Bose-Einstein condensation: Specific heat

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Using the exercise of Huang, we discuss the temperature dependence of specific heat for the Bose-Einstein condensation.

((**Example**)) **Huang Problem 18-4**
Critical behavior of specific heat for bosons in the vicinity of T_E

Show that the slope of the heat capacity of an ideal Bose gas has a discontinuity at $T = T_E$ given by

$$\left(\frac{\partial C_V}{\partial T}\right)_{T \to T_E^+} - \left(\frac{\partial C_V}{\partial T}\right)_{T \to T_E^-} = 3.66 \frac{N k_B}{T_E}$$

Hint: Calculate the internal energy via $U = \frac{3}{2} PV$.

((**Solution**))
The pressure is given by

$$P(T, z) = k_B T n_Q(T) \varsigma_{5/2}(z)$$

The internal energy can be derived as

$$\begin{aligned} U(T, z) &= \frac{3}{2} P(T, z) V \\ &= V \frac{3}{2} k_B T n_Q(T) \varsigma_{5/2}(z) \qquad \text{for } T > T_E \\ &= V \frac{3k_B}{2c} T^{5/2} \varsigma_{5/2}(z) \end{aligned}$$

$$\begin{aligned} U(T, z=1) &= \frac{3}{2} P(T, z=1) V \\ &= V \frac{3k_B}{2c} T^{5/2} \varsigma_{5/2}(z=1) \end{aligned}$$

for $T < T_E$

where T_E is the Bose-Einstein condensation temperature, $n_Q(T)$ is the quantum concentration

$$n_Q(T) = \left(\frac{mk_B T}{2\pi\hbar^2}\right)^{3/2} = \left(\frac{mk_B}{2\pi\hbar^2}\right)^{3/2} T^{3/2} = \frac{1}{c} T^{3/2}$$

with

$$c = \left(\frac{mk_B}{2\pi\hbar^2}\right)^{-3/2}.$$

The heat capacity is

$$C = \frac{dU}{dT} = V\frac{3k_B}{2c}[\frac{5}{2}T^{3/2}\varsigma_{5/2}(z) + T^{5/2}\frac{dz}{dT}\frac{d}{dz}\varsigma_{5/2}(z)$$

for $T > T_E$

$$C = \frac{dU(T, z=1)}{dT} = V\frac{3k_B}{2c}\frac{5}{2}T^{3/2}\varsigma_{5/2}(z=1)$$

for $T < T_E$

We note that for $T > T_E$, the number density is independent of *T*. So we have

$$\frac{d}{dT}n(T,z) = \frac{d}{dT}n = 0,$$

with

$$n(T,z) = n = n_Q(T)\varsigma_{3/2}(z) = \frac{1}{c}T^{3/2}\varsigma_{3/2}(z).$$

((**Note**)) Definition of T_E

T_E is defined as

$$n = n_Q(T_E)\varsigma_{3/2}(z=1)\,,$$

or

$$\boxed{T_E = \frac{2\pi\hbar^2}{mk_B}[\frac{n}{\varsigma_{3/2}(z=1)}]^{2/3} \approx 3.3125\frac{\hbar^2 n^{3/2}}{mk_B}}$$

Thus

$$\begin{aligned}\frac{d}{dT}n(T,z) &= \frac{d}{dT}[\frac{1}{c}T^{3/2}\varsigma_{3/2}(z)] \\ &= \frac{1}{c}[\frac{3}{2}T^{1/2}\varsigma_{3/2}(z) + T^{3/2}\frac{dz}{dT}\frac{d}{dz}\varsigma_{3/2}(z)] \\ &= \frac{d}{dT}n \\ &= 0\end{aligned}$$

or

$$\frac{3}{2}T^{1/2}\varsigma_{3/2}(z) + T^{3/2}\frac{dz}{dT}\frac{d}{dz}\varsigma_{3/2}(z)] = 0$$

or

$$\frac{dz}{dT} = -\frac{3}{2T}\frac{\varsigma_{3/2}(z)}{\frac{d}{dz}\varsigma_{3/2}(z)} = -\frac{3z}{2T}\frac{\varsigma_{3/2}(z)}{\varsigma_{1/2}(z)}$$

or

$$\boxed{\frac{T}{z}\frac{dz}{dT} = -\frac{3}{2}\frac{\varsigma_{3/2}(z)}{\varsigma_{1/2}(z)}}$$

We make a plot of this as a function of z around $z = 1$.

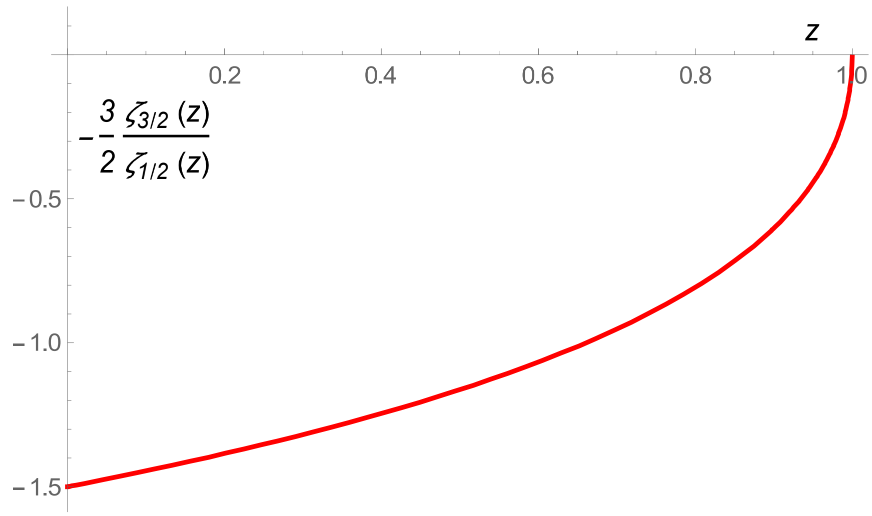


Fig. Plot of $\frac{T}{z}\frac{dz}{dT}=-\frac{3}{2}\frac{\varsigma_{3/2}(z)}{\varsigma_{1/2}(z)}$ as a function of z. This function becomes zero at $z = 1$.

Here we use

$$\varsigma_{1/2}(z)=z\frac{d}{dz}\varsigma_{3/2}(z)$$

Using the above relation, we get

$$\begin{aligned}\frac{C}{Vk_B}&=\frac{3}{2c}T^{3/2}[\frac{5}{2}\varsigma_{5/2}(z)+T\frac{dz}{dT}\frac{d}{dz}\varsigma_{5/2}(z)]\\&=\frac{3}{2c}T^{3/2}[\frac{5}{2}\varsigma_{5/2}(z)+\frac{T}{z}\frac{dz}{dT}\varsigma_{3/2}(z)]\\&=\frac{3}{2c}T^{3/2}\{\frac{5}{2}\varsigma_{5/2}(z)-\frac{3}{2}\frac{[\varsigma_{3/2}(z)]^2}{\varsigma_{1/2}(z)}\}\end{aligned}$$

or

$$\frac{C}{Vk_B}=\frac{3n}{2}\left(\frac{T}{T_E}\right)^{3/2}\frac{1}{\varsigma_{3/2}(z=1)}\{\frac{5}{2}\varsigma_{5/2}(z)-\frac{3}{2}\frac{[\varsigma_{3/2}(z)]^2}{\varsigma_{1/2}(z)}\}$$

or

$$\frac{C}{Nk_B} = \frac{3}{2}\left(\frac{T}{T_E}\right)^{3/2} \frac{1}{\varsigma_{3/2}(z=1)}\{\frac{5}{2}\varsigma_{5/2}(z) - \frac{3}{2}\frac{[\varsigma_{3/2}(z)]^2}{\varsigma_{1/2}(z)}\}$$
$$= \frac{3}{2}\left(\frac{T}{T_E}\right)^{3/2} \frac{1}{\varsigma_{3/2}(z=1)}\{\frac{5}{2}\varsigma_{5/2}(z) + \frac{T}{z}\frac{dz}{dT}\varsigma_{3/2}(z)]\}$$

for $T > T_E$,

where $n = \frac{N}{V}$,

$$n = n(T_E, z=1) = n_Q(T_E)\varsigma_{3/2}(z=1) = \frac{1}{c}T_E^{\ 3/2}\varsigma_{3/2}(z=1),$$

or

$$\frac{\varsigma_{3/2}(z)}{\varsigma_{3/2}(z=1)} = \frac{n_Q(T_E)}{n_Q(T)} = \left(\frac{T_E}{T}\right)^{3/2}$$

and

$$\varsigma_{3/2}(z) = z\frac{d}{dz}\varsigma_{5/2}(z).$$

For $T < T_E$, we have

$$\frac{C}{Vk_B} = \frac{15}{4c}T^{3/2}\varsigma_{5/2}(z=1)$$
$$= \frac{15}{4c}T^{3/2}\varsigma_{5/2}(z=1)\frac{nc}{T_E^{\ 3/2}\varsigma_{3/2}(z=1)}$$
$$= \frac{15n}{4}\left(\frac{T}{T_E}\right)^{3/2}\frac{\varsigma_{5/2}(z=1)}{\varsigma_{3/2}(z=1)}$$

or

$$\frac{C}{Nk_B} = \frac{15}{4}\left(\frac{T}{T_E}\right)^{3/2}\frac{\varsigma_{5/2}(z=1)}{\varsigma_{3/2}(z=1)}$$

for $T < T_E$,

We now calculate

$$
\begin{aligned}
C_+ - C_- &= Nk_B \frac{3}{2}\left(\frac{T}{T_E}\right)^{3/2} \frac{1}{\varsigma_{3/2}(z=1)} \{\frac{5}{2}\varsigma_{5/2}(z) + \frac{T}{z}\frac{dz}{dT}\varsigma_{3/2}(z)]\} - \frac{15}{4}\left(\frac{T}{T_E}\right)^{3/2} \frac{\varsigma_{5/2}(z=1)}{\varsigma_{3/2}(z=1)} \\
&= Nk_B \frac{3}{2}\left(\frac{T}{T_E}\right)^{3/2} \frac{\varsigma_{3/2}(z)}{\varsigma_{3/2}(z=1)} \frac{T}{z}\frac{dz}{dT} \\
&\approx \frac{3}{2} Nk_B \frac{T}{z}\frac{dz}{dT}
\end{aligned}
$$

Since $\frac{T}{z}\frac{dz}{dT} = -\frac{3}{2}\frac{\varsigma_{3/2}(z)}{\varsigma_{1/2}(z)}$ approaches zero as $z \to 1$, because $\varsigma_{1/2}(z) \to \infty$. The heat capacity C_V is continuous at $T = T_E$. How about the discontinuity of the derivative of heat capacity with respect to *T* around $T = T_E$?

$$
\begin{aligned}
\frac{d}{dT}(C_+ - C_-)|_{T=T_E} &= \frac{3}{2} Nk_B T_E \frac{d}{dT}(\frac{1}{z}\frac{dz}{dT})|_{T=T_E} \\
&= \frac{3}{2} Nk_B T_E \frac{d^2 \ln z}{d^2 T}|_{T=T_E} \\
&= \frac{3}{2} Nk_B T_E \frac{1}{T_E{}^2}\frac{d^2 \ln z}{d^2 t}|_{t=1} \\
&= \frac{3}{2}\frac{Nk_B}{T_E}\frac{d^2 \ln z}{d^2 t}|_{t=1} \\
&= (3.66484)\frac{Nk_B}{T_E}
\end{aligned}
$$

which mean that dC/dT has a discontinuity at $T = T_E$.
Using the Mathematica, we examine the *T* dependence of dC/dT in the vicinity of $T = T_E$, showing a jump.

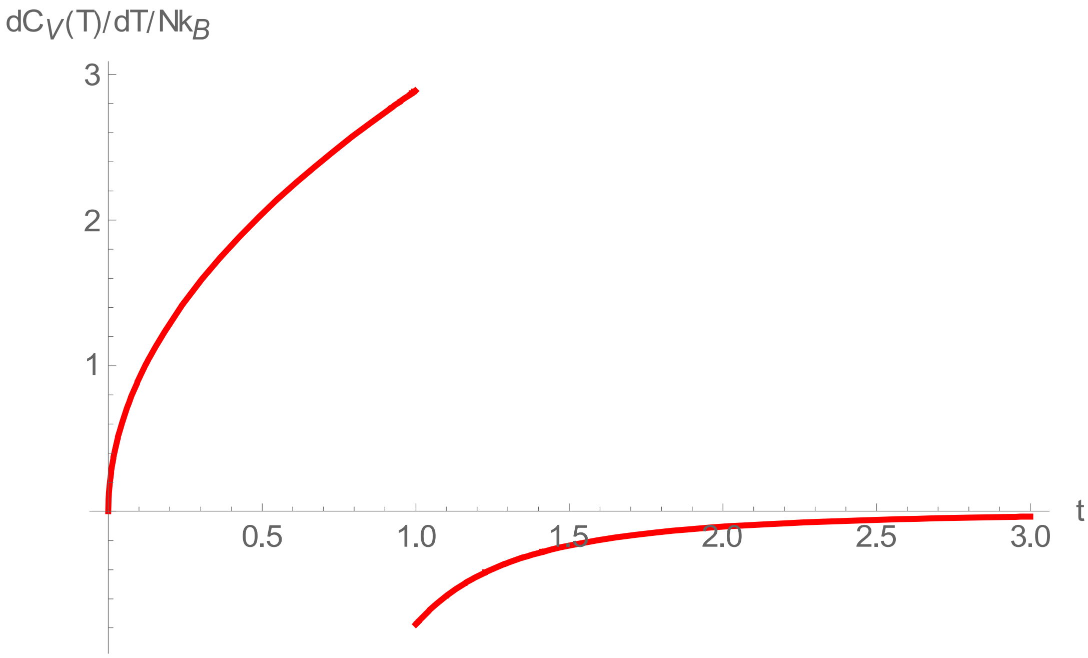


Fig. $dC_V / dT / Nk_B$ as a function of T around t =1. ($t = T/T_E$). It changes discontinuously from the positive value (2.88851) to a negative value (-0.776333) at t = 1. The universal constant for the jump is 3.66484.

Heat capacity of the Bose-Einstein condensation

```
Clear["Global`*"];

k1[t_] := PolyLog[3/2, λ] - PolyLog[3/2, 1]/t^(3/2);

Lamda[t_] := Module[{eq1, eq2, λ1},
  eq1 = FindRoot[k1[t] == 0, {λ, 0.1, 1}];
  λ1 = λ /. eq1[[1]]];
```

Interpolation and its derivative

```
E1[t_] := 3/2 t PolyLog[5/2, Lamda[t]]/PolyLog[3/2, Lamda[t]];

g1 = Table[{t, E1[t]}, {t, 1, 10, 0.01}];
g11 = Interpolation[g1]; CU = g11';
CUU = g11'';
```

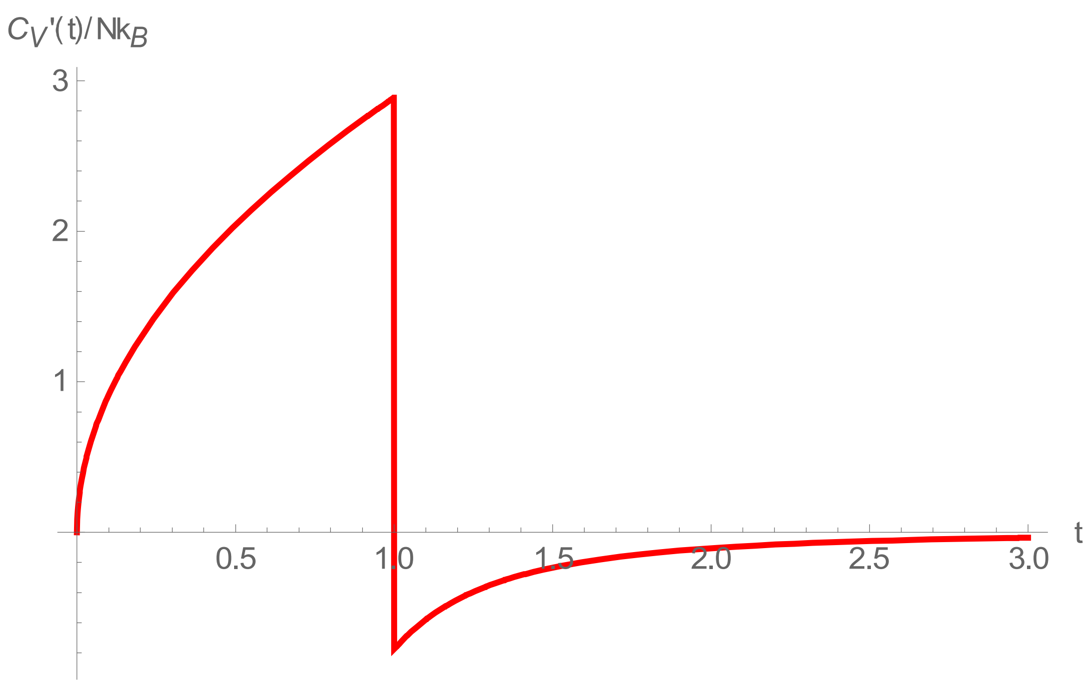
CU :heat capacity normalized by $\frac{3}{2}$ $\mathrm{N}k_{\mathrm{B}}$ for T>TE

CD: heat capacity normalized by $\frac{3}{2}$ $\mathrm{N}k_{\mathrm{B}}$ for T<TE

```
CD[t_] := 3/2 1.2837825 t^(3/2);

CDD[t_] := 9/4 1.2837825 t^(1/2)

CDUU = Which[0 < t < 1, CDD[t], t > 1, CUU[t]];
p1 = Plot[CDUU, {t, 0, 3}, PlotStyle → {Red, Thick},
  AxesLabel → {"t", "CV'(t)/NkB"}];
p2 =
 Graphics[
  {Text[Style["Heat capacity of BE condensation",
     Black, 12], {2.0, 0.4}], Green, Thick,
   Line[{{1, 0}, {1, CD[1]}}], Dashed, Thin, Black,
   Line[{{0, 1.5}, {3, 1.5}}] }];
Show[p1]
```



```
a1 = CUU[1]
```

-0.776333

```
a2 = CDD[1]
```

2.88851

```
a2 - a1
```

3.66484

REFERENCES

K. Huang, Introduction to Statistical Physics, second edition (CRC Press, 2010).

H.S. Robertson, Statistical Thermodynamics (PTR Prentice Hall, 1993).