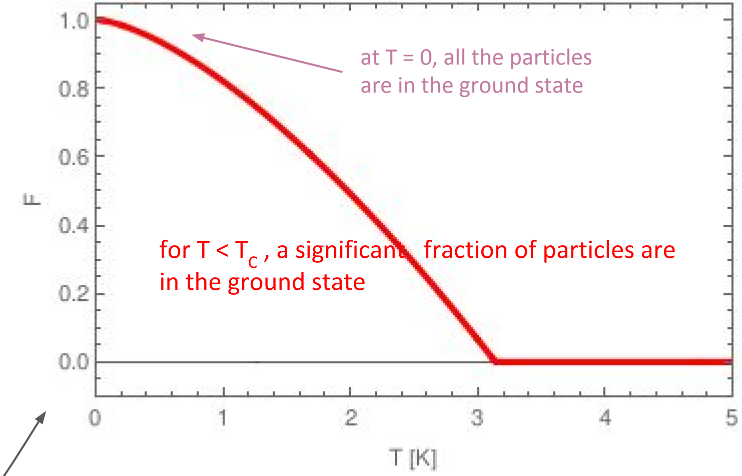
$\hookrightarrow C = e^{x_0} \to 1$
$(x_0 \to 0)$

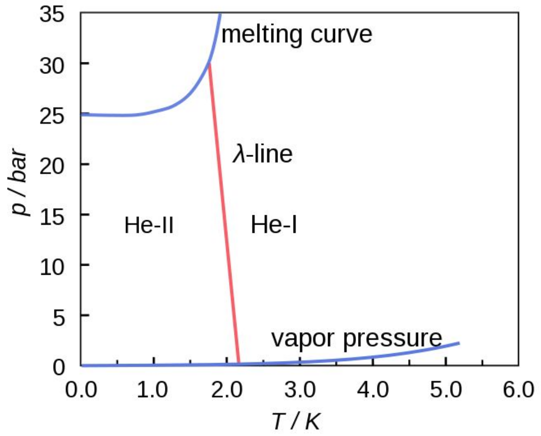
$$(1-F)\frac{N_{tot}}{\Omega} = \frac{\sqrt{2}}{2\pi^2}\left(\frac{mkT}{\hbar^2}\right)^{3/2} f(0)$$

$\hookrightarrow = T^{3/2}\ \nu / T_c^{3/2}$

$$F = 1 - \left(\frac{T}{T_c}\right)^{3/2}$$

In fact liquid He-4 does have a phase transition, at ~ 2 deg Kelvin, to a superfluid phase. Roughly speaking, the superfluid is the BE condensate.





Homework Assignment due Friday, February 26

Problem 24. Derive the equilibrium Bose-Einstein distribution, from the condition $R_1 + R_2 = 0$. (The rates R_1 and R_2 are defined in the lecture of Feb. 15.)

Problem 25.
(a) Assume an ideal gas of spin-0 bosons, with these parameter values (= the values for He-4 atoms):
atomic mass = m = 4 u ;
density = ρ = 0.14 g/cc ;
Starting from the Bose-Einstein distribution, calculate the temperature for Bose-Einstein condensation.
(b) Repeat the calculation for these parameter values (= the values for Ne-20 atoms):
atomic mass = m = 20 u ;
density = ρ = 1.4 g/cc .
(c) Explain why Ne-20 does not have a superfluid phase.