(Section numbering of 2nd edition)

Bose-Einstein condensation

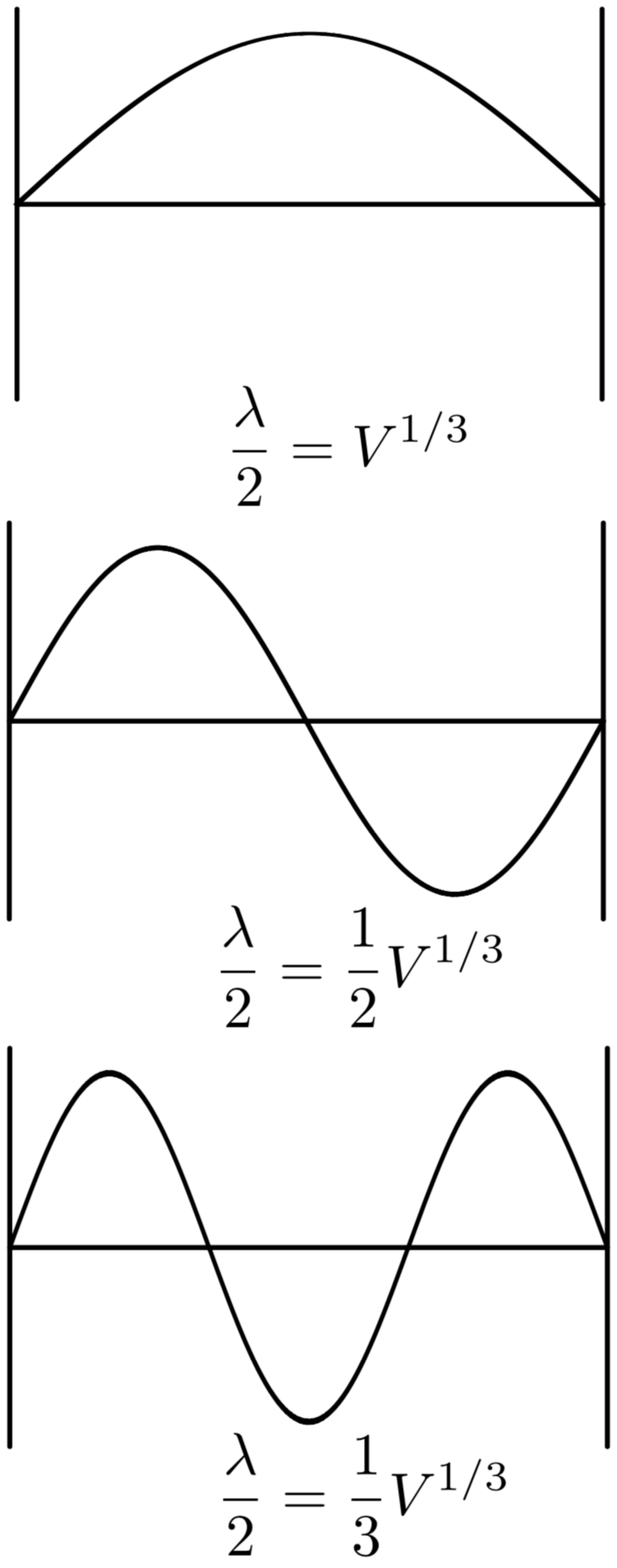
2.1.5 Density of states

$$\sum_j e^{-E_j/kT} \quad \rightarrow \quad \int_0^\infty g(\varepsilon)\, e^{-\varepsilon/kT} \mathrm{d}\varepsilon$$

density of states ↑

- Cubic box, side $V^{1/3}$
- Standing waves $\lambda_{n_x} = 2\frac{V^{1/3}}{n_x}, \lambda_{n_y} = 2\frac{V^{1/3}}{n_y}, \lambda_{n_z} = 2\frac{V^{1/3}}{n_z}$
- Momenta $p_x = \frac{\pi\hbar}{V^{1/3}} n_x,\ p_y = \frac{\pi\hbar}{V^{1/3}} n_y,\ p_z = \frac{\pi\hbar}{V^{1/3}} n_z$

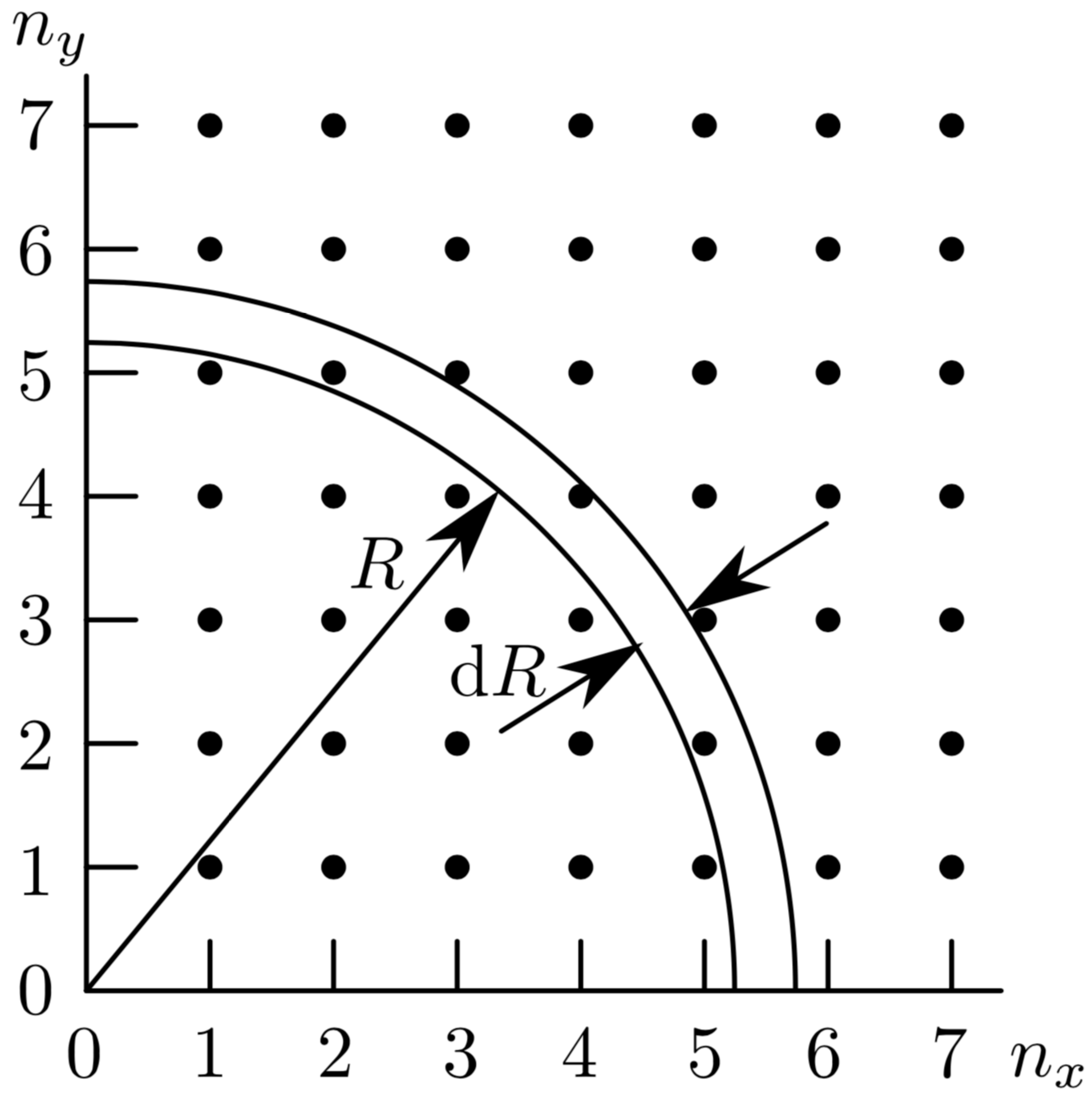
$$n_x, n_y, n_z = 1,2,3,\ldots, \infty$$



$$p_x = \frac{\pi\hbar}{V^{1/3}} n_x, \; p_y = \frac{\pi\hbar}{V^{1/3}} n_y, \; p_z = \frac{\pi\hbar}{V^{1/3}} n_z$$

- Energy: $\varepsilon = (p_x^2 + p_y^2 + p_z^2)/2m$
- So $\varepsilon = \dfrac{\pi^2\hbar^2}{2mV^{2/3}} R^2$ where $R^2 = n_x^2 + n_y^2 + n_z^2$
- No of states up to energy ε is volume of octant of radius R:

$$\mathcal{N}(\varepsilon) = \frac{1}{8}\frac{4}{3}\pi R^3 = \frac{1}{6}\frac{V}{\pi^2\hbar^2}(2m\varepsilon)^{3/2}.$$



$$\mathcal{N}(\varepsilon) = \frac{1}{6}\frac{V}{\pi^2\hbar^2}(2m\varepsilon)^{3/2}$$

- Density of states $$g(\varepsilon)\mathrm{d}\varepsilon = \mathcal{N}(\varepsilon + \mathrm{d}\varepsilon) - \mathcal{N}(\varepsilon)$$

  so that $$g(\varepsilon) = \frac{\mathrm{d}\mathcal{N}(\varepsilon)}{\mathrm{d}\varepsilon}.$$

- Differentiating $\mathcal{N}(\varepsilon)$ gives

$$g(\varepsilon) = \frac{1}{4}\frac{V}{\pi^2\hbar^3}(2m)^{3/2}\varepsilon^{1/2}$$

2.6.1 General procedure

- Bose-Einstein distribution

$$n(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/kT} - 1}$$

- Average of $f(\varepsilon)$

$$\bar{f} = \sum_i f(\varepsilon_i)\, n(\varepsilon_i)$$

(ignore spin degeneracy)

- Approximate sum by integral

$$\bar{f} = \int_0^\infty f(\varepsilon)\, n(\varepsilon)\, \mathrm{d}\varepsilon$$

we have

$$g(\varepsilon) = \frac{1}{4}\frac{V}{\pi^2\hbar^3}(2m)^{3/2}\varepsilon^{1/2}.$$

Need to determine μ first (from N)

2.6.2 Ground state occupation — chemical potential

- At $T = 0$ all bosons will be in the ground state.

$$N_0 = \frac{1}{e^{(\varepsilon_0 - \mu)/kT} - 1} = \quad \frac{1}{e^{-\mu/kT} - 1}$$ in thermodynamic limit.

- When N_0 is significant, μ/kT will be small (and negative), so expand exponential:

$$\mu \sim -kT/N_0$$

so $\mu = 0$ when N_0 is macroscopic

- Macroscopic occupation of ground state associated with zero chemical potential

2.6.3 Number of particles

Add up number of particles $N = \sum_i n_i \;\rightarrow\; \int_0^\infty g(\varepsilon)\, n(\varepsilon)\, \mathrm{d}\varepsilon$??

- The $\varepsilon^{1/2}$ in $g(\varepsilon)$ gives the ground state zero weight !!
- Failure of the continuum approximation; discounts the ground state.
- But for bosons at low temperature this is problematic.
- So, since $g(\varepsilon)$ neglects the ground state occupation, let's add this "by hand"

$$N = N_0 + \frac{V}{4\pi^2\hbar^3}(2m)^{3/2} \int_0^\infty \frac{\varepsilon^{1/2}}{e^{(\varepsilon-\mu)/kT-1}}\, \mathrm{d}\varepsilon$$

2.6.4 Low temperature behaviour — Bose-Einstein condensation

- Macroscopic occupation of ground state $\Longrightarrow$ put $\mu = 0$. So

$$N = N_0 + \frac{V}{4\pi^2\hbar^3}(2m)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}}{e^{\varepsilon/kT-1}}\,\mathrm{d}\varepsilon.$$

- Change variable of integration: $x = \varepsilon/kT$ gives

$$N = N_0 + V\left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2}\frac{2}{\sqrt{\pi}}\int_0^\infty \frac{x^{1/2}}{e^x - 1}\,\mathrm{d}x$$

- Physics comes outside of integral, the integral is just a number.

Integral is $$\int_0^\infty \frac{x^{1/2}}{e^x - 1}\,\mathrm{d}x = \frac{\sqrt{\pi}}{2}\zeta(\tfrac{3}{2})$$ (details in book/problems)

where $\zeta()$ is Riemann's zeta function, and $\zeta(\frac{3}{2}) = 2.612...$

- So N is

$$N = N_0 + V\left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2}\zeta(\tfrac{3}{2}).$$

- As T increases above $T = 0$ the ground state becomes depleted.

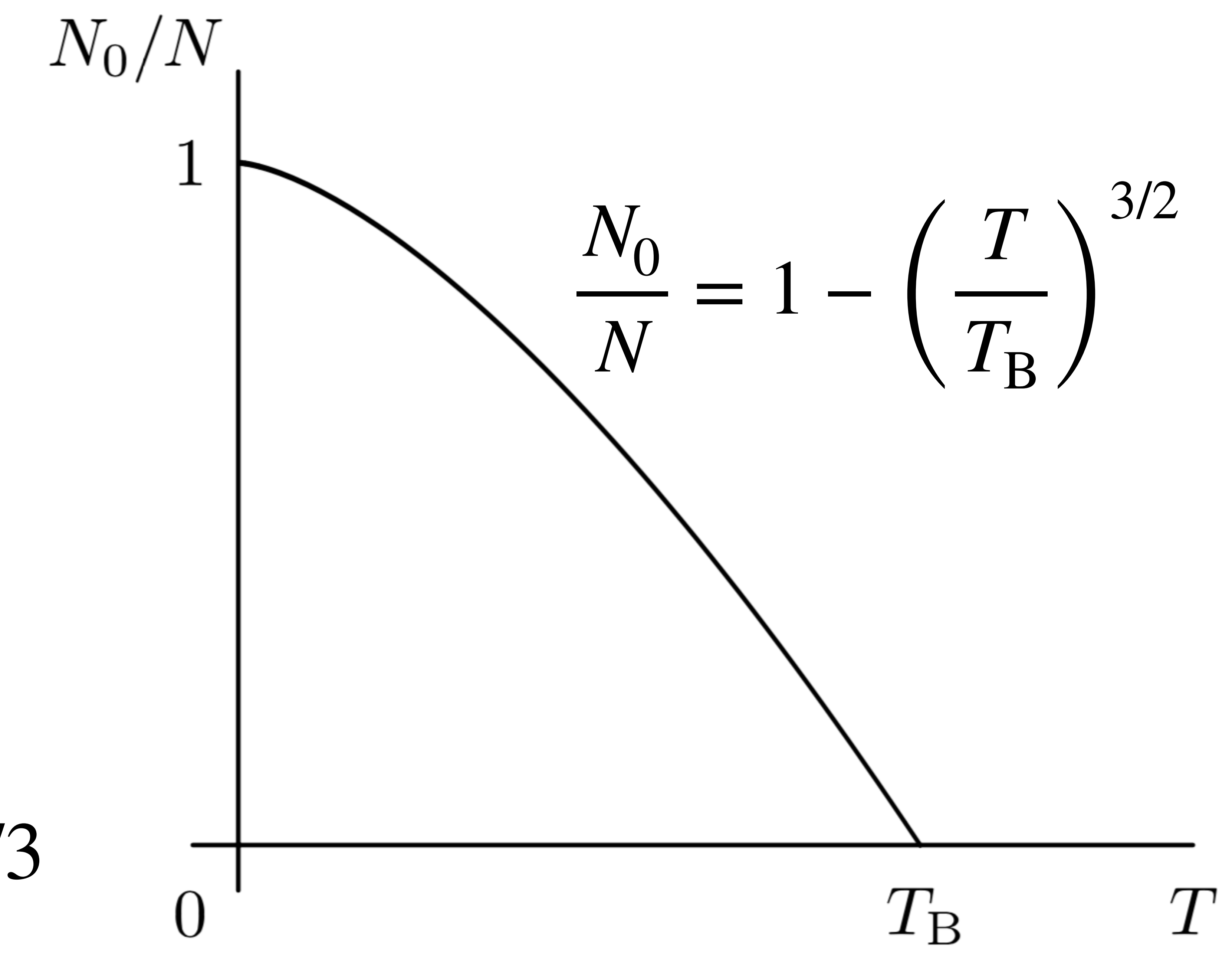
$$N_0 = N - V\left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2}\zeta(\tfrac{3}{2}).$$

- Ground state fraction

$$\frac{N_0}{N} = 1 - \frac{V}{N}\left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2}\zeta(\tfrac{3}{2}).$$

- Ground state fraction goes to zero at

$$T_\text{B} = \frac{2\pi\hbar^2}{mK}\left\{\frac{1}{\zeta(\frac{3}{2})}\frac{N}{V}\right\}^{2/3} = 3.313\frac{\hbar^2}{mK}\left\{\frac{N}{V}\right\}^{2/3}$$



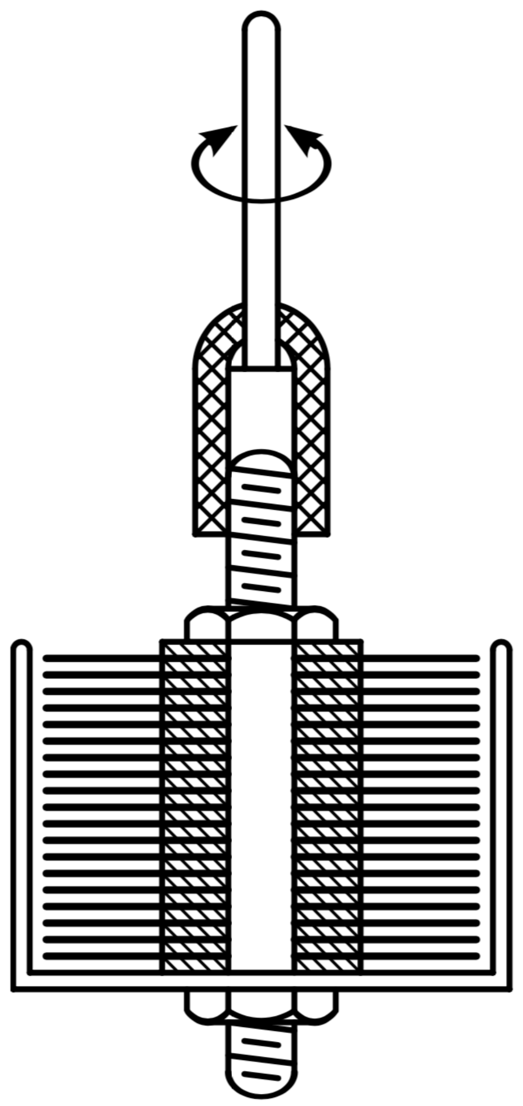
- Thermodynamic limit ?

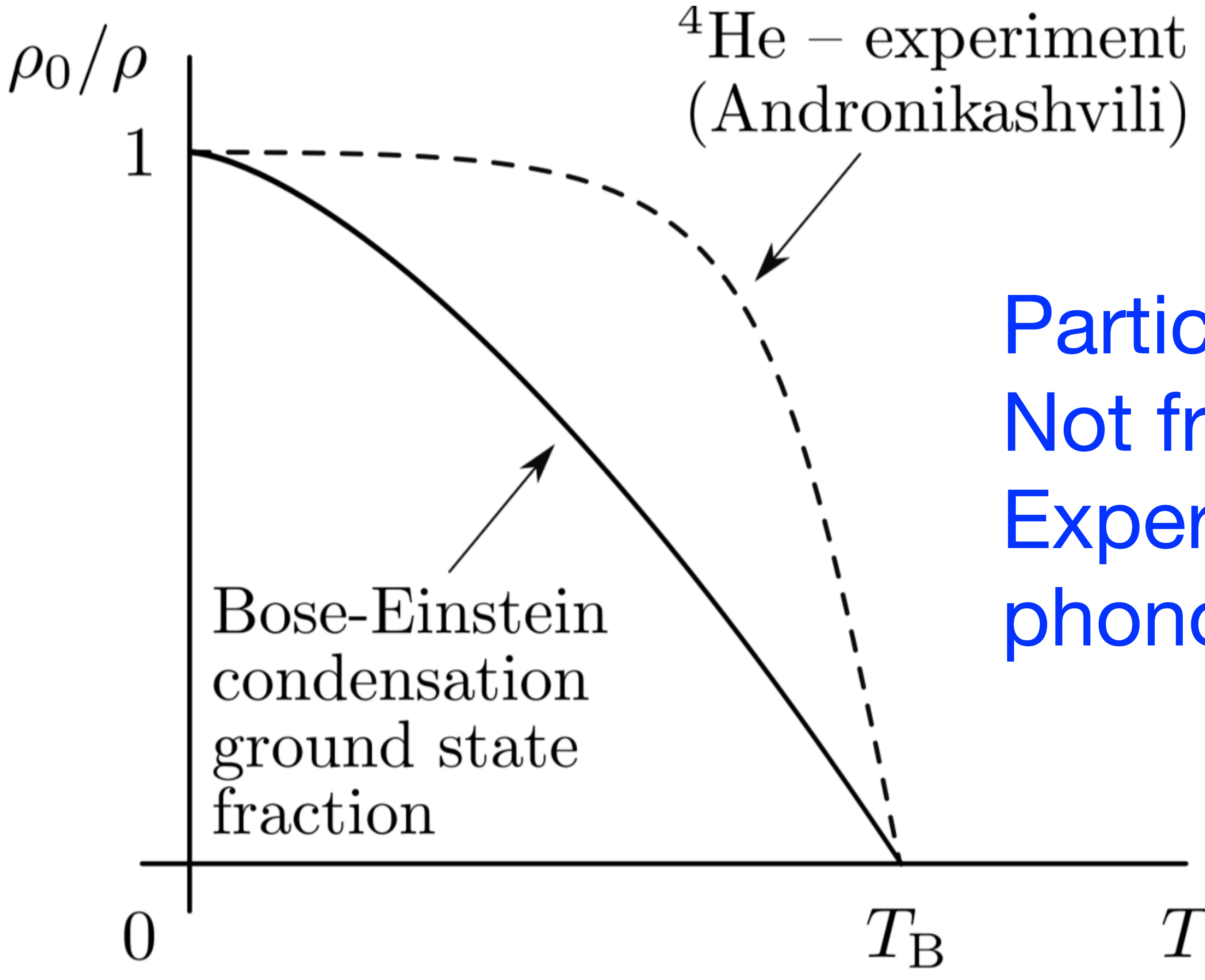
- Phase transition at $T = T_\text{B}$ called Bose-Einstein condensation.

- Roughly, transition is where Λ is comparable with inter-particle spacing.

2.6.6 Comparison with superfluid ^{4}He

- Superfluid transition in liquid ^{4}He observed at $T = 2.17$ K.
- Calculated T_{B} at liquid ^{4}He density is $T_{\mathrm{B}} = 3.13$ K. — similar??
- Suggestion by F. London and by L. Tisza that the superfluid transition *was* BEC.
- Andronikashvili experiment:





Particles are not free.
Not free-particle excitations.
Experiment consistent with
phonon and "roton" excitations.

2.6.5 Heat capacity of Bose gas

- Start from internal energy

$$E = \int_0^\infty \varepsilon\, g(\varepsilon)\, n(\varepsilon)\, \mathrm{d}\varepsilon.$$

Don't need to worry about ground state — it doesn't contribute to E.

- We'll just look at $T \le T_\mathrm{B}$, so we take $\mu = 0$.

$$E = \frac{V}{4\pi^2\hbar^3}(2m)^{3/2} \int_0^\infty \frac{\varepsilon^{3/2}}{e^{\varepsilon/kT} - 1}\, \mathrm{d}\varepsilon$$

Change variables:

$$E = \frac{V}{4\pi^2\hbar^3}(2m)^{3/2}(kT)^{5/2} \int_0^\infty \frac{x^{3/2}}{e^x - 1}\, \mathrm{d}x.$$

$$E = \frac{V}{4\pi^2\hbar^3}(2m)^{3/2}(kT)^{5/2}\int_0^\infty \frac{x^{3/2}}{e^x - 1}\,\mathrm{d}x$$

Integral is $\displaystyle\int_0^\infty \frac{x^{3/2}}{e^x - 1}\,\mathrm{d}x = \frac{3\sqrt{\pi}}{4}\zeta(\tfrac{5}{2}), \qquad \zeta(\tfrac{5}{2}) = 1.342...$

express E in terms of T_B

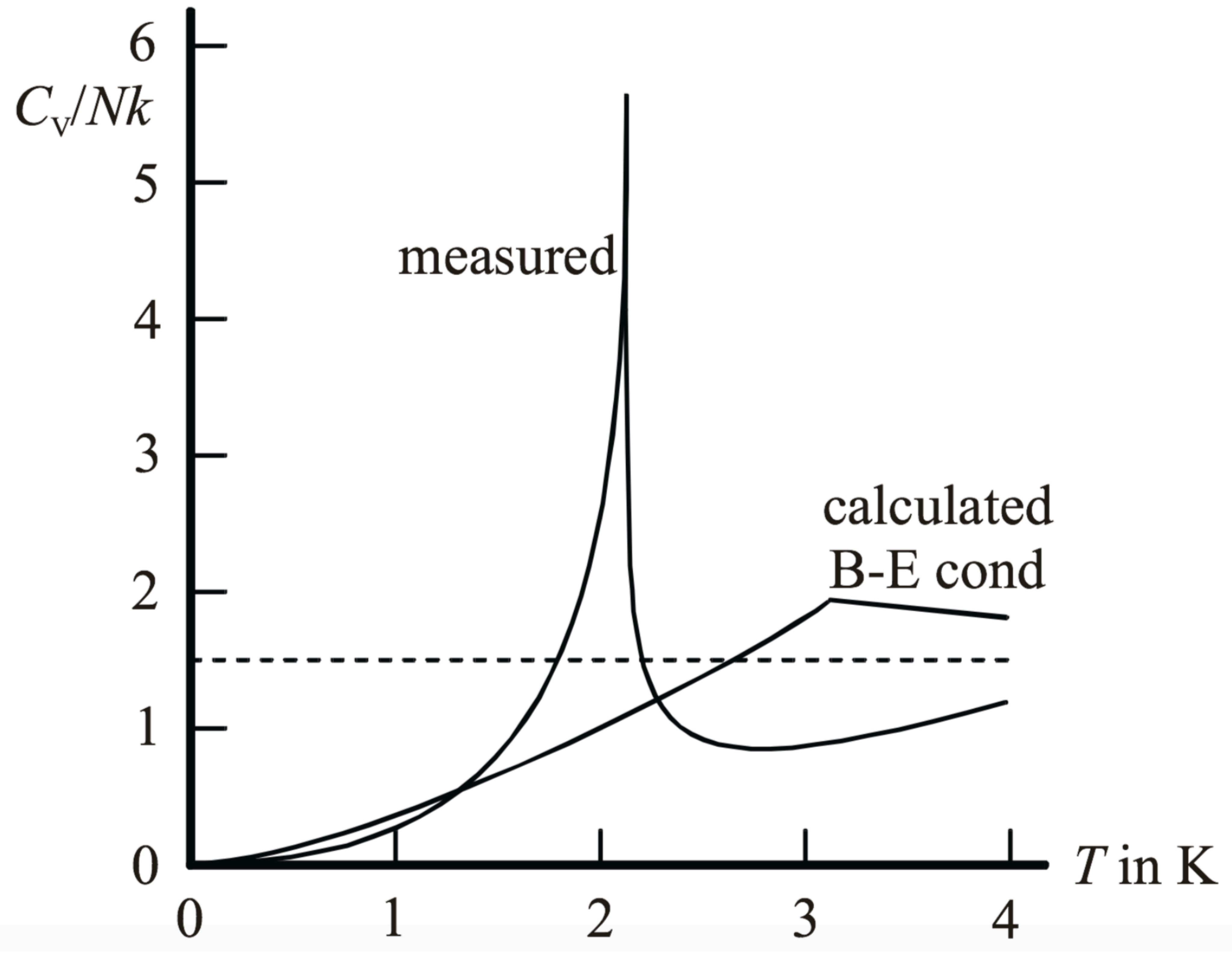
$$E = \frac{3}{2}Nk\frac{\zeta(\frac{5}{2})}{\zeta(\frac{3}{2})}\frac{T^{5/2}}{T_\mathrm{B}^{3/2}}\,.$$

Differentiate to get heat capacity

$$C_V = \frac{15}{4}Nk\frac{\zeta(\frac{5}{2})}{\zeta(\frac{3}{2})}\left(\frac{T}{T_\mathrm{B}}\right)^{3/2} = \frac{15}{4}Nk\left(\frac{T}{T_\mathrm{B}}\right)^{3/2}\times\frac{1.342}{2.612} = 1.926Nk\left(\frac{T}{T_\mathrm{B}}\right)^{3/2}$$

$$C_V = 1.926Nk\left(\frac{T}{T_B}\right)^{3/2}$$

- Classical value: $C_V = \frac{3}{2}Nk$.
  High temp value approaches this.
- Low temp BEC $C_V \sim T^{3/2}$.
- Low temp experiment $C_V \sim T^3$.
  Phonons - collective excitations.



2.8 BEC of a gas in a harmonic trap

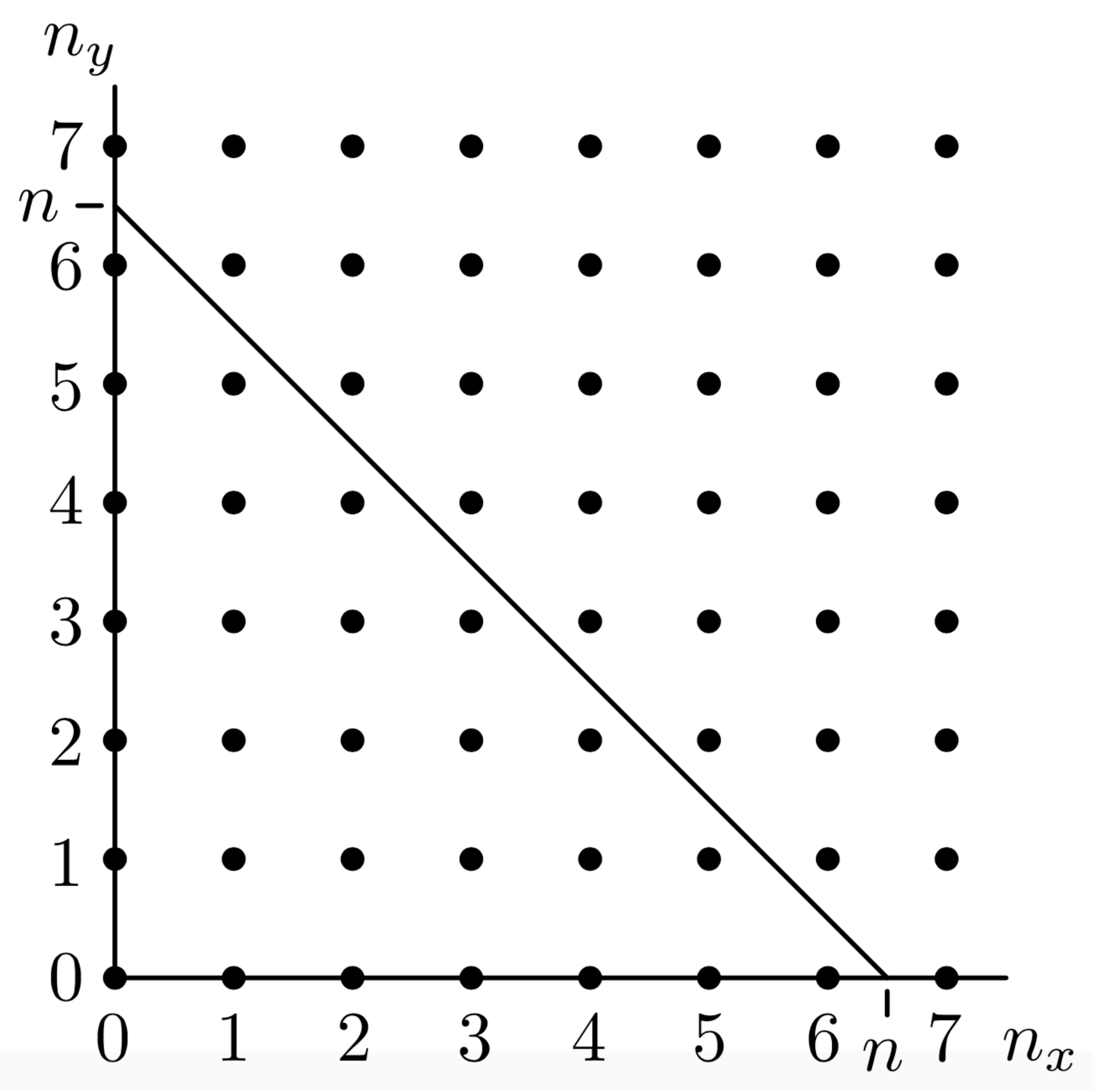
- Helium is a *liquid* — interactions — so is superfluidity true BEC?
- Would like to study a low density gas — negligible interactions.
- But $T_{\mathrm{B}} \sim (N/V)^{2/3}$, so if you go to lower densities, you must go to lower T.
- Laser cooling of trapped gases can do it. (really atomic physics, - not low temp)!

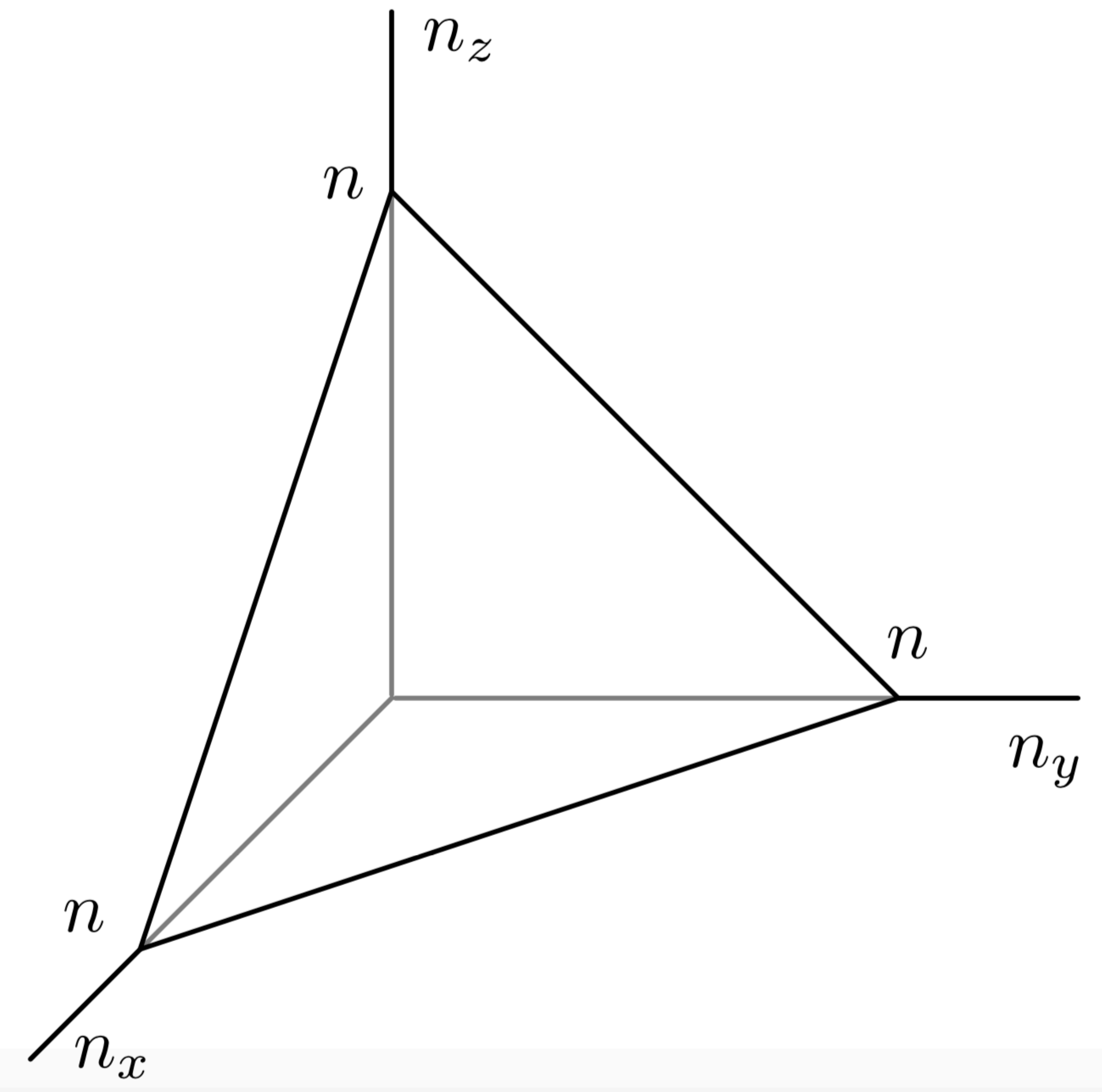
- We will study a gas trapped in a harmonic potential.

2.8.1 Enumeration and counting of states

- Energy of a 1d harmonic oscillator $\varepsilon = (n + \frac{1}{2})\hbar\omega$
- where ω is angular frequency, and quantum number n is integer: $n = 0,1,2\dots$
- For convenience, let's ignore ground state energy.
- In 3d need 3 quantum numbers: $\varepsilon = (n_x + n_y + n_z)\hbar\omega$
- Triple $\{n_x, n_y, n_z\}$ defines a point on a cubic grid.
- Energy: $\varepsilon = n\hbar\omega$ where $n = n_x + n_y + n_z$.

- $$\varepsilon = (n_x + n_y + n_z)\hbar\omega = n\hbar\omega.$$
- No of states up to energy $\varepsilon = n\hbar\omega$, denoted by $\mathcal{N}(\varepsilon)$ is the number of grid points $\{n_x, n_y, n_z\}$ satisfying
$$n_x + n_y + n_z < n$$
- In 3d $\mathcal{N}(\varepsilon)$ is the volume of the oblique pyramid $= \frac{1}{3}$base $\times$ height
$$\mathcal{N}(\varepsilon) = \frac{1}{6}n^3 = \frac{1}{6}\left(\frac{\varepsilon}{\hbar\omega}\right)^3$$
Differentiate to get $g(\varepsilon)$
$$g(\varepsilon) = \frac{d\mathcal{N}(\varepsilon)}{d\varepsilon}: \quad g(\varepsilon) = \frac{1}{2}\frac{\varepsilon^2}{(\hbar\omega)^3}$$





Chemical potential

- Bosons: low temperatures $\Longrightarrow$ macroscopic occupation of the ground state.
- As before, when N_0 is large $\mu \sim -kT/N_0$

so $\mu = 0$ when N_0 is macroscopic

- Macroscopic occupation of ground state associated with zero chemical potential

Number of particles

- The $g(\varepsilon)$ (now $\propto \varepsilon^2$) gives zero weight to the ground state occupation.
- So must put this in "by hand":

$$N = N_0 + \frac{1}{2}\frac{1}{(\hbar\omega)^3}\int_0^\infty \frac{\varepsilon^2 \, \mathrm{d}\varepsilon}{e^{(\varepsilon-\mu)/kT}+1}$$

Put $\mu \to 0$ (below transition), and change variables $x = \varepsilon/kT$, gives

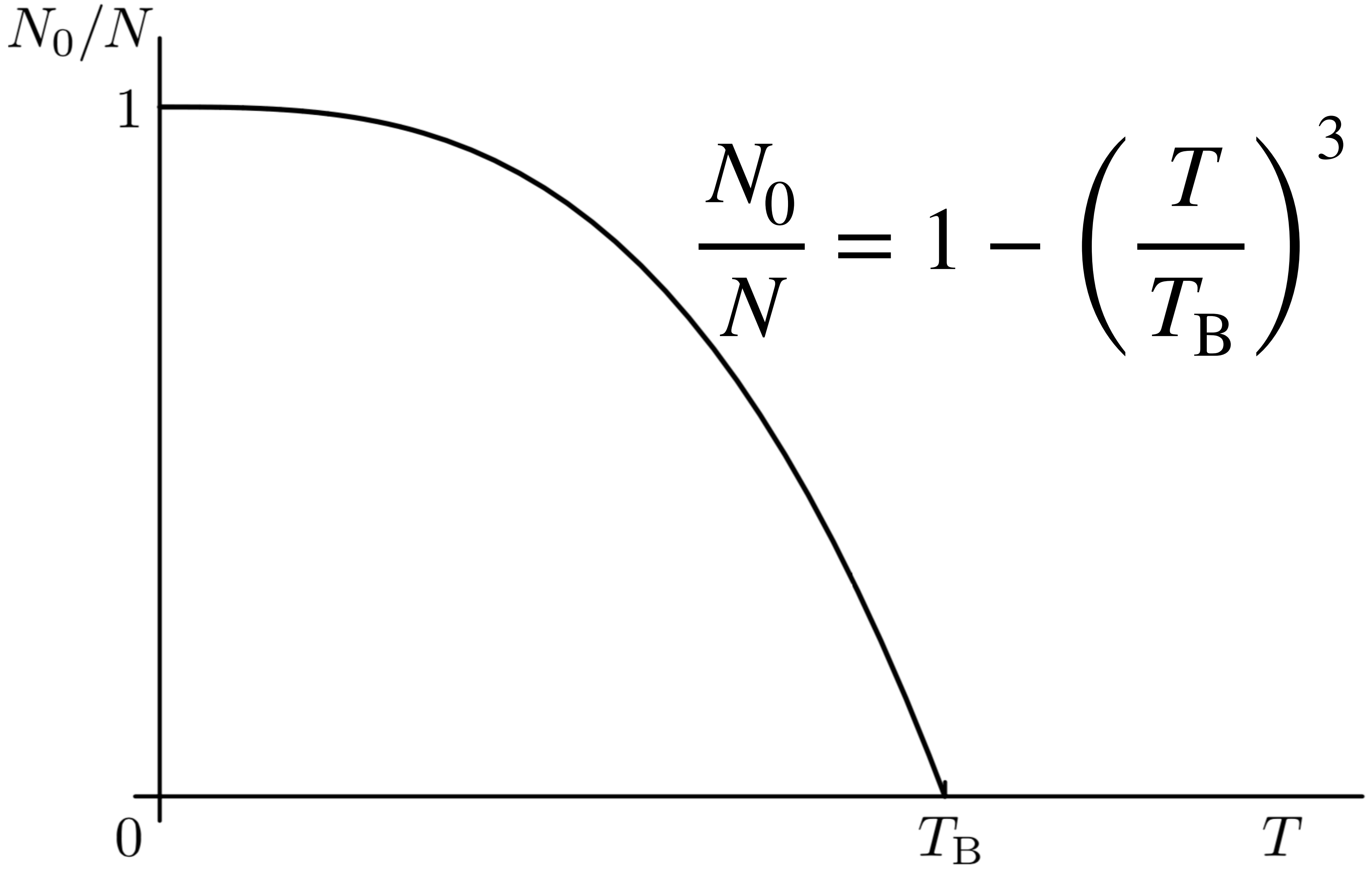
$$N = N_0 + \frac{1}{2}\left(\frac{kT}{\hbar\omega}\right)^3 \int_0^\infty \frac{x^2 \, \mathrm{d}x}{e^x+1},$$ integral is a number: $$\int_0^\infty \frac{x^2 \, \mathrm{d}x}{e^x+1} = 2\zeta(3)$$

- Below transition $$N = N_0 + \left(\frac{kT}{\hbar\omega}\right)^3 \zeta(3).$$

$$N = N_0 + \left(\frac{kT}{\hbar\omega}\right)^3 \zeta(3)$$

- As T increases above $T = 0$ the ground state becomes depleted

$$N_0 = N - \left(\frac{kT}{\hbar\omega}\right)^3 \zeta(3)$$



- Ground state fraction goes to zero at

$$T_B = \frac{\hbar\omega}{k}\left(\frac{N}{\zeta(3)}\right)^{1/3} = 0.940\frac{\hbar\omega}{k}N^{1/3}$$

Particle density

- Gas sits in a harmonic potential.

- Density *decreases* with *increasing temperature*. Mean square displacement:

$$\langle x^2 \rangle_T = \frac{kT}{m\omega^2}.$$

- Corresponds to an effective volume $V = \left(\langle x^2 \rangle_T\right)^3 = \left(\frac{kT}{m}\right)^{3/2} \omega^{-3}$

- Effective density $\frac{N}{V} = \left(\frac{m}{kT}\right)^{3/2} N\omega^2$, effective particle separation $l = (N/V)^{1/3}$:

$$l = \left(\frac{kT}{m}\right)^{1/2} \frac{1}{\omega N^{1/3}}.$$

$$l = \left(\frac{kT}{m}\right)^{1/2} \frac{1}{\omega N^{1/3}}$$

- Recall argument that at transition thermal de Broglie wavelength Λ should be comparable with mean particle spacing l:

$$\sqrt{\frac{2\pi\hbar^2}{mkT_c}} \approx \left(\frac{kT_B}{m}\right)^{1/2} \frac{1}{\omega N^{1/3}},$$

about 2.4 times the exact expression for T_B.

Exact result gives

$$\Lambda = \sqrt{2\pi}\,\zeta(3)^{1/3} l = 2.67\, l.$$

Spatial extent

- We had, for particles at temperature T:

$$\langle x^2 \rangle_T = \frac{kT}{m\omega^2}.$$

  This is the mean square spatial extent of (a normal) confined gas.

- For the particles in the SHO ground state (condensate), the probability of being found a distance x from the minimum is

$$|\Psi(x)|^2 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-m\omega x^2/\hbar}$$

  a mean square displacement

$$\langle x^2 \rangle_0 = \frac{\hbar}{2m\omega}$$

  (typo in book!)

We found $\langle x^2 \rangle_T = \dfrac{kT}{m\omega^2}$ and $\langle x^2 \rangle_0 = \dfrac{\hbar}{2m\omega}$.

- Ratio:

$$\frac{\langle x^2 \rangle_T}{\langle x^2 \rangle_0} = 2\frac{kT}{\hbar\omega}$$

better to use T_{B} instead of ω, then

$$\frac{\langle x^2 \rangle_T}{\langle x^2 \rangle_0} = 2\zeta(3)^{-1/3} N^{1/3} \frac{T}{T_{\mathrm{B}}} = 1.88\, N^{1/3} \frac{T}{T_{\mathrm{B}}}$$

- This indicates that as one cools through the transition a much narrower (ground state) peak will appear in the particle density.

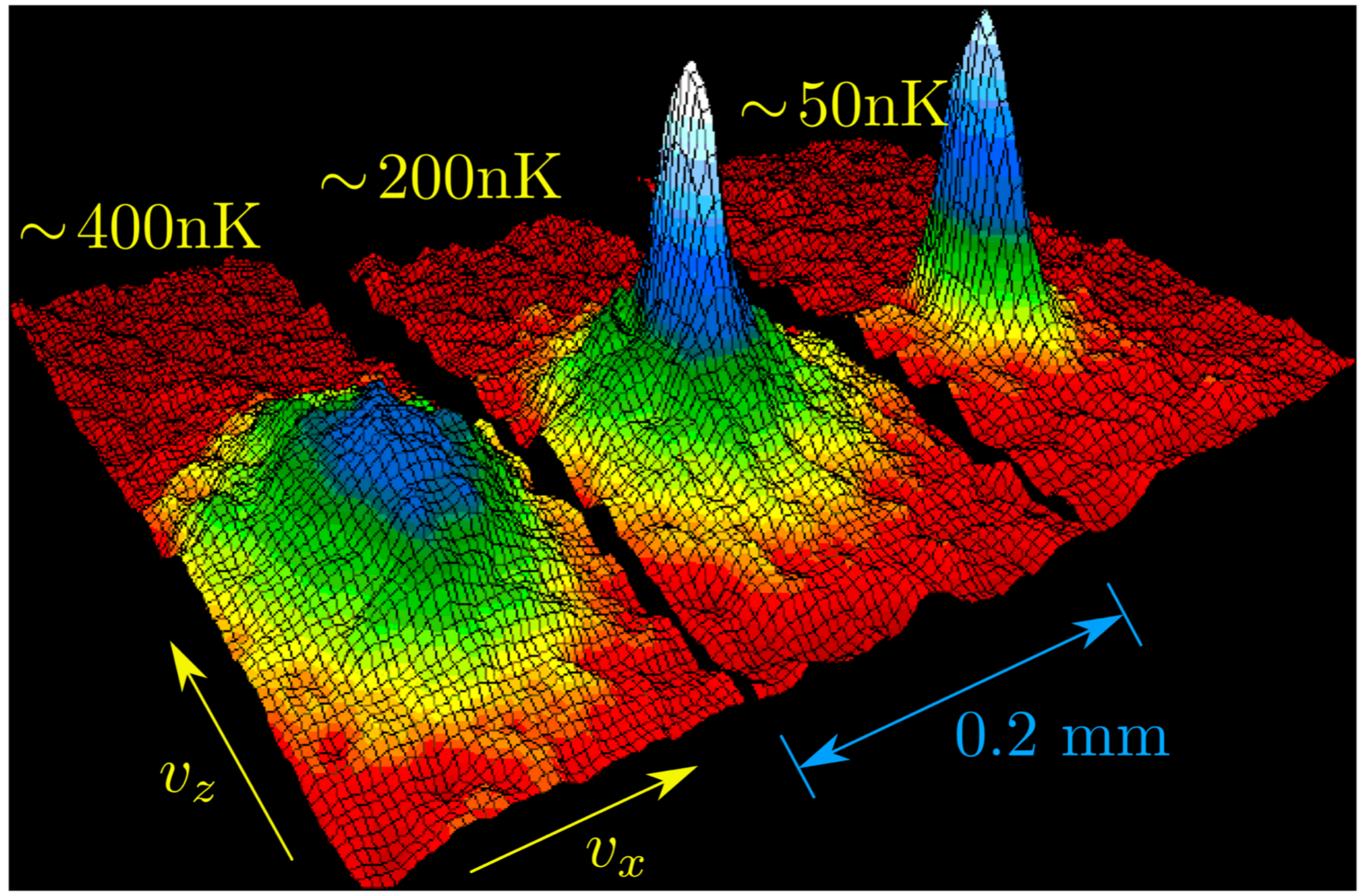
Experimental observation

- First observation in 1995. Rubidium vapour
  E. Cornell, W. Ketterle, C.Wieman
  — Nobel prize 2001

- Left image: velocity distribution at 400 nK, just before the appearance of the BEC.

- Centre image: at 200 nK, just after the appearance of the BEC

- Right image: at 50 nK, after further evaporation leaves a sample of nearly pure condensate.



Bose-Einstein condensation in rubidium vapour. Velocity distributions of the atoms at three different temperatures.

- Rubidium has a small repulsive interaction. Interest in effect of repulsion on BEC.