``Enseigner la recherche en train de se faire''

COLLÈGE DE FRANCE
1530

Chaire de
Physique de la Matière Condensée

PETITS SYSTEMES THERMOELECTRIQUES: *CONDUCTEURS MESOSCOPIQUES ET GAZ D'ATOMES FROIDS*

Cycle « Thermoélectricité »
2012 - 2014

Antoine Georges

Séance du 10 décembre 2013
Cours 5

Building Thermal Engines with Ultra-Cold Atomic Gases:

Thermomechanical, Mechanocaloric and Thermo-`Electric' effects

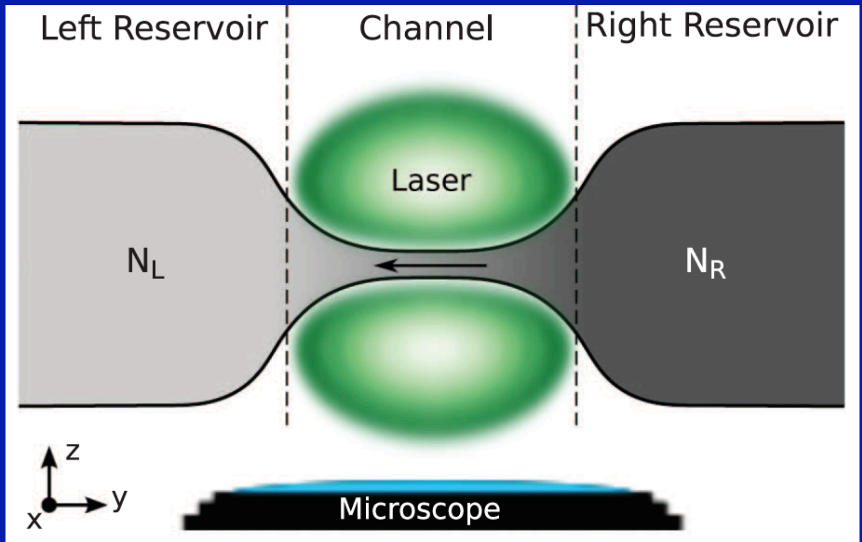
Séminaires du 10/12/2014 :

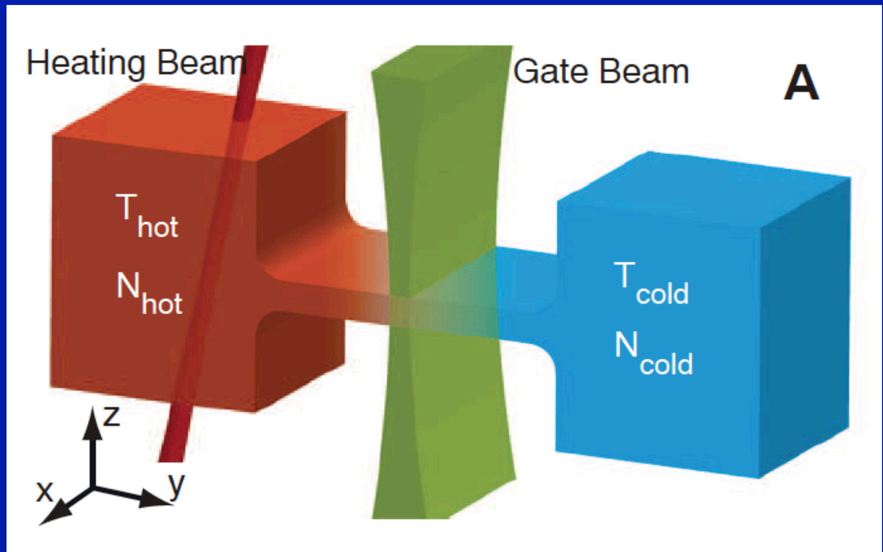
- Jean-Philippe Brantut (ETH-Zürich)

Transport experiments with ultra-cold atoms

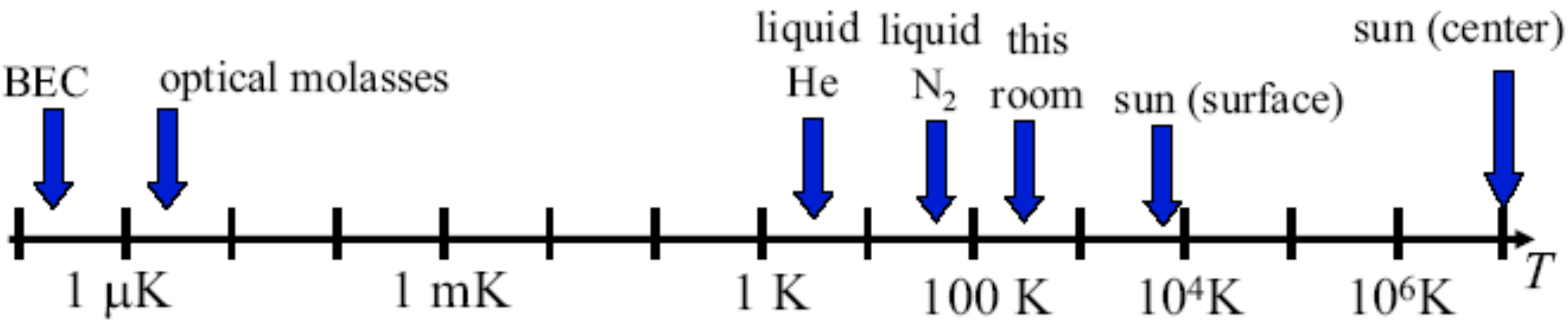
- Charles Grenier (ETH-Zürich)

Thermoelectric transport of ultracold fermions: theory.





Ultra-Cold Atomic Gases



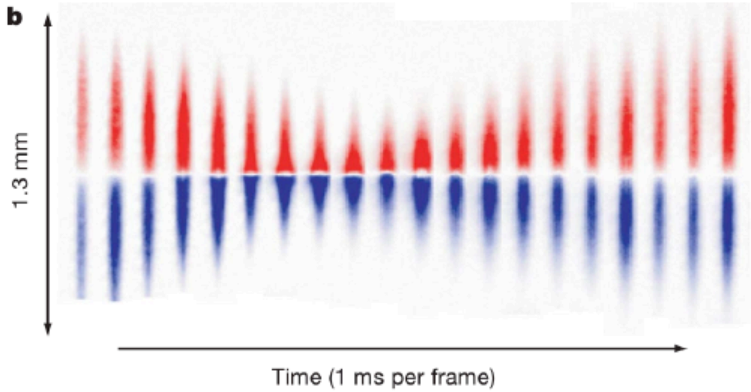
Nobel 2001
E. Cornell , W. Ketterle , C. Wieman

Nobel 1997
S. Chu, C. Cohen-Tannoudji, W. Phillips

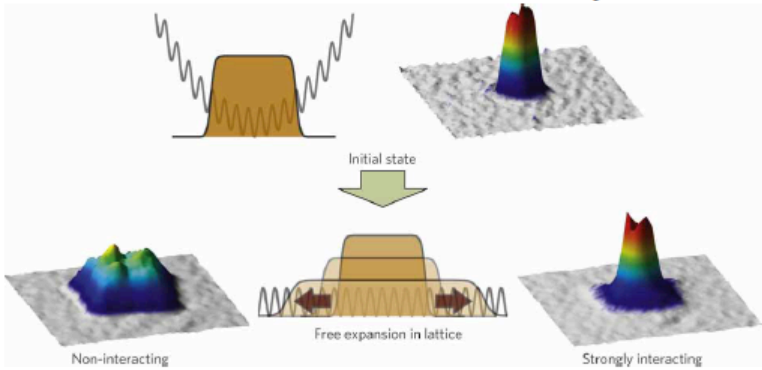
An emerging field: transport experiments with ultra-cold atomic gases → seminars

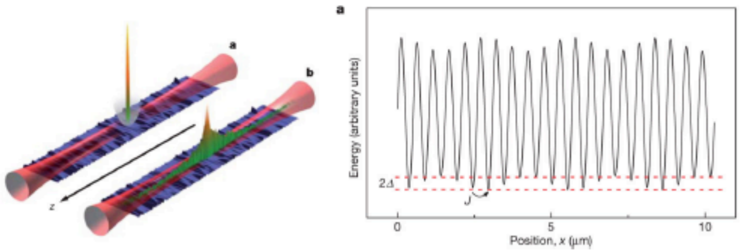
Introduction - Transport and cold atoms

Spin transport (MIT, 2011)
A. Sommer *et al.*, Nature



Interactions (LMU, 2012)
U. Schneider *et al.*, Nat. Phys.

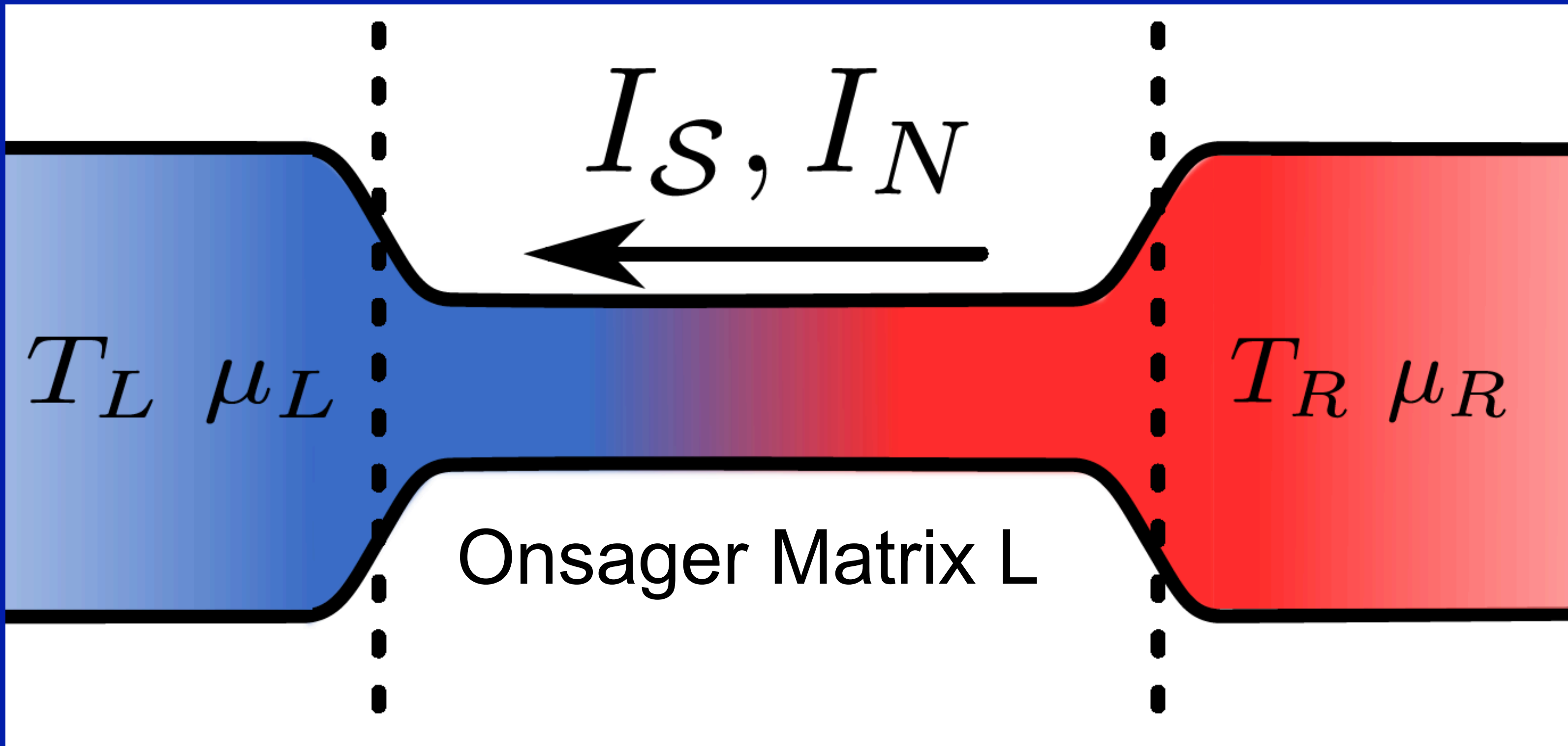




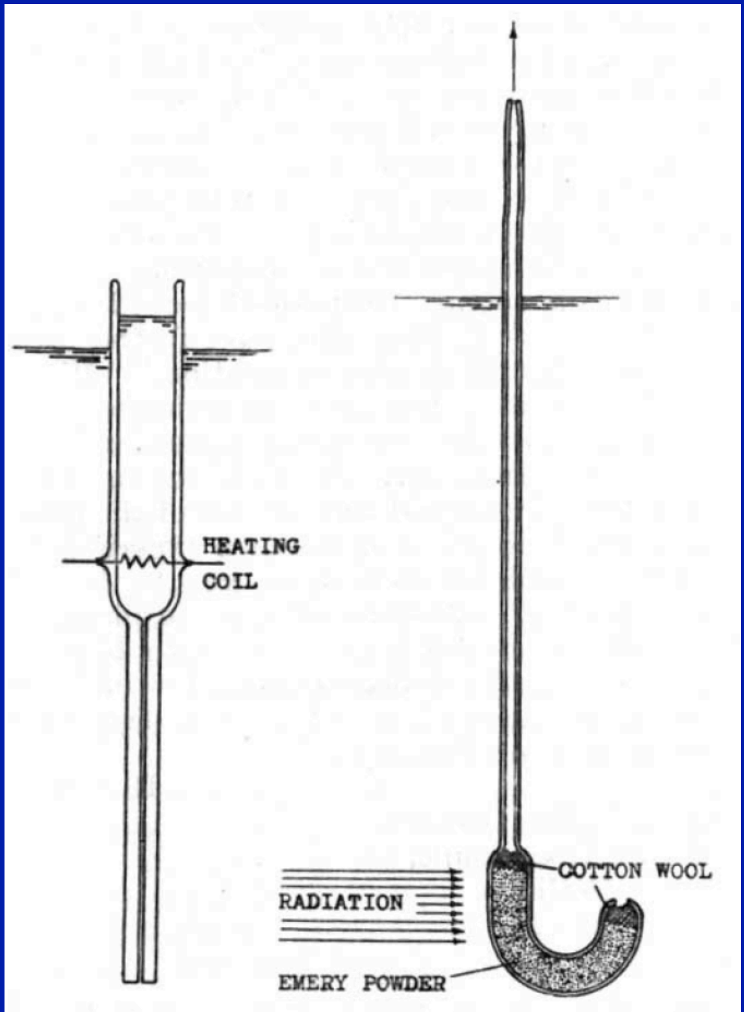
Disorder (Inst. d'optique - LENS, 2008)
J. Billy *et al.*-G. Roati *et al.*, Nature

Also:
H. Ott *et al*, Phys. Rev. Lett. 92, 160601 (2004)
S. Palzer *et al*, Phys. Rev. Lett. 103, 150601 (2009)
J. Catani *et al*, Phys. Rev. A 85, 023623 (2012)
K.K. Das *et al*, Phys. Rev. Lett. 103, 123007 (2009)
And many others ...

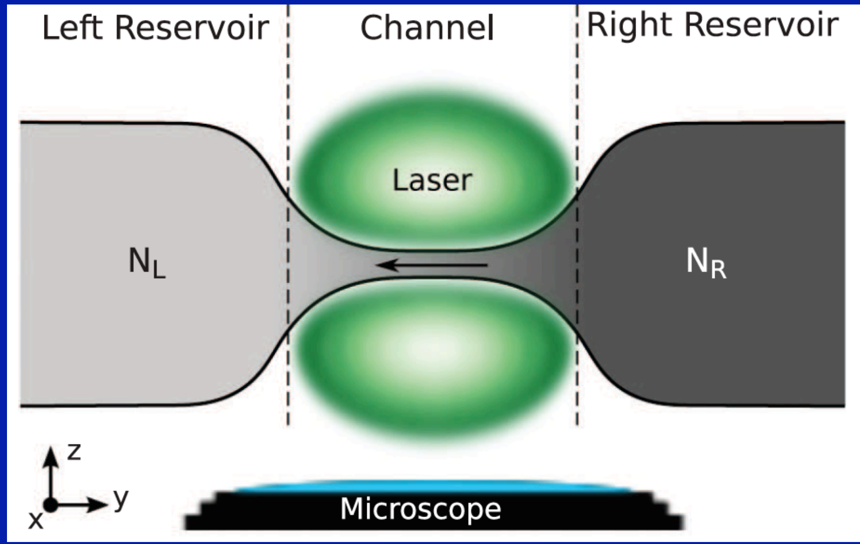
Generic set-up in the following:
Two reservoirs and a constriction



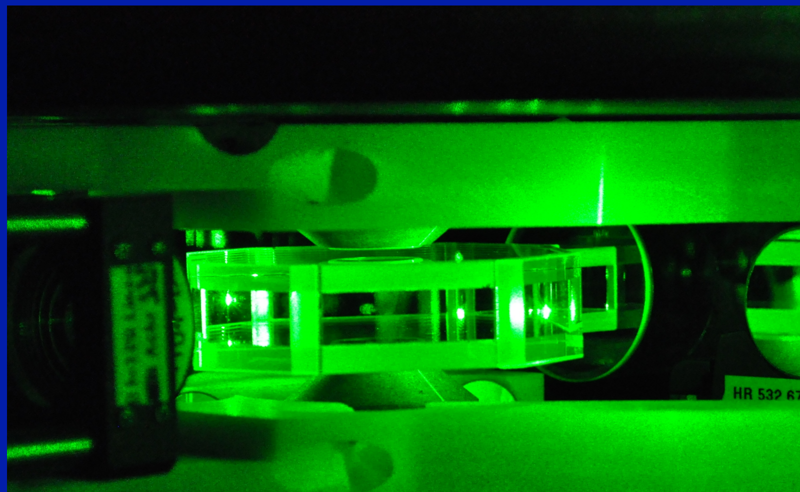
Older and Newer Incarnations:



Allen and Jones,
Nature, 1938



Brantut et al.
Science, 337, 1071 (2012)



Picture:
Courtesy T.Esslinger et al. ETH

Reminder from Lecture 2: Matrix of Onsager Coefficients for the constriction in the linear response regime

Particle and entropy currents:

$$\boxed{\begin{aligned} I_N &= L_{11}\Delta\mu + L_{12}\Delta T \\ I_S &= L_{21}\Delta\mu + L_{22}\Delta T \end{aligned}}$$

N,S particle number and entropy
I_N,I_S: currents

$$\Delta\mu \equiv \mu_L - \mu_R$$
$$\Delta T \equiv T_L - T_R$$

Reminders from lecture 2: Conductance, Thermopower, and Thermal Conductance:

$$L_{11} = \frac{2}{h} I_0$$

$$L_{12} = \frac{2}{h} k_B\, I_1$$

$$L_{22} = \frac{2}{h} k_B^2\, I_2$$

$$G = \frac{2e^2}{h} I_0 \ , \quad \left(\frac{h}{e^2} = 25.81 k\Omega \right)$$

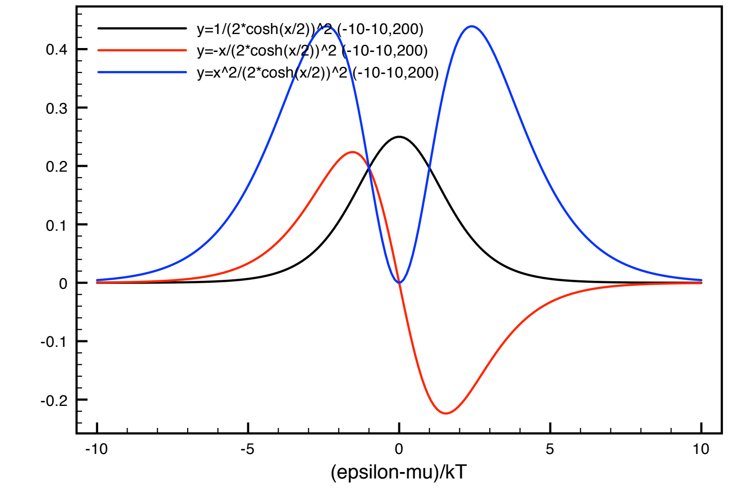
$$\alpha = -\frac{k_B}{e} \frac{I_1}{I_0} \ , \quad \left(\frac{k_B}{e} = 86.3\, \mu V K^{-1} \right)$$

$$\frac{G_{th}}{T} = \frac{2}{h} k_B^2 \left[I_2 - \frac{I_1^2}{I_0} \right]$$

$$\mathcal{L} \equiv \frac{G_{th}}{TG} = \left(\frac{k_B}{e} \right)^2 \left[\frac{I_2}{I_0} - \left(\frac{I_1}{I_0} \right)^2 \right]$$

Dimensionless integrals:

$$I_n \equiv \int d\varepsilon\, \mathcal{T}(\varepsilon) \left(\frac{\varepsilon - \mu}{k_B T} \right)^n \left(-\frac{\partial f}{\partial \varepsilon} \right)$$



Dynamics of equilibration:

The thermodynamics of the reservoirs
AND the transport in the constriction
BOTH play a role

Consider the simplest case with no temperature imbalance, L_{12}=0, and linear-response applies (small deviations from equilibrium) :

Dynamics of the particle flow:

$$\frac{d}{dt}\Delta N = -I_N = -L_{11}\,\Delta\mu$$

Thermodynamics in the reservoirs: $\Delta N = \kappa\,\Delta\mu \ , \ \kappa \equiv \frac{\partial N}{\partial \mu}\Big|_T$

(κ ~ compressibility, see below)

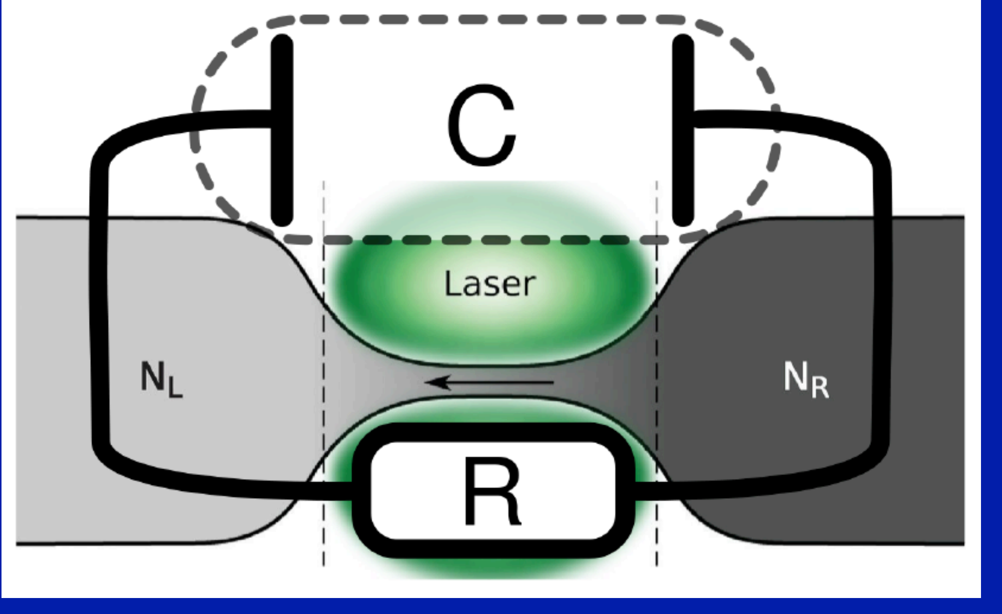
Combining:

$$\frac{d}{dt}\Delta\mu = -\frac{L_{11}}{\kappa}\,\Delta\mu$$

Same for ΔN

$$\boxed{\{\Delta N(t), \Delta\mu(t)\} = \{\Delta N_0, \Delta\mu_0\}\, e^{-t/\tau_\mu} \quad , \quad \tau_\mu = \frac{\kappa}{L_{11}}}$$

cf. discharge of a capacitor:



$$Q(t) = Q_0\, e^{-t/\tau} \quad , \quad \tau = RC = \frac{C}{G} = \frac{C}{e^2 L_{11}}$$

Similarly, thermal equilibration: (assuming no off-diagonal terms e.g. L_{12}=0)

$$\Delta T(t) = \Delta T_0 \, e^{-t/\tau_T} \quad , \quad \tau_T = \frac{C_\mu/T}{L_{22}} = \frac{C_\mu/T}{G_{th}/T}$$

With the heat capacity at constant chemical potential:

$$C_\mu = T \, \frac{\partial S}{\partial T}\Big|_\mu$$

In the presence of coupling between T and μ either via transport (L_{12}) or thermodynamics (dilatation coeff.), <u>the evolution of μ and T become coupled</u>: see seminars by J-P Brantut and C.Grenier

A note in passing: A dynamical interpretation of Wiedemann-Franz law

For a free Fermi gas, as T→0 (cf. previous lectures):

$$\frac{G_{th}/T}{G} \to \frac{\pi^2}{3} \;, \quad \frac{C_\mu/T}{\kappa} \to \frac{\pi^2}{3}$$

Hence, the particle and thermal equilibration times are the same as T→ 0 !

$$\boxed{\frac{\tau_\mu}{\tau_T} \to 1}$$

More on the thermodynamics of the reservoirs: including the non-diagonal terms

$$\begin{pmatrix} \Delta N \\ \Delta S \end{pmatrix} = \underline{K} \begin{pmatrix} \Delta \mu \\ \Delta T \end{pmatrix} = \begin{pmatrix} \kappa & \kappa\alpha_r \\ \kappa\alpha_r & C_\mu/T \end{pmatrix} \begin{pmatrix} \Delta \mu \\ \Delta T \end{pmatrix}$$

$$K_{11} \equiv \kappa = \frac{\partial N}{\partial \mu}\Big|_T = -\frac{\partial^2 \Omega}{\partial \mu^2}$$

$$K_{12} = K_{21} \equiv \alpha_r \kappa = \frac{\partial N}{\partial T}\Big|_\mu = -\frac{\partial^2 \Omega}{\partial \mu \partial T} = \frac{\partial S}{\partial \mu}\Big|_T$$

$$K_{22} \equiv \frac{C_\mu}{T} = \frac{\partial S}{\partial T}\Big|_\mu = -\frac{\partial^2 \Omega}{\partial T^2}$$

Grand-potential: $\Omega \equiv -k_B T \ln Z_{gc} \;,\; S = -\frac{\partial \Omega}{\partial T}\Big|_\mu \;,\; N = -\frac{\partial \Omega}{\partial \mu}\Big|_T$

Expressions for a free Fermi gas:

For a free Fermi gas, these coefficients are easily calculated from:

$$N(\mu,T) = \int d\varepsilon D(\varepsilon) f\left(\frac{\varepsilon-\mu}{k_B T}\right)$$

$$S(\mu,T) = -k_B \int d\varepsilon D(\varepsilon) \left[f \ln f + (1-f)\ln(1-f)\right]$$

with $D(\varepsilon)$ the density of states. This leads to:

$$K_{11} = J_0 \ , \ K_{12} = K_{21} = k_B J_1 \ , \ K_{22} = k_B^2 J_2$$

where J_n are integrals with the *dimension of energy*:

$$J_n = \int d\varepsilon D(\varepsilon) \left(\frac{\varepsilon-\mu}{k_B T}\right)^n \left(-\frac{\partial f}{\partial \varepsilon}\right)$$

Note formal similarity with the expression of the Onsager coefficients for transport !

Same (general) constraints apply (around equilibrium state):

$$K_{11} \geq 0 \, , \, K_{22} \geq 0 \, , \, \det K \geq 0$$

Reminders from lecture 2: Conductance, Thermopower, and Thermal Conductance:

$$L_{11} = \frac{2}{h} I_0$$
$$L_{12} = \frac{2}{h} k_B\, I_1$$
$$L_{22} = \frac{2}{h} k_B^2\, I_2$$

$$G = \frac{2e^2}{h} I_0 \ , \quad \left(\frac{h}{e^2} = 25.81 k\Omega \right)$$
$$\alpha = -\frac{k_B}{e} \frac{I_1}{I_0} \ , \quad \left(\frac{k_B}{e} = 86.3\, \mu V K^{-1} \right)$$
$$\frac{G_{th}}{T} = \frac{2}{h} k_B^2 \left[I_2 - \frac{I_1^2}{I_0} \right]$$
$$\mathcal{L} \equiv \frac{G_{th}}{TG} = \left(\frac{k_B}{e} \right)^2 \left[\frac{I_2}{I_0} - \left(\frac{I_1}{I_0} \right)^2 \right]$$

Dimensionless integrals:

$$I_n \equiv \int d\varepsilon\, \mathcal{T}(\varepsilon) \left(\frac{\varepsilon - \mu}{k_B T} \right)^n \left(-\frac{\partial f}{\partial \varepsilon} \right)$$

Physical Interpretation of the Coefficients of the Thermodynamic Matrix :

K_{11} ~ Compressibility :

Pressure in grand-canonical ensemble, given extensivity of $\Omega = V\omega(\mu, T)$:

$$p(\mu, T) = -\frac{\partial \Omega}{\partial V} = -\frac{1}{V}\Omega(\mu, T)$$

With $n \equiv N/V$ the density, the equation of state will be given by:

$$p(n, T) = p_{gc}\left[\mu(n, T), T\right]$$

From which it follows that:

$$\frac{\partial p}{\partial n}|_T = \frac{\partial p}{\partial \mu}|_T \frac{\partial \mu}{\partial n}|_T = n\frac{\partial \mu}{\partial n}|_T$$

A variation of volume corresponds to (from $n = N/V$):

$$\frac{\delta V}{V} = -\frac{\delta n}{n}$$

The isothermal compressibility is usually defined as:

$$\kappa_T \equiv -\frac{1}{V}\frac{\partial V}{\partial p}|_T = \frac{1}{n}\frac{\partial n}{\partial p}|_T$$

So that:

$$\boxed{\kappa_T = \frac{1}{n^2}\frac{\partial n}{\partial \mu}|_T = \frac{1}{n^2 V}K_{11} \equiv \frac{1}{n^2 V}\kappa}$$

Must be positive (otherwise phase separation)

We have seen that $K_{22} = C_\mu / T$

At constant density: "stopping condition"

$$K_{11}\delta\mu + K_{12}\delta T = 0 \Rightarrow \delta\mu = -\frac{K_{12}}{K_{11}}\delta T$$

$$\delta S = K_{21}\delta\mu + K_{22}\delta T = \left(K_{22} - \frac{K_{12}^2}{K_{11}}\right)\delta T = \frac{\det K}{K_{11}}\delta T$$

cf. analogy with thermal conductivity calculation

$$\boxed{\det K = \kappa \frac{C_N}{T} \geq 0}$$

Positivity of K_{22} and det K follows from the second principle of thermodynamics

K_{12} ~ Thermal expansion coefficient at constant μ:

$$\alpha_\mu \equiv \frac{1}{V}\frac{\partial V}{\partial T}|_\mu = -\frac{1}{n}\frac{\partial n}{\partial T}|_\mu$$

$$\boxed{K_{12} \equiv \kappa\alpha_r = V\frac{\partial n}{\partial T}|_\mu = -N\alpha_\mu}$$

Importantly for the following, this coefficient <u>can be positive or negative</u>. Alternatively its sign can be related to the variation of μ as a function of temperature at constant density:

We note that a variation at constant density implies:

$$K_{11}\delta\mu + K_{12}\delta T = 0 \Rightarrow \frac{\partial \mu}{\partial T}|_n = -\frac{K_{12}}{K_{11}} = -\alpha_r$$

Hence:

$$\boxed{\frac{\partial n}{\partial T}|_\mu = -n^2\kappa_T\frac{\partial \mu}{\partial T}|_n \quad \left(= n^2\kappa_T\alpha_r = \frac{1}{V}K_{12}\right)}$$

μ decreases with T → $\alpha_r > 0$ → Δn , ΔT same sign at constant μ

Enough with Thermodynamics,
Let's turn to some physical
effects !

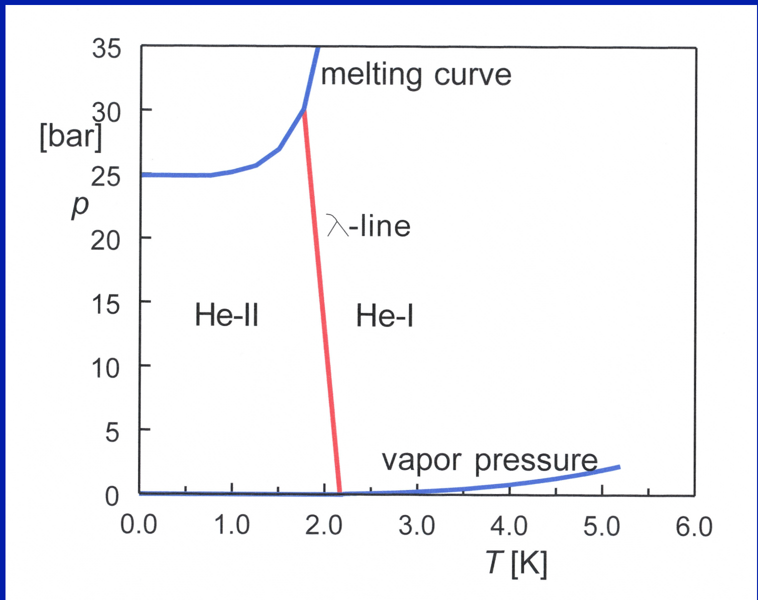
SUPERFLUIDS:

Thermomechanical and Mechanocaloric effects

The Fountain Effect

Superfluid Helium 4: some reminders

- On the fascinating history of the discovery of superfluidity
- Sébastien Balibar:
- J. Low Temp Phys 146, 441 (2007)
- La pomme et l'atome (Odile Jacob, 2005)
- Slides on website @ENS
- Also: A.Griffin, J.Phys. Cond. Mat. 21, 164220 (2009)



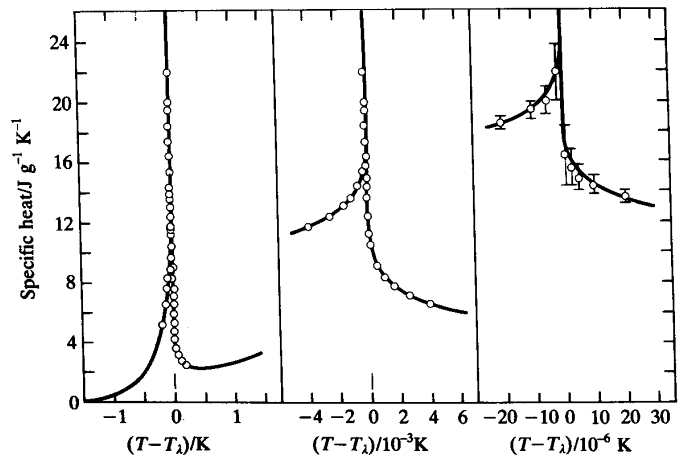


Fig. 15.3. The specific heat of liquid ^{4}He under the saturated vapour pressure as a function of $T - T_\lambda$. The width of the small vertical line just above the origin indicates the portion of the diagram shown expanded (in width) in the curve directly to the right (after Buckingham and Fairbank [193].)

Fountain Effect: The Movie

A 1963 film by Alfred Leitner

Find it on You Tube
(Alfred Leitner Helium II the Superfluid Part 4)

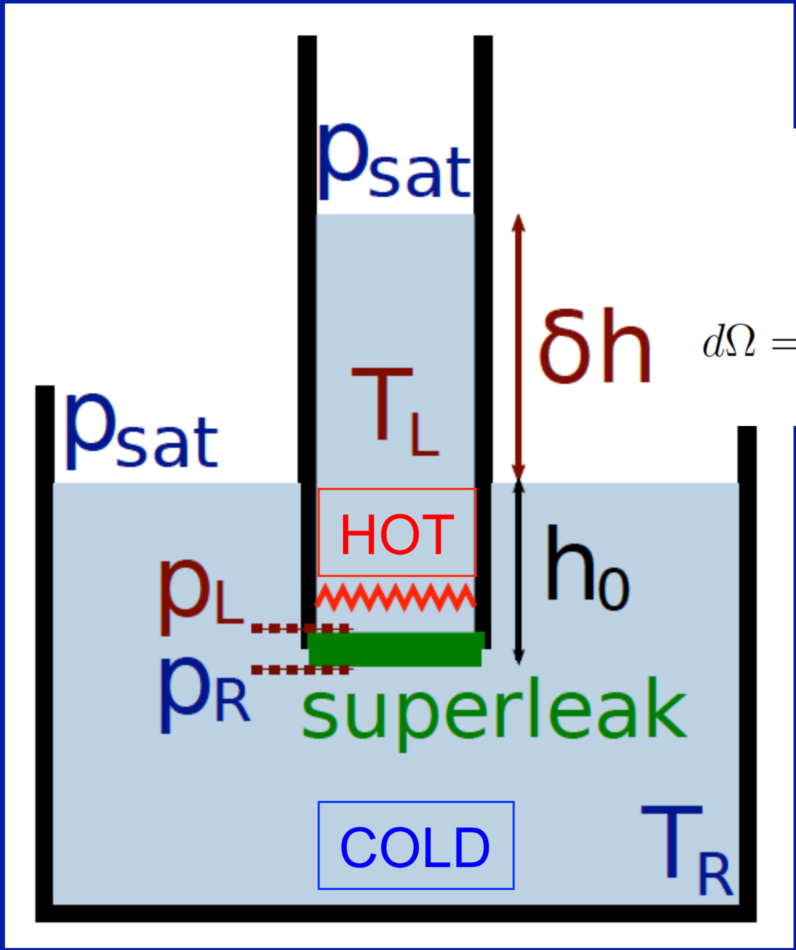
Or rather, in this context: The "U-tube" movie ☺

Also: alfredleitner.com

The fountain effect in Helium

- Key point:
- The superfluid component carries NO ENTROPY (no heat)
- Entropy of each vessel remains separately constant
- In contrast, fast equilibration of chemical potential

Fountain effect: conventional setup



$$\mu(T_L, p_L) \;=\; \mu(T_R, p_R)$$

$$\frac{\partial \mu}{\partial T}|_p \delta T + \frac{\partial \mu}{\partial p}|_T \delta p = 0$$

$$d\Omega = -V dp = -N d\mu - S dT \Rightarrow \frac{\partial \mu}{\partial T}|_p = -\frac{S}{N} \;,\; \frac{\partial \mu}{\partial p}|_T = \frac{V}{N}$$

$$\boxed{\delta p \;=\; \frac{S}{V}\,\delta T\,(=\rho g\,\delta h)}$$

Pressure increases on the hot side

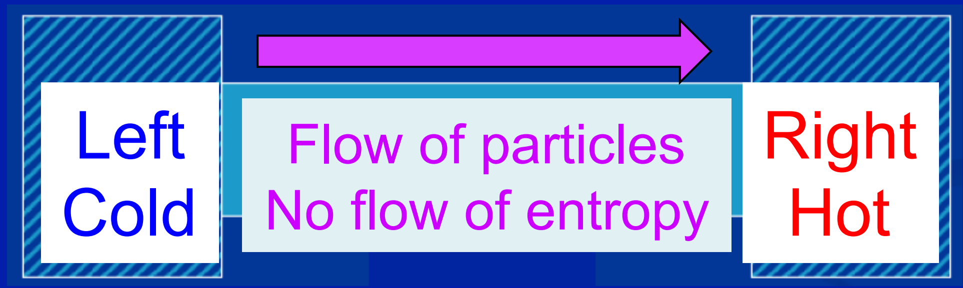
Thermo-mechanical effect

Fig: courtesy David Papoular
(as several others below)

$$\frac{\partial \mu}{\partial T}|_p = -\frac{S}{V} \leq 0 \Rightarrow$$

Flow during equilibration is from cold to hot

Reverse effect: Mechano-caloric (cf. Peltier vs. Seebeck)



$$\Delta S_A = s_A \Delta N_A + N_A \Delta s_a = 0 \Rightarrow \Delta s_A = -\frac{s_A}{N_A}\Delta N_A \geq 0$$

→ Local heating of left (cold) reservoir
(cooling of right hot reservoir)

If thermostats keep the temperature of each reservoir constant.
The left (cold) reservoir releases heat to the thermostat
The right (hot) reservoir takes heat from the thermostat

Predicted by Tisza (1938), Observed by Daunt and Mendelssohn (1939)
cf. Fritz London's book "Superfluids"

A novel setup for the fountain effect: ultra-cold gases

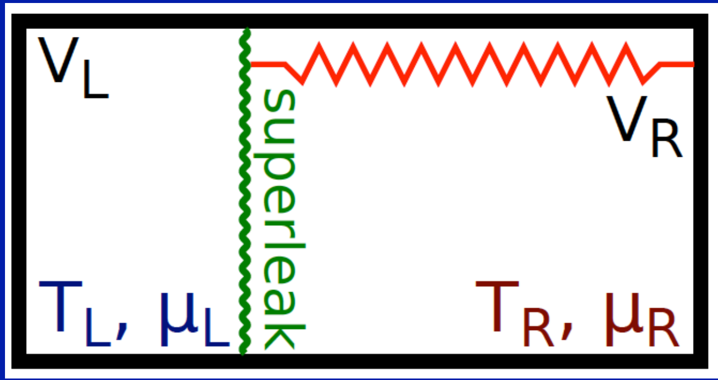
- Marques et al. PRA 69, 053808 (2004)
- Karpiuk et al. PRA 86, 033619 (2012)
- Papoular, Ferrari, Pitaevskii and Stringari PRL 109, 084501 (2012)

  → Thermodynamic considerations

  → The following slides borrow from that work

Fountain effect at constant volume of the containers:

(e.g. cold atomic gas in a box-shaped trapping potential – not harmonic)



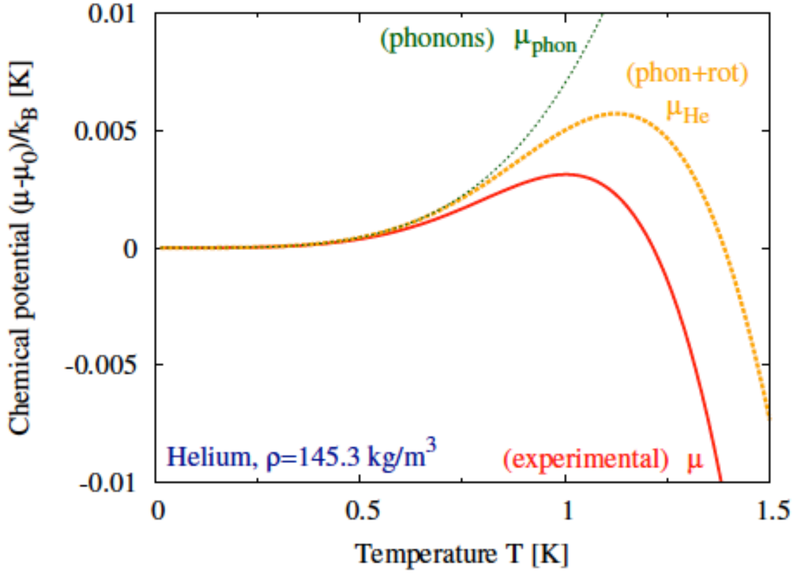
$$\boxed{\mu(T_R, n_R) \;=\; \mu(T_L, n_L)}$$

$$\delta n \;=\; \frac{\partial n}{\partial T}\Big|_\mu \delta T \;=\; -n^2 \kappa_T \frac{\partial \mu}{\partial T}\Big|_n \delta T$$

Two cases depending on whether μ(T) at constant n is:

- Decreasing: net flow from cold to hot (positive flow, as above)
- Increasing: net flow from hot to cold (negative flow) !
- In this case cold reservoir becomes colder → cooling method ?

Thermomechanical effect at constant V: Helium 4 (I)



$$\left.\frac{\partial n}{\partial T}\right|_\mu = -n^2\kappa_T \left.\frac{\partial \mu}{\partial T}\right|_n$$

- $\partial\mu/\partial T|_\mu$ changes sign for $T \approx 1\,\mathrm{K}$ because of roton contribution.

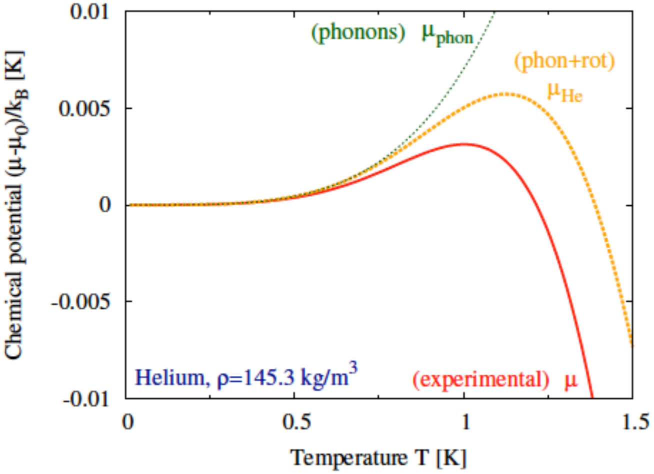
$$\boxed{\mu_{\mathrm{rot}}(n,T) = f(k_B T)^{1/2} \left.\frac{\partial\Delta}{\partial n}\right|_T e^{-\Delta/k_B T}}$$

1. Higher–T regime ($T \gtrsim 1\,\mathrm{K}$): **Positive flow**

For $\rho = 145.3\,\mathrm{kg\,m^{-3}}$ and $T = 1.8\,\mathrm{K}$, $\displaystyle \frac{T}{\rho}\left.\frac{\partial\rho}{\partial T}\right|_\mu$ is of the order of $+10^{-2}$.

Slide: courtesy D.Papoular

Thermomechanical effect at constant V: Helium 4 (II)



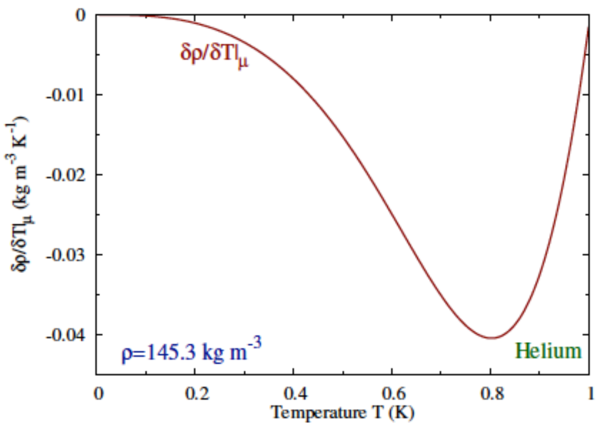
$$\left.\frac{\partial n}{\partial T}\right|_{\mu} = -n^2 \kappa_T \left.\frac{\partial \mu}{\partial T}\right|_{n}$$

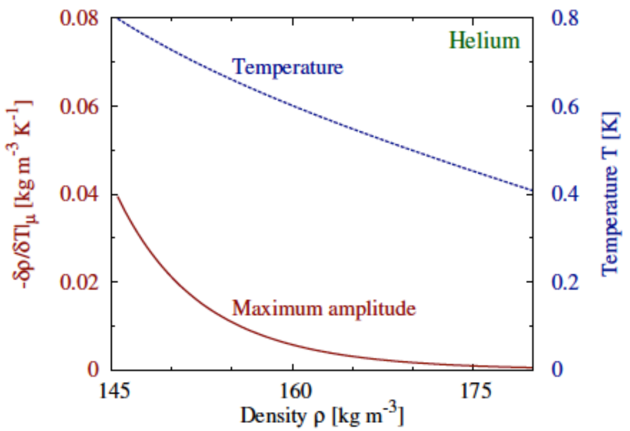
- $\partial\mu/\partial T|_{\mu}$ changes sign for $T \approx 1\,\mathrm{K}$ because of roton contribution.

$$\mu_{\text{phon}}(n,T) = \frac{\pi^2}{30}\frac{(k_B T)^4}{\hbar^3 c_0^4}\left.\frac{\partial c_0}{\partial n}\right|_{T},$$

2. Phonon regime ($T \lesssim 1\,\mathrm{K}$): Negative flow

- Maximum negative flow for $\rho \approx 145.3\,\mathrm{kg\,m^{-3}}$, $T = 0.8\,\mathrm{K}$
- $(T/\rho)\,\partial\rho/\partial T|_{\mu}^{\max} \approx -2\cdot 10^{-4}$ experimentally observable!





Slide: courtesy D.Papoular

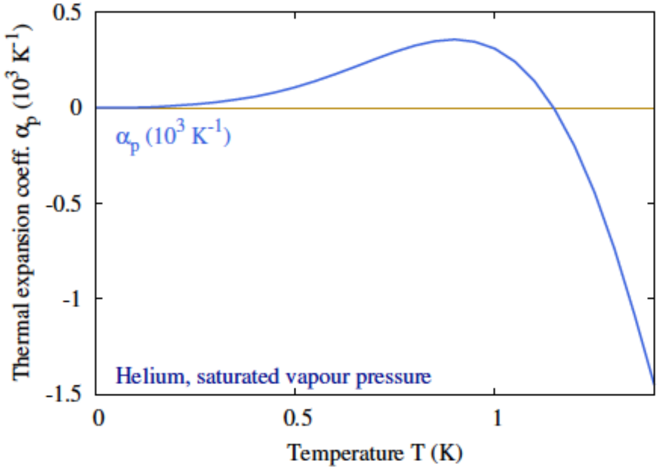
Helium 4: Orders of magnitude

1. Amplitudes for positive and negative flow differ by 2 orders of magnitude

$T = 0.8\,\mathrm{K}$: $\quad \frac{T}{\rho}\frac{\partial \rho}{\partial T}\Big|_{\mu} \approx -2 \cdot 10^{-4}$ $\qquad$ $T = 1.8\,\mathrm{K}$: $\quad \frac{T}{\rho}\frac{\partial \rho}{\partial T}\Big|_{\mu} \approx +10^{-2}$

$$\frac{T}{\rho}\frac{\partial \rho}{\partial T}\Big|_{\mu} = T\,(\kappa_T\, s - \alpha_p)$$

- $T = 1.8\,\mathrm{K}$: $\quad \alpha_p < 0 \longrightarrow$ build–up
- $T = 0.8\,\mathrm{K}$: $\quad \alpha_p > 0 \longrightarrow$ cancellation



---

2. Amplitude of constant–V effect determined by compressibility κ_T

$$\frac{\partial n}{\partial T}\Big|_{\mu} = -\,n^2\,\kappa_T\,\frac{\partial \mu}{\partial T}\Big|_{n}$$

- Gases much more compressible than liquids
- Look for this effect in ultracold bosonic gases !

Slide: courtesy D.Papoular

Thermomechanical effect at constant V: Bose gases

- Model for the homogeneous interacting Bose gas: $\left(\Lambda_T^2 = \frac{2\pi\hbar^2}{mk_B T}\right)$

Ideal–gas entropy:

$$\frac{S}{k_B} = \frac{5}{2}\zeta(3/2)\,\frac{V}{\Lambda_T^3}$$

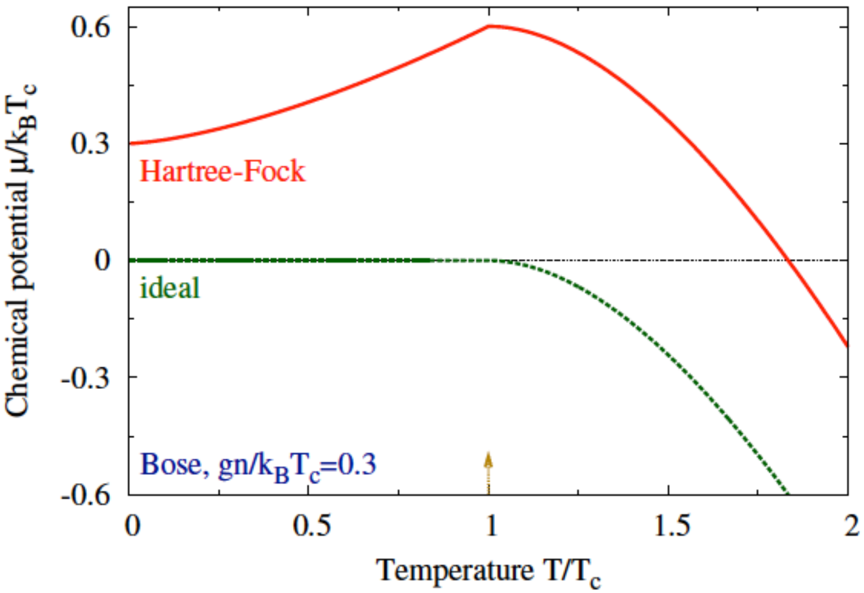
Hartree–Fock chemical potential:

$$\mu = g(n_0 + 2n_T) = g\left[n + \frac{\zeta(3/2)}{\Lambda_T^3}\right]$$

$$\left.\frac{\partial n}{\partial T}\right|_\mu = -n^2\kappa_T \left.\frac{\partial \mu}{\partial T}\right|_n$$

- $\left.\frac{T}{n}\frac{\partial n}{\partial T}\right|_\mu = -\frac{3}{2}\left(\frac{T}{T_c}\right)^{3/2}$

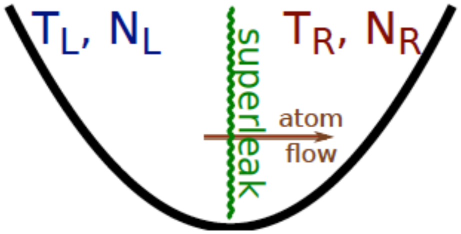
1. Negative flow for all $T < T_c$
2. Amplitude ≈ 1 for $T \lesssim T_c$

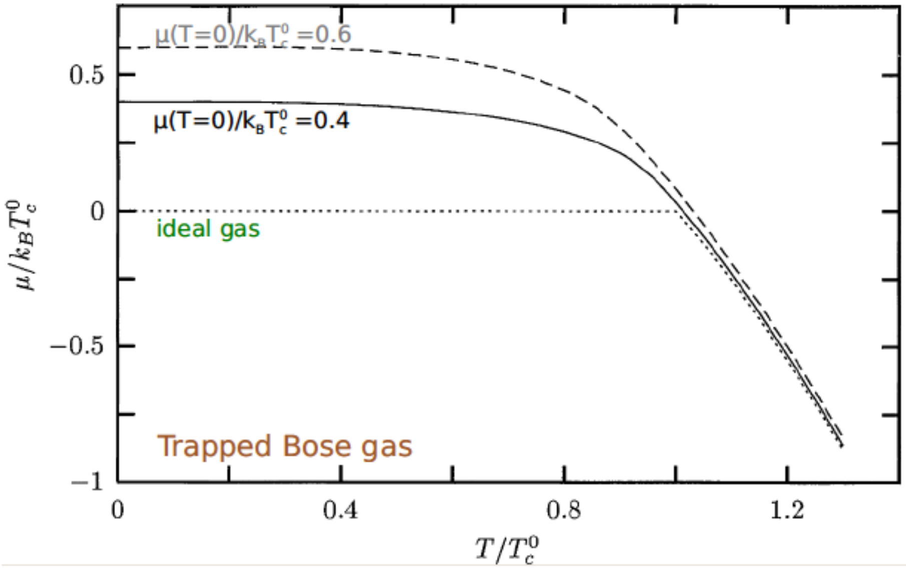


Slide: courtesy D.Papoular

What about the trapping potential?

- Experiments are usually performed with trapped atoms



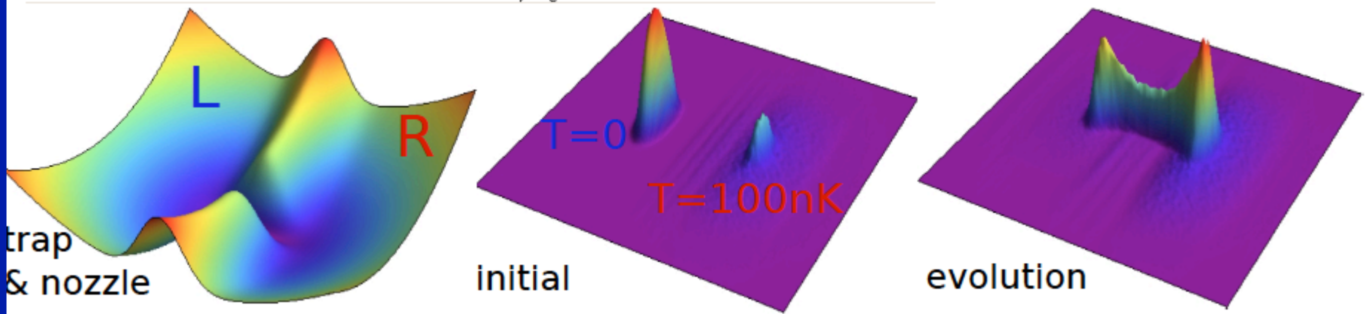


- In a harmonic trap, $\mu(T)\searrow$

$$\left.\frac{\partial n}{\partial T}\right|_{\mu} = -n^2\kappa_T \left.\frac{\partial \mu}{\partial T}\right|_{n}$$

$\longrightarrow$ atoms flow from (L) to (R)

Seen numerically (Karpiuk & al 2010)



Karpiuk & al, PRA 2012

- To observe negative flow, use a box–like potential [Meyrath 2005]

Slide: courtesy D.Papoular

Observation of thermo-`electric' effects in ultra-cold gases

- Theoretical predictions: C.Grenier, C.Kollath and A.G. arXiv:1209.3942
- Recent experimental observation in cold fermionic gases: Brantut et al. Science 342, 713 (2013) http://www.ethlife.ethz.ch/archive_articles/131024_thermoelektrische_materialien_red/index_EN
- See Todays' seminars (Brantut, Grenier) Bosons: Cheng Chin's group, see arXiv:1306.4018 and arXiv:1311.0769.