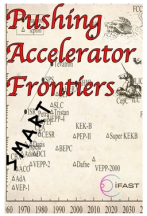
Beam losses induced by trapping of neutral molecules by the beam

G. Franchetti, GSI, JWGU & HFHF

F. Zimmermann, CERN

ECloud22, 26/9/2022



Topics

- Motivation
- Forces and torques on molecules with dipole moments
- Dynamics of molecules and trapping
- Enhancement of residual gas density
- Impact on beam lifetime
- Phenomenology
- Summary

Motivation

Density of vacuum atoms or molecules → Beamlifetime

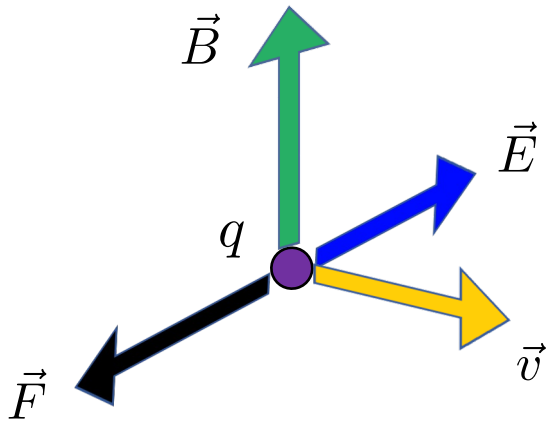
Collision Beam - vacuum molecules

1) Emission of beamstrahlung photons by beam electrons or positrons
2) Stripping of electrons from partially stripped heavy-ion beam
3) Fragmentation of the neutral molecule itself
4) Ionized gas molecules or liberated electrons: electron cloud

Here: a study of the dynamics of neutral molecules under the effect of the beam electromagnetic fields, estimated on the beam lifetime

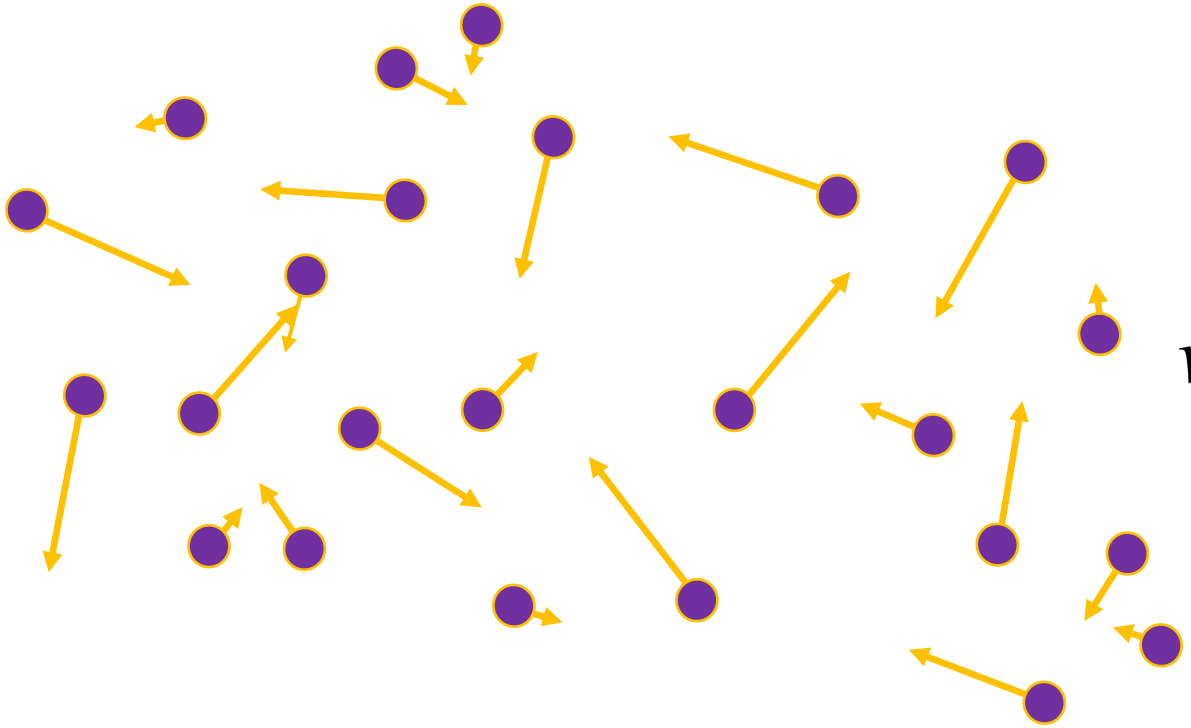
Dynamics of charged particles

$$\frac{d\vec{p}}{dt} = q\vec{E} + q\vec{v} \times \vec{B}$$



The dynamics is determined by the initial condition of the particle, and by the electromagnetic field

Dynamics of neutral molecules



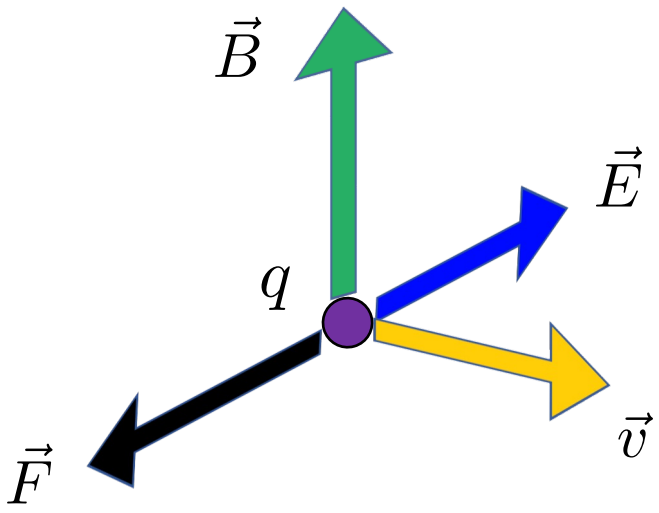
$$v_{rms} = \sqrt{\frac{k_b T}{M}}$$

Thermodynamics → Maxwell-Boltzmann velocity distribution
→ Temperature

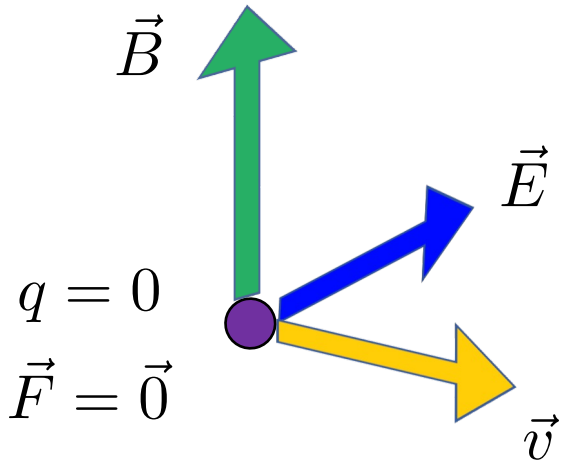
Properties → Collisions, Mean free path,
Impingement rate, Pressure

Charged particles vs neutral at first sight

Charged molecule/particle

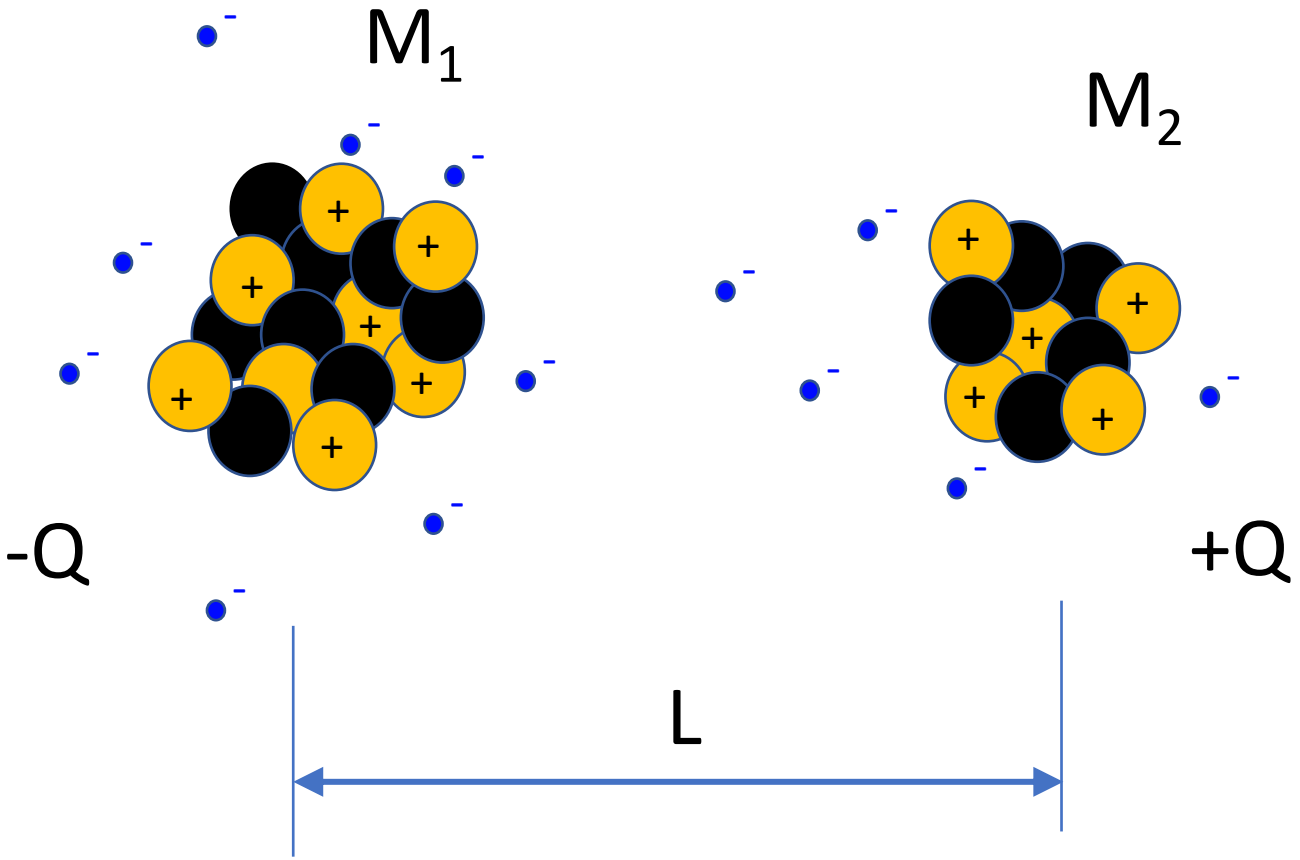


Neutral molecule

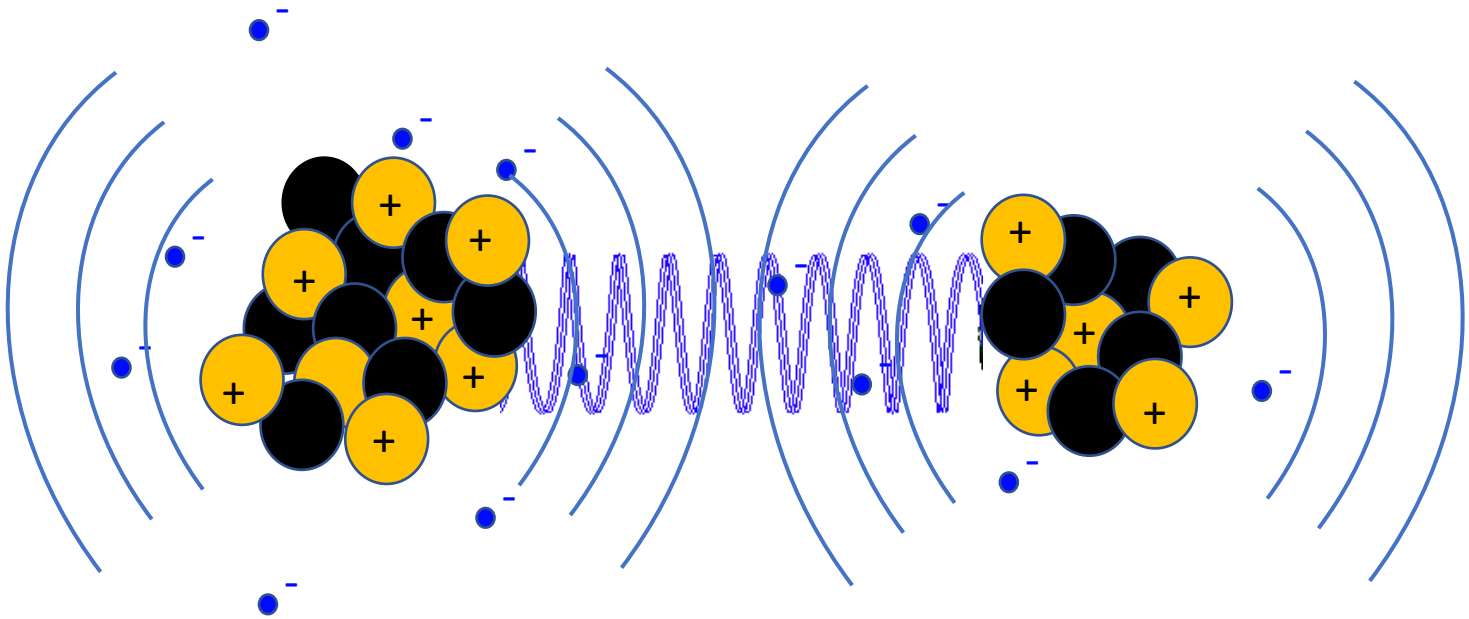


Apparently →
no forces on the molecule

Structure of molecules

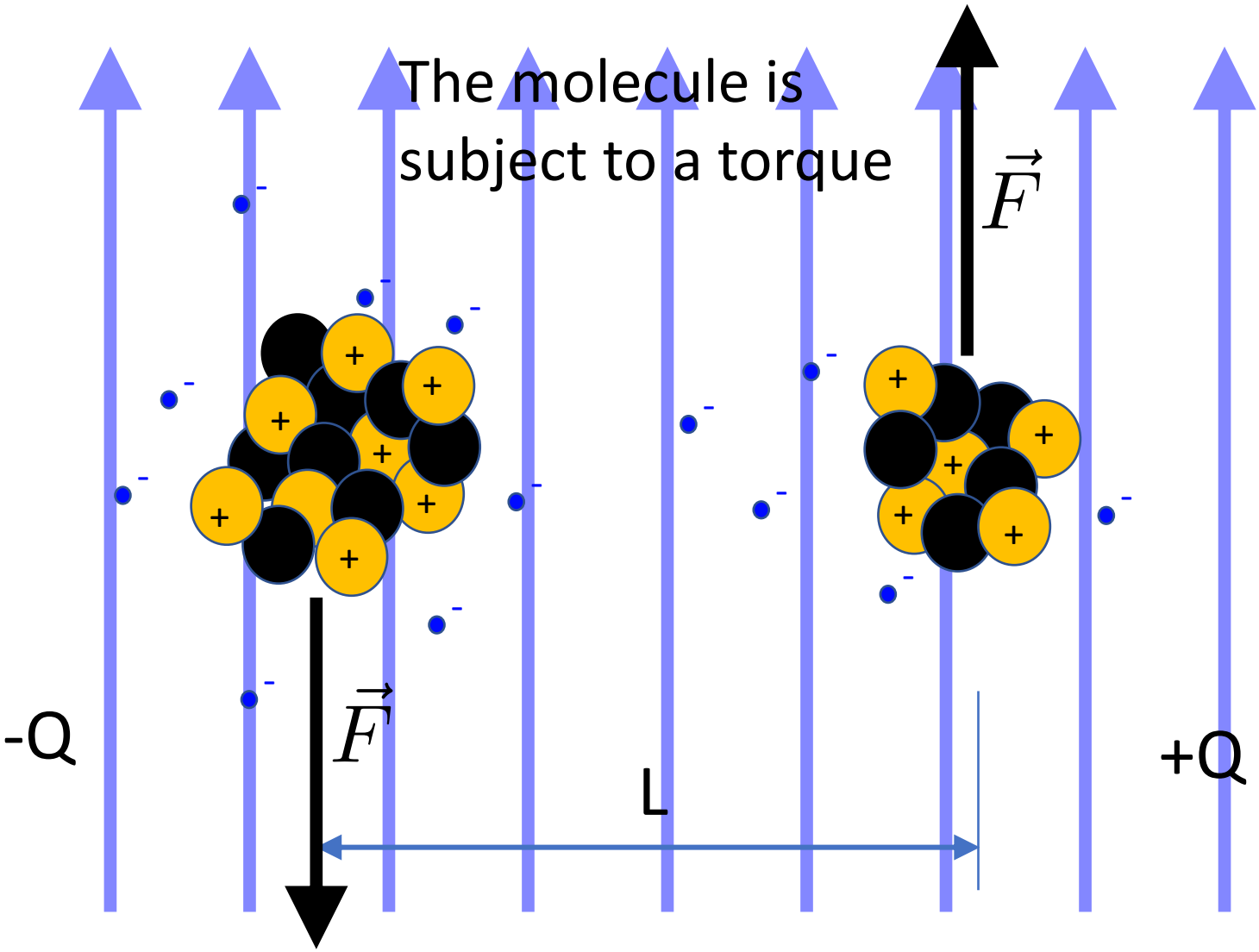


Vibrational state

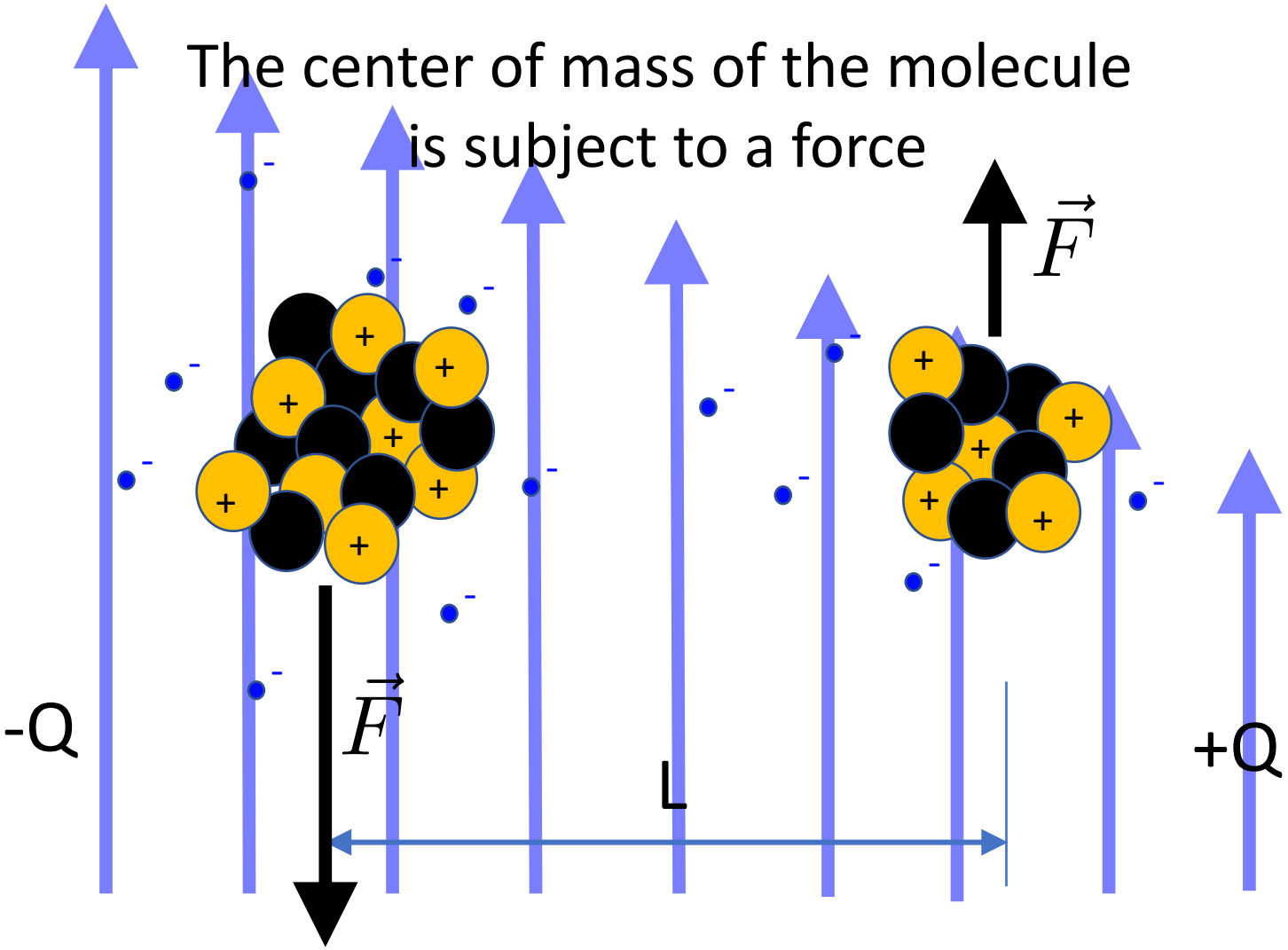


Characteristic molecular vibrational frequency → very large

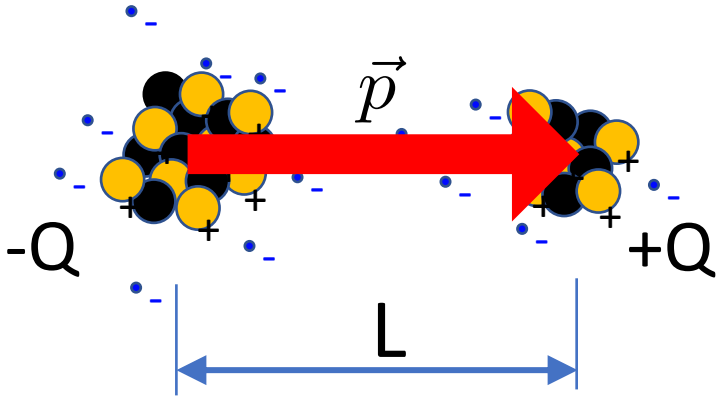
Molecules and electric fields



Molecules and electric fields



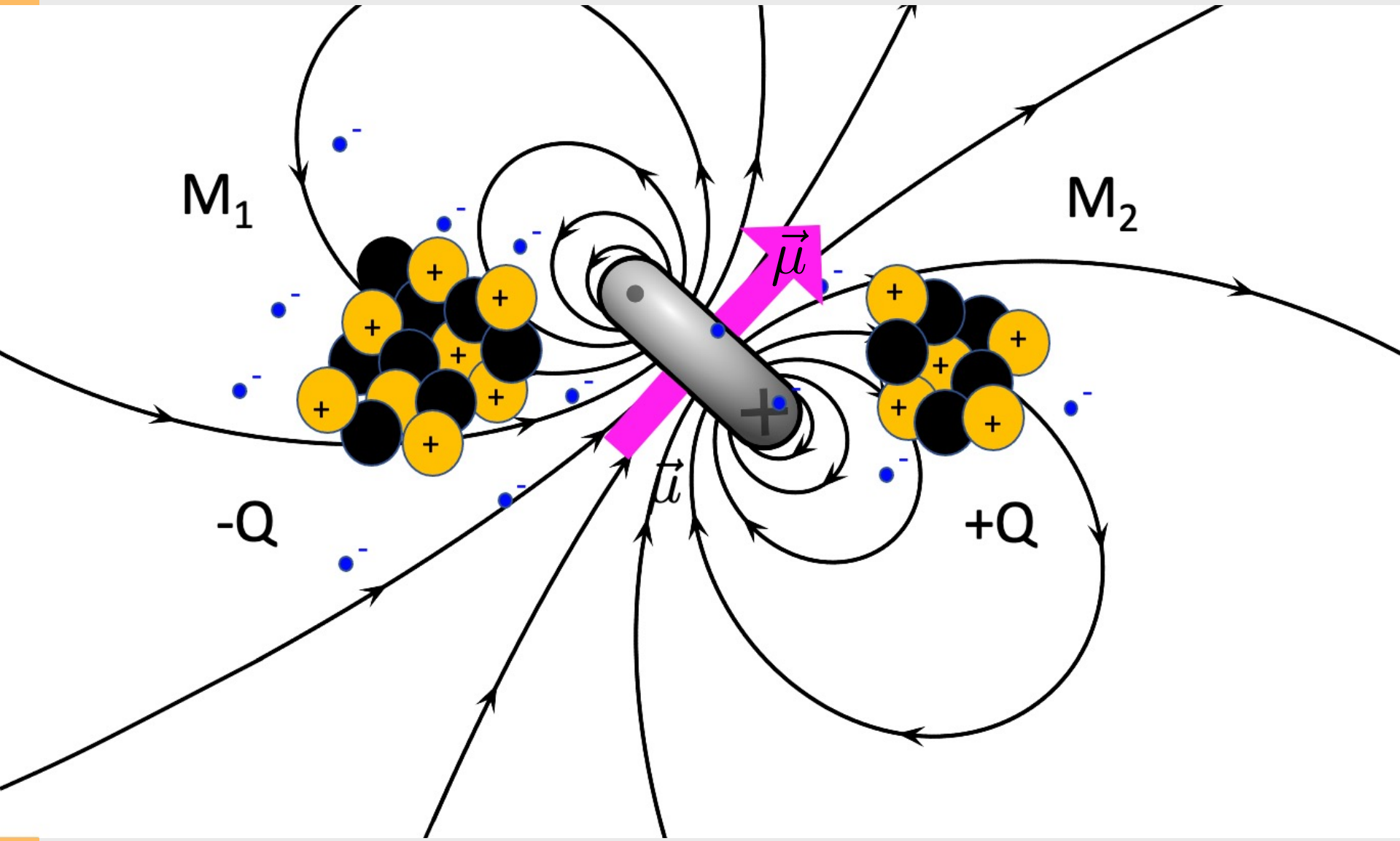
Electric dipole moment



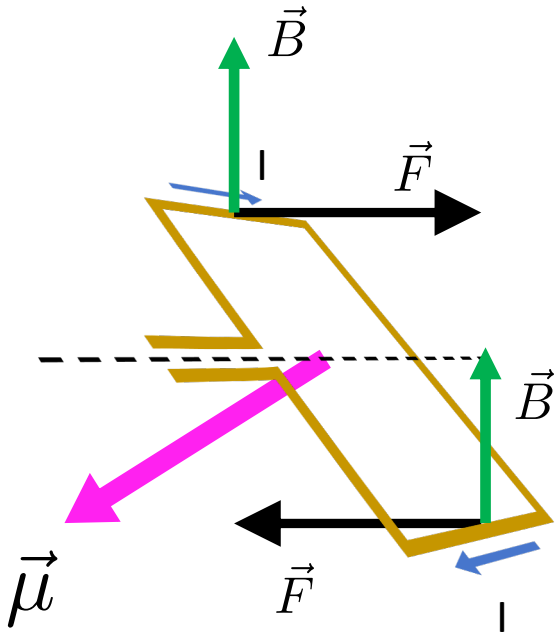
$$\vec{p} = Q\vec{L}$$

$$\begin{cases} \vec{F}_{cm} = (\vec{p}\cdot\nabla)\vec{E} & \leftarrow \text{Force on the center of mass} \\ \vec{\tau} = \vec{p}\times\vec{E} & \leftarrow \text{Torque} \end{cases}$$

Molecules and magnetic fields



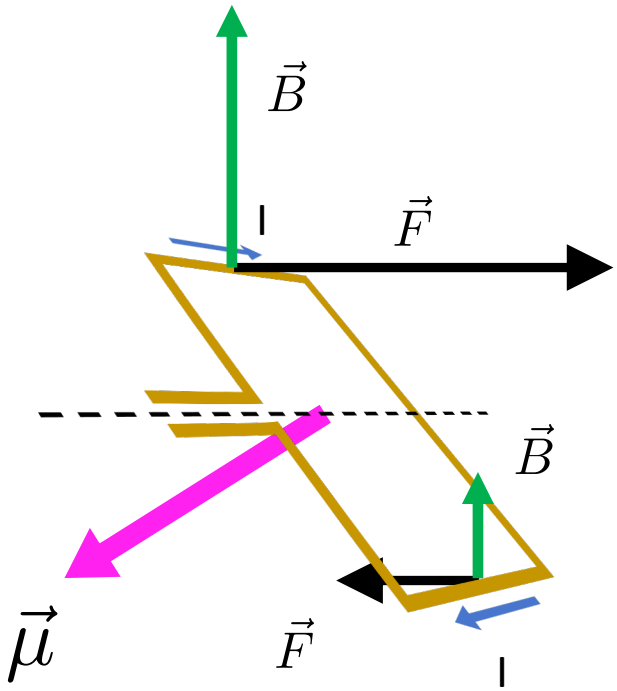
Molecules and magnetic fields



Torque

$$\vec{\tau} = \vec{\mu} \times \vec{B}$$

Molecules and magnetic fields



If the magnetic field is not uniform the force on the center of mass is

$$\vec{F}_{cm} = (\vec{\mu} \cdot \nabla)\vec{B}$$

Dynamics of neutral molecules

$$\begin{cases} \vec{F}_{cm} = (\vec{p}\cdot\nabla)\vec{E} + (\vec{\mu}\cdot\nabla)\vec{B} \\ \vec{\tau} = \vec{p}\times\vec{E} + \vec{\mu}\times\vec{B} \end{cases}$$

In general:

3 coordinates for the position of the center of mass

3 coordinates for the molecule “orientation”

3 velocities for the center of mass

3 “velocities” for the orientation

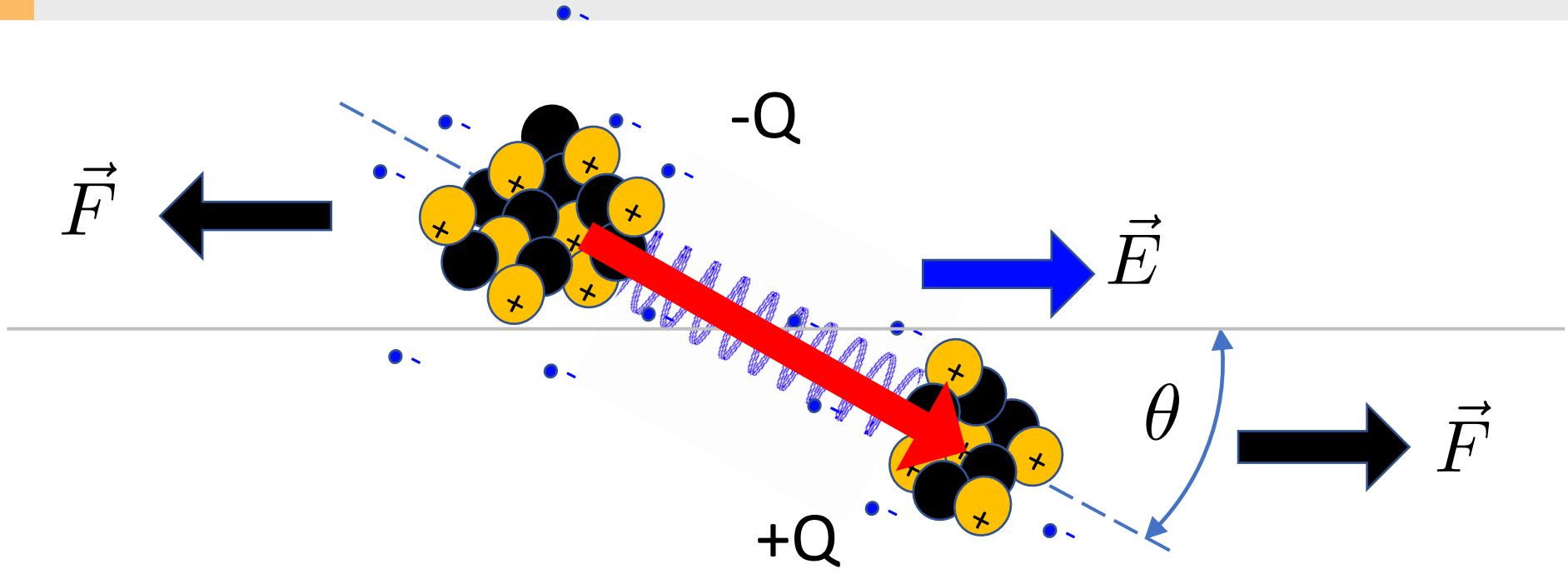
Molecules of interest

Molecule	EDM [D]	MDM [BM]	M [amu]
H_2O	1.87	0	18
O_2	0	2.8	32
CO	0.025	0	28
N_2	0	0	28
CO_2	0	0	44

[D] = Debye, 1 D ≈ 0.21 *e*Å with *e* the electron charge, 1 Å = 0.1 nm

[BM] = Bohr magneton, its value is 9.27×10^{-24} J/T

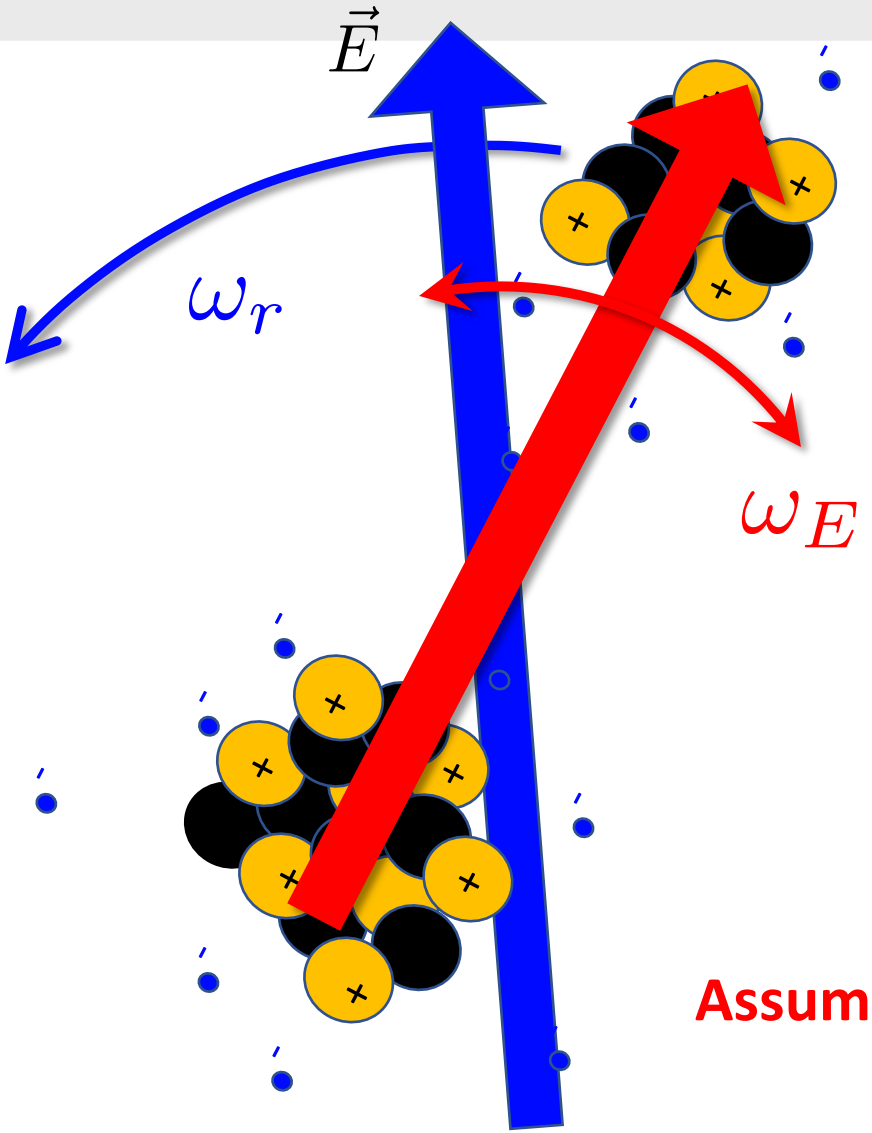
Dipole moment alignment and intrinsic time scale



The dipole tends to align to the field →fast frequency of oscillation

$$\theta'' + \omega_E^2 \theta = 0 \qquad \omega_E = \sqrt{\frac{pE}{I_i}}$$

Closed alignment condition



$$\omega_E = \sqrt{\frac{pE}{I_i}}$$

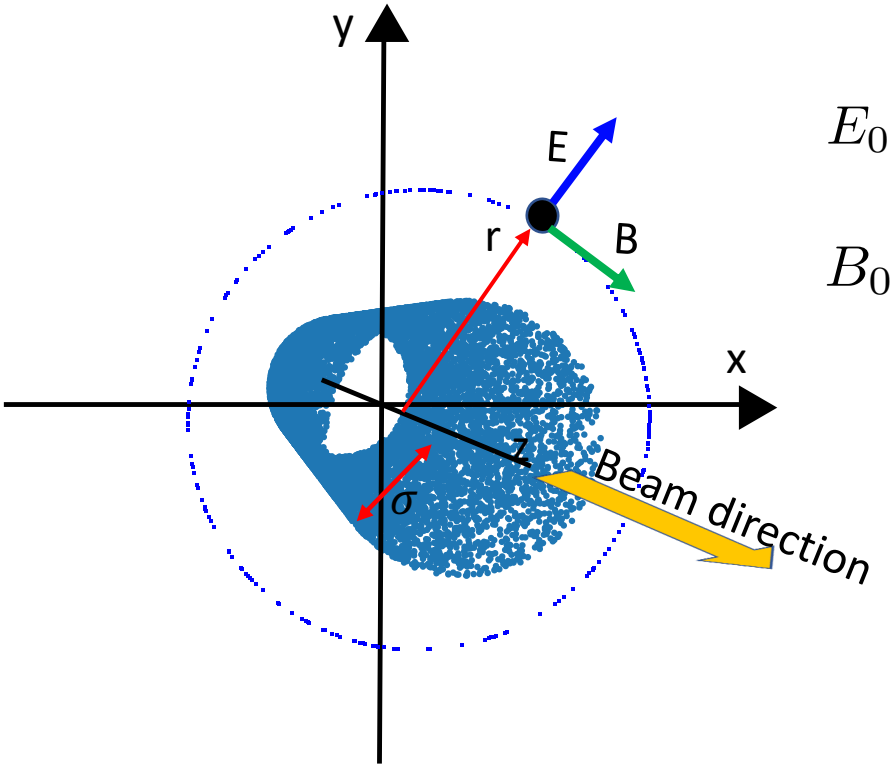
$$\omega_r = \frac{v_{cm}}{r_c}$$

$$\frac{\omega_r}{\omega_E} \ll 1$$

Assumption: the dipole is aligned to the local field

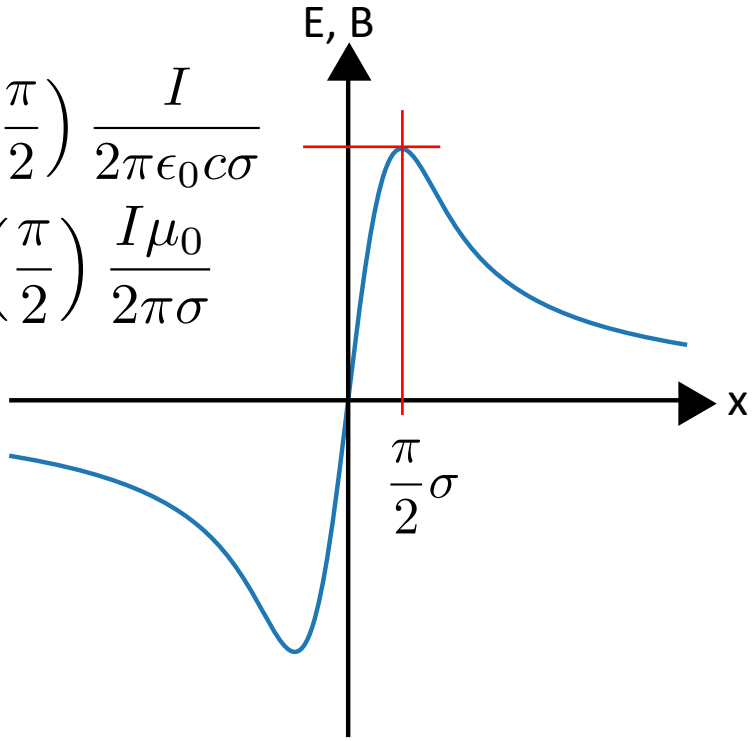
Electromagnetic beam field

Transverse Gaussian beam distribution



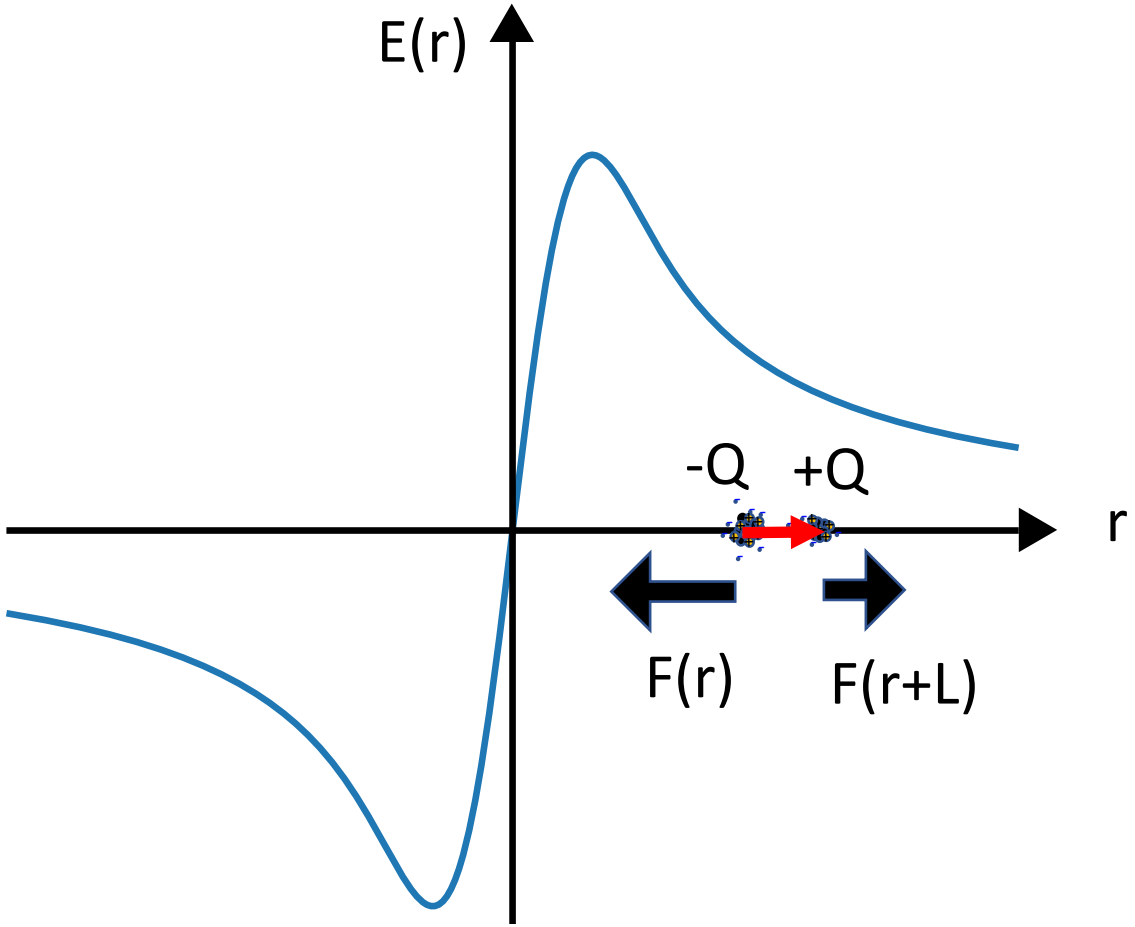
$$E_0 = \ln\left(\frac{\pi}{2}\right)\frac{I}{2\pi\epsilon_0 c\sigma}$$

$$B_0 = \ln\left(\frac{\pi}{2}\right)\frac{I\mu_0}{2\pi\sigma}$$



For LHC
- $E_0 \approx 4 \times 10^6$ V/m
- $B_0 = 137 \times 10^{-4}$ T = 137 Gauss

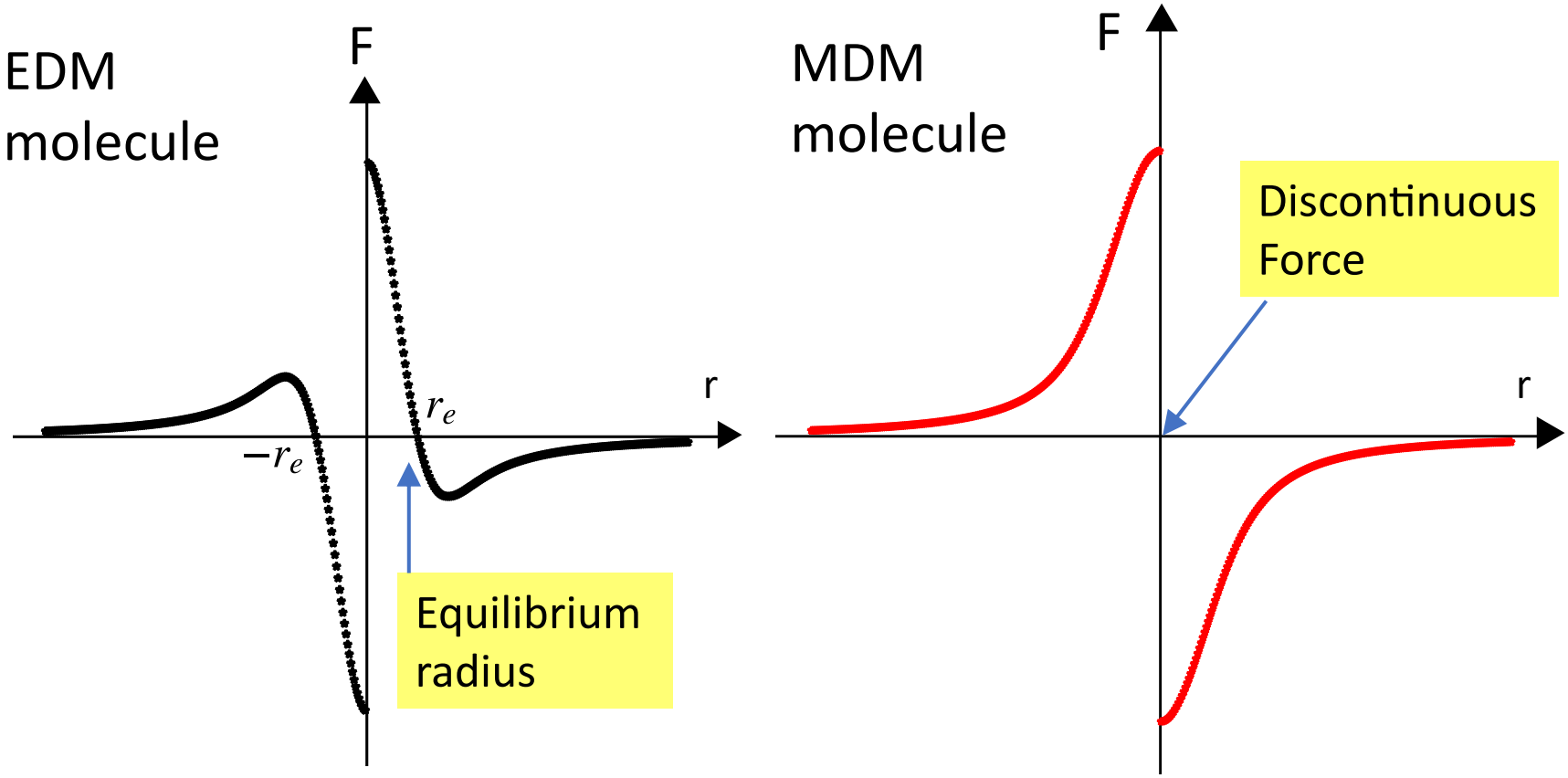
Force on a molecule from $\vec{E}$



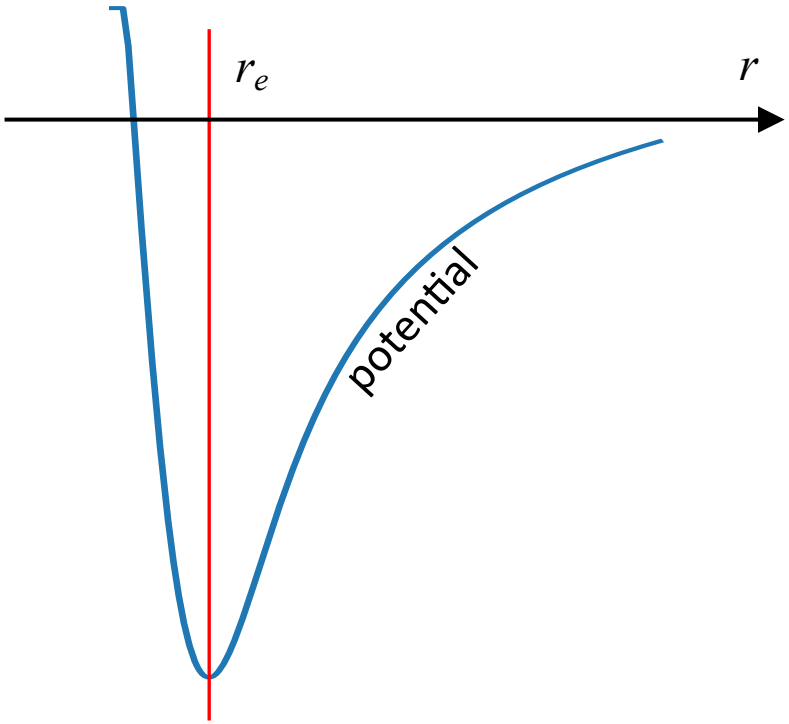
$$F = +QE(r+L) - QE(r) = QLE'(r) = pE'(r)$$

For molecules with dipole moment aligned, the Force on the center of mass is:

$$\vec{F}(\vec{r}) = \left[p\frac{dE(r)}{dr} - \mu\frac{B(r)}{r} \right] \frac{\vec{r}}{r}$$



Trapping of neutral molecules



This force produces a potential Well

Molecules Trapping

If the kinetic energy of molecules is small enough to remain inside the potential Well

Initial kinetic energy ←→ Temperature

Potential Well → Trapping temperature T^*

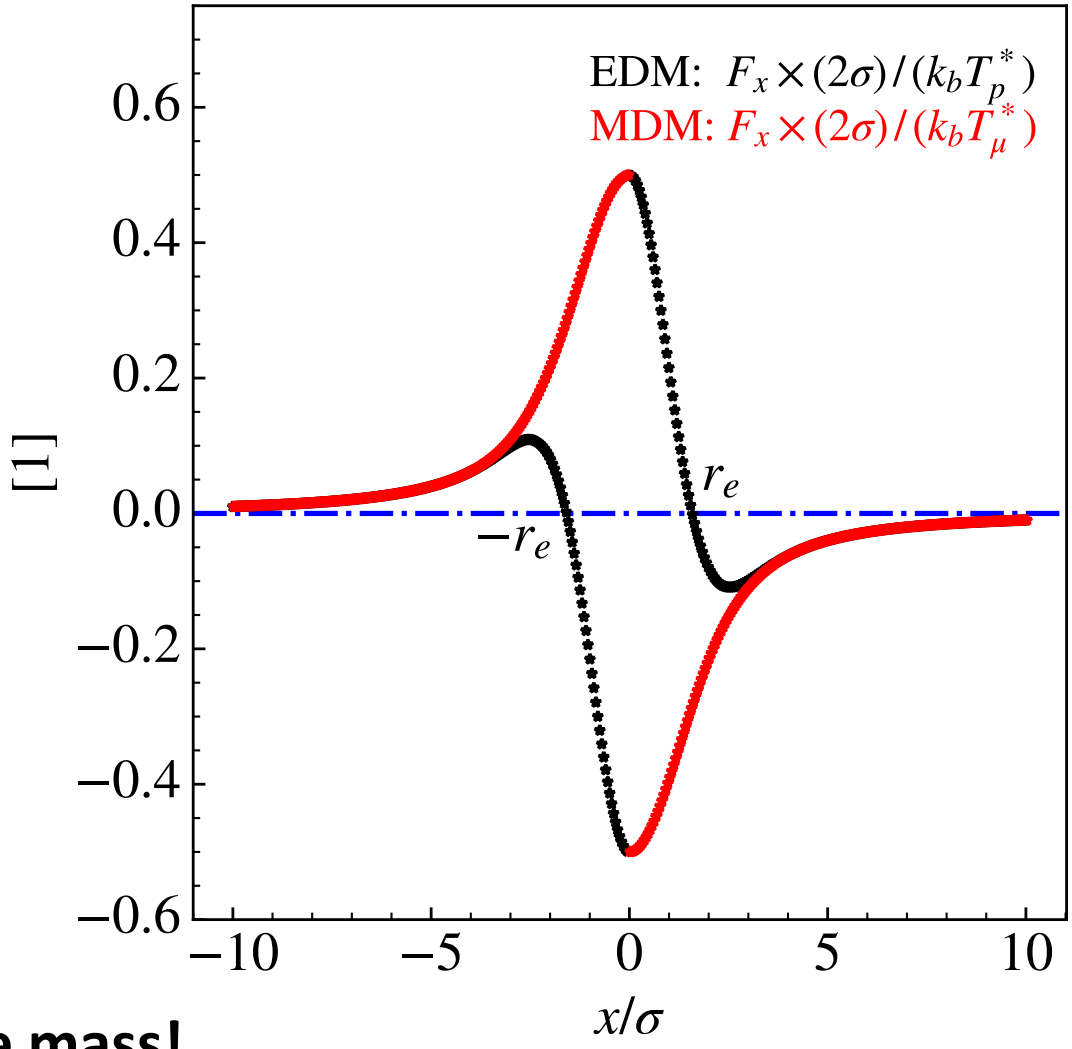
The amount of trapping depends on T/T^*

Trapping temperature and Forces

$$T_p^* = \frac{1}{\pi \epsilon_0 k_b c} \frac{I}{\sigma} p$$

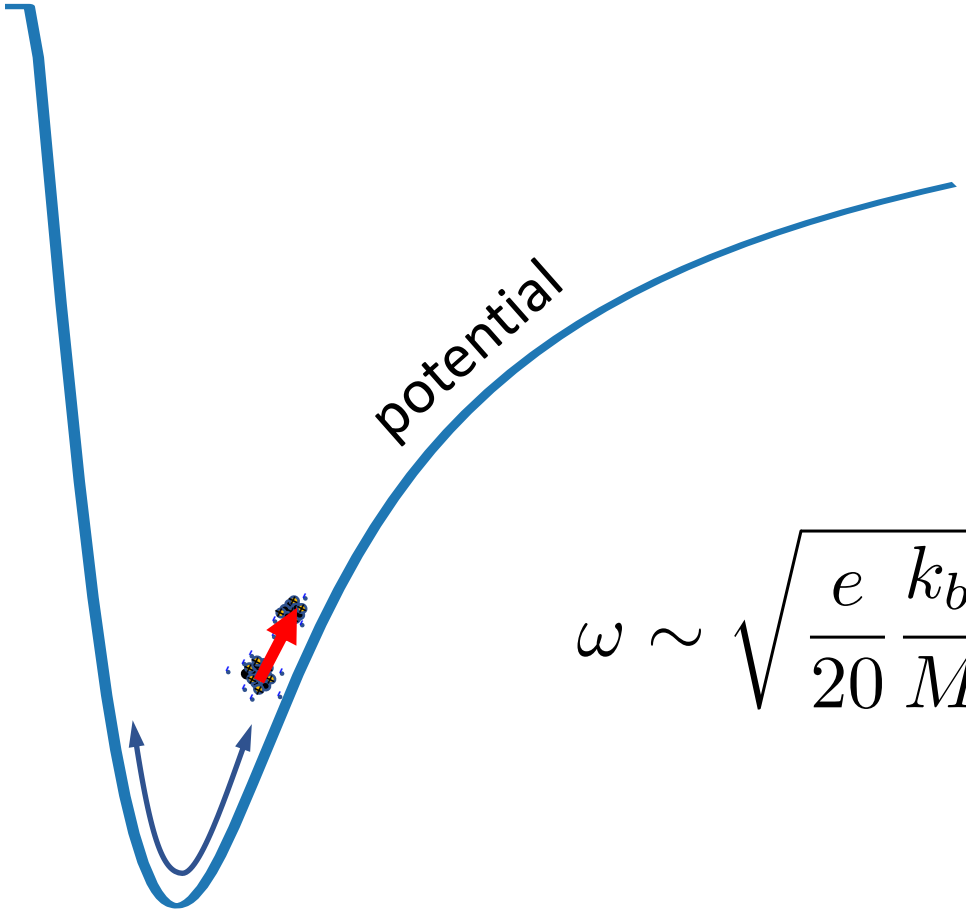
$$T_\mu^* = \frac{1}{\pi \epsilon_0 k_b c} \frac{I}{\sigma} \frac{\mu}{c}$$

The trapping temperature is a combination of the beam properties and the dipole moment of the molecules



Independent on the molecule mass!

Oscillations around the equilibrium radius



$$\omega \sim \sqrt{\frac{e}{20}\frac{k_b T_p^*}{M\sigma^2}}$$

Time scales

Vibrational	Very fast
Oscillation around E-field	$\omega_E = \sqrt{\frac{pE}{I}} \quad \omega_E^2 \simeq \ln\left(\frac{\pi}{2}\right) \frac{k_b}{mL^2} T_p^*$
Oscillation around the equilibrium radius r_e	$\omega \sim \sqrt{\frac{e}{20} \frac{k_b T_p^*}{M\sigma^2}}$

LHC Beam

Coasting beam

$\sigma = 3 \times 10^{-4}$ m

I = 1 A

$E_0 = 9 \times 10^4$ V/m

$B_0 = 3 \times 10^{-4}$ T = 3 Gauss

Bunched beam

$\sigma = 2 \times 10^{-4}$ m

$\sigma_z = 0.076$ m

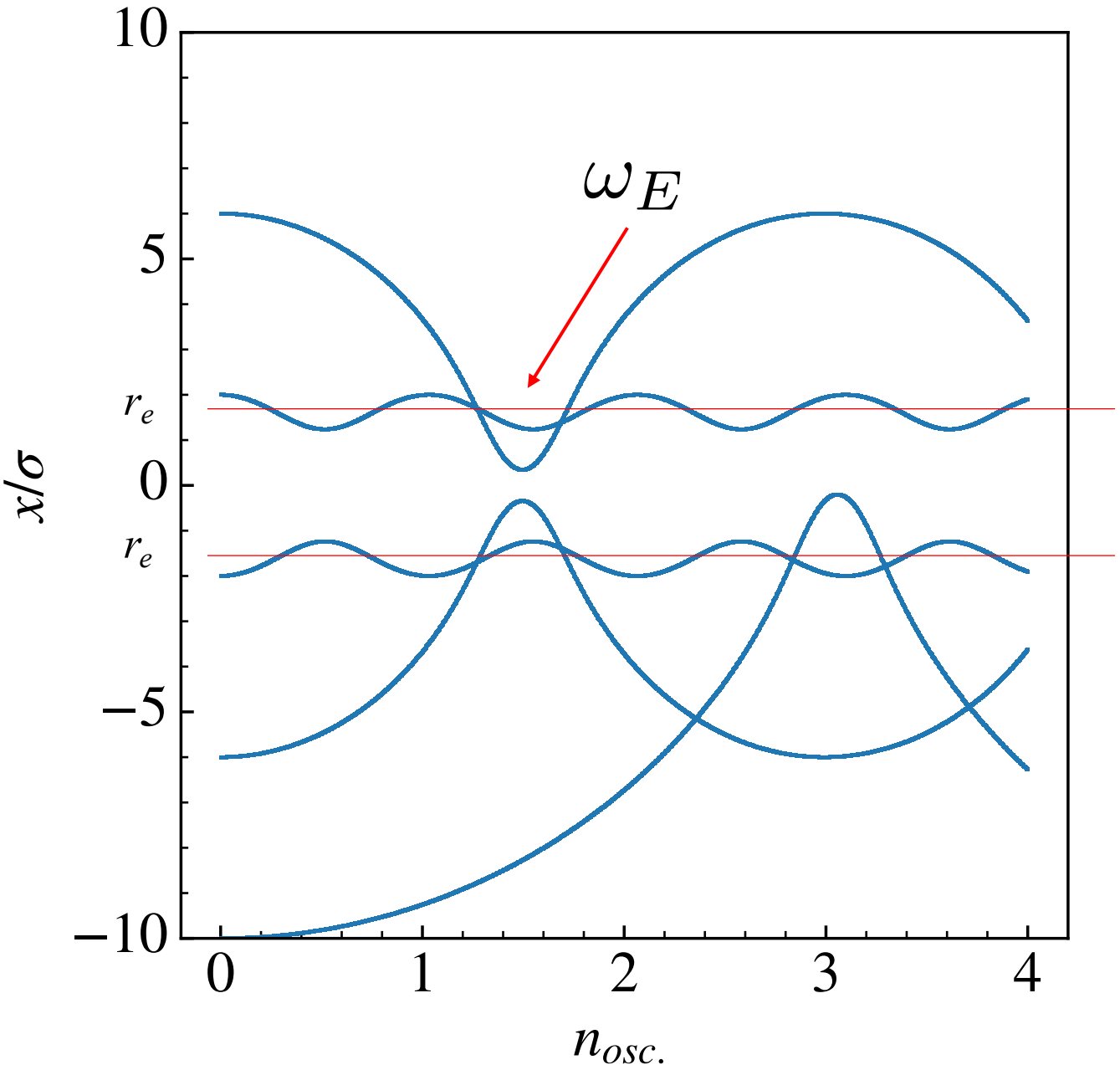
$N_b = 1.2 \times 10^{11}$ protons

$E_0 = 4 \times 10^6$ V/m

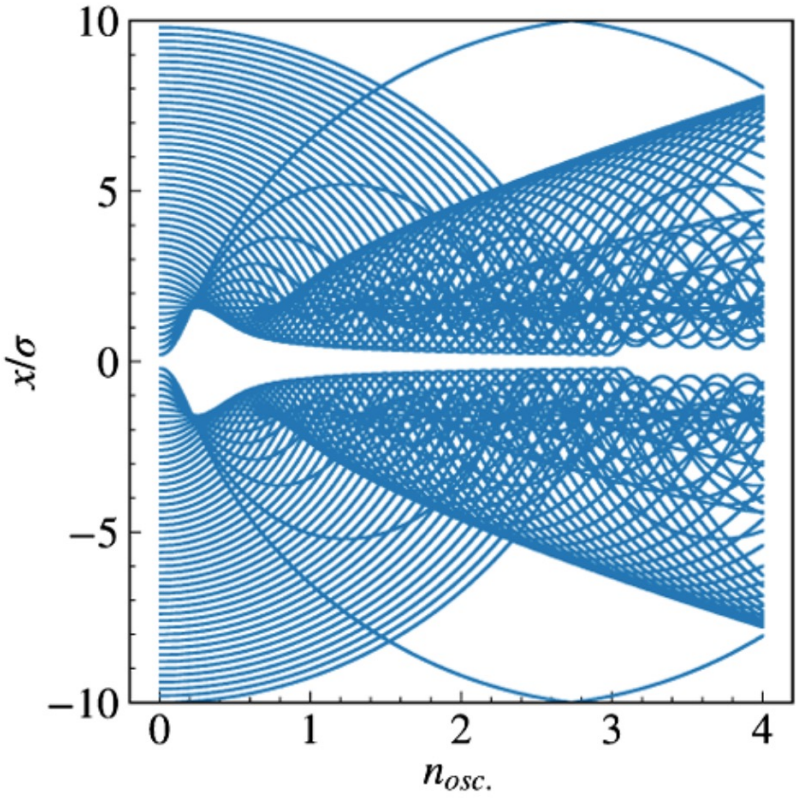
$B_0 = 137 \times 10^{-4}$ T = 137 Gauss

Vaccum temperature T = 2 K

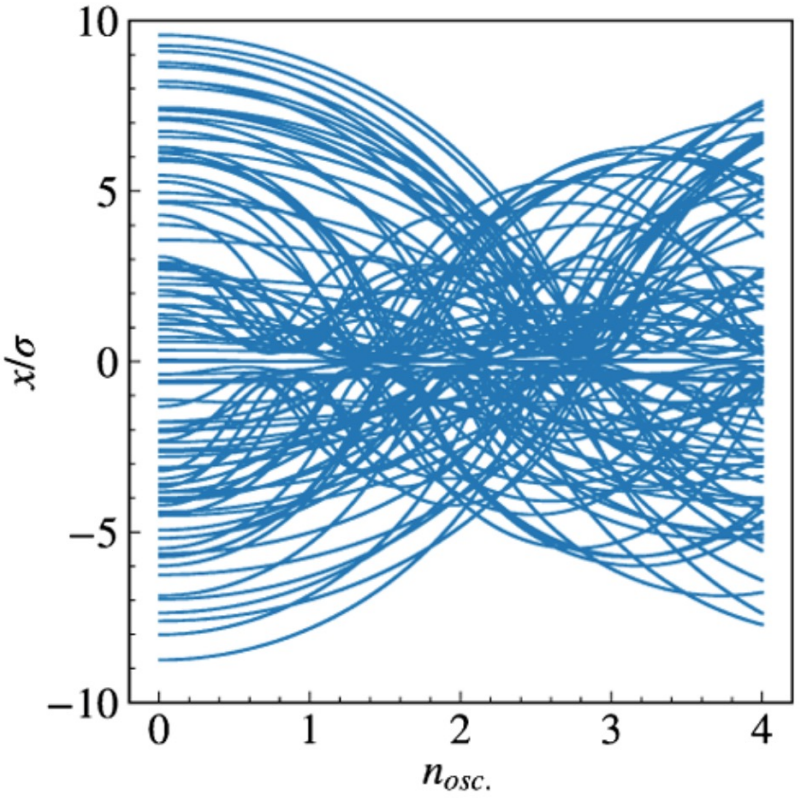
H_2O	O_2
$p = 6.2 \times 10^{-30}$ Cm	$\mu = 2.8$ BM $= 2.6 \times 10^{-23}$ J/K
$M = 3 \times 10^{-26}$ Kg	$M = 5.3 \times 10^{-26}$ Kg
$\omega_E \approx 9.0 \times 10^{11}$ rad/s	$\omega_B = 4.27 \times 10^{10}$ rad/s
$T^*_p = 0.18$ K	$T^*_\mu = 2.5$ mK
$\omega = 11189$ rad/s	
f = 1780 Hz	


10
5
0
−5
−10
x/σ
r_e
r_e
ω_E
0
1
2
3
4
$n_{osc.}$

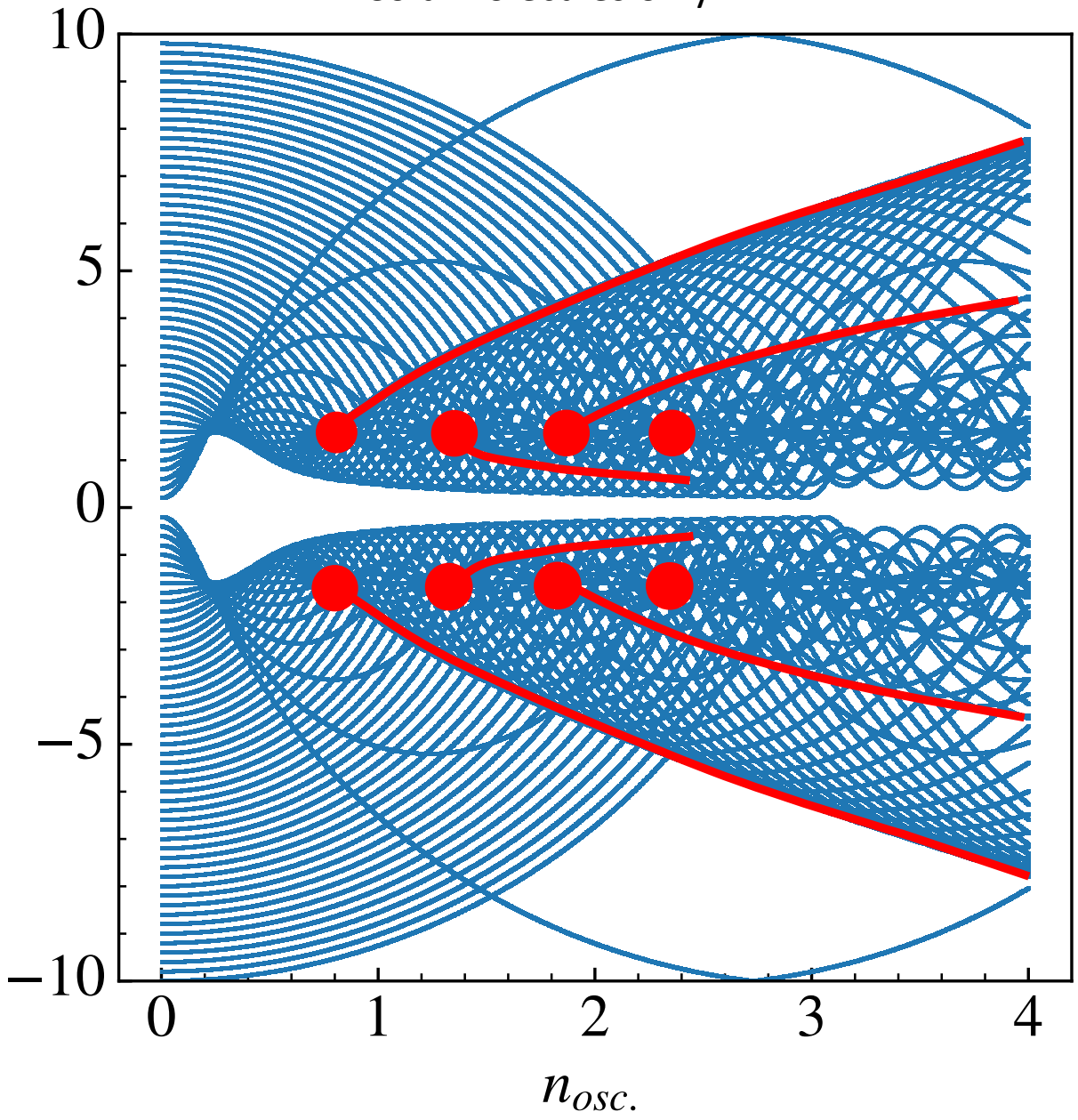
Cold molecules only in x



Cold molecules in xy



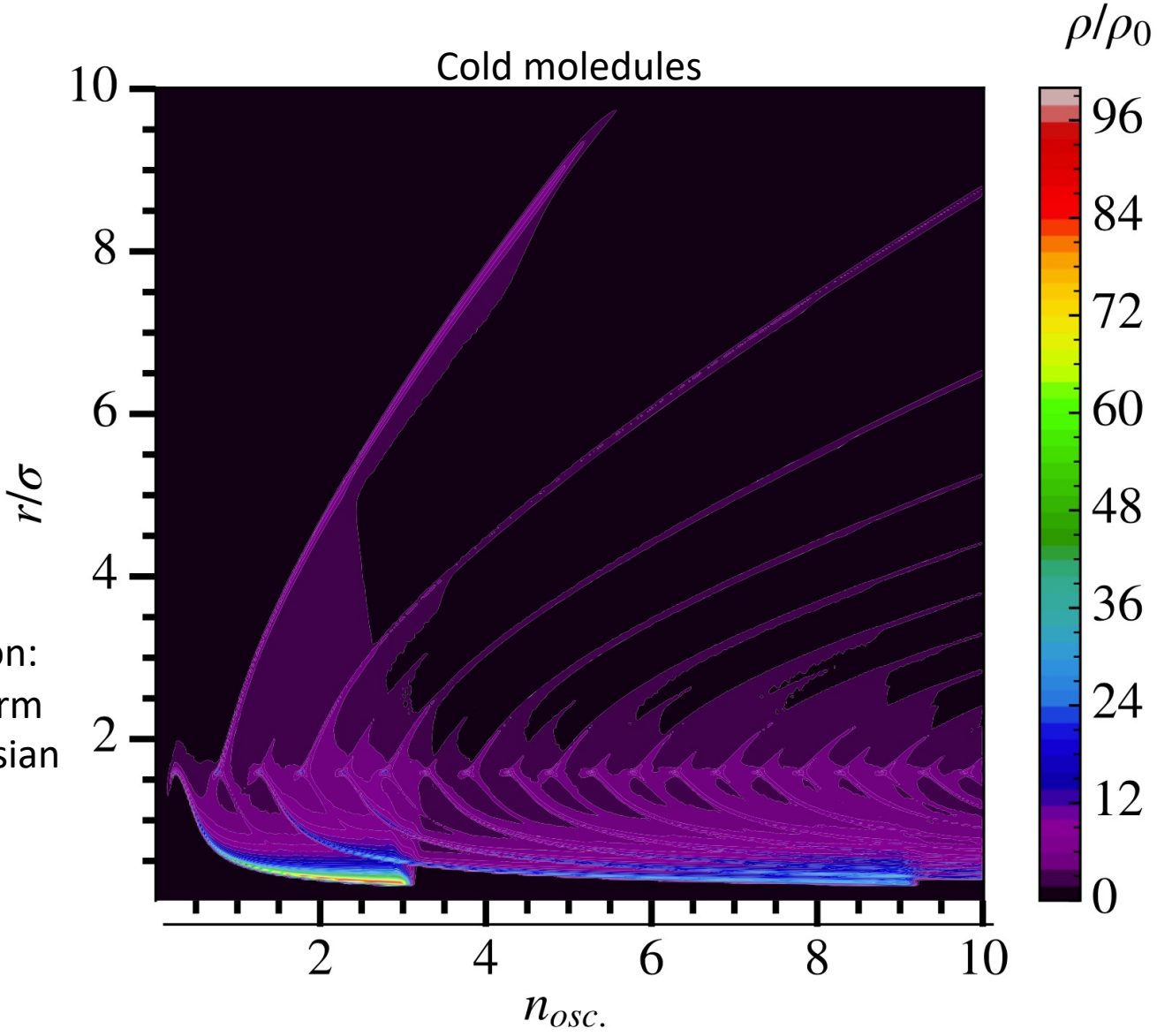
Cold molecules only in x



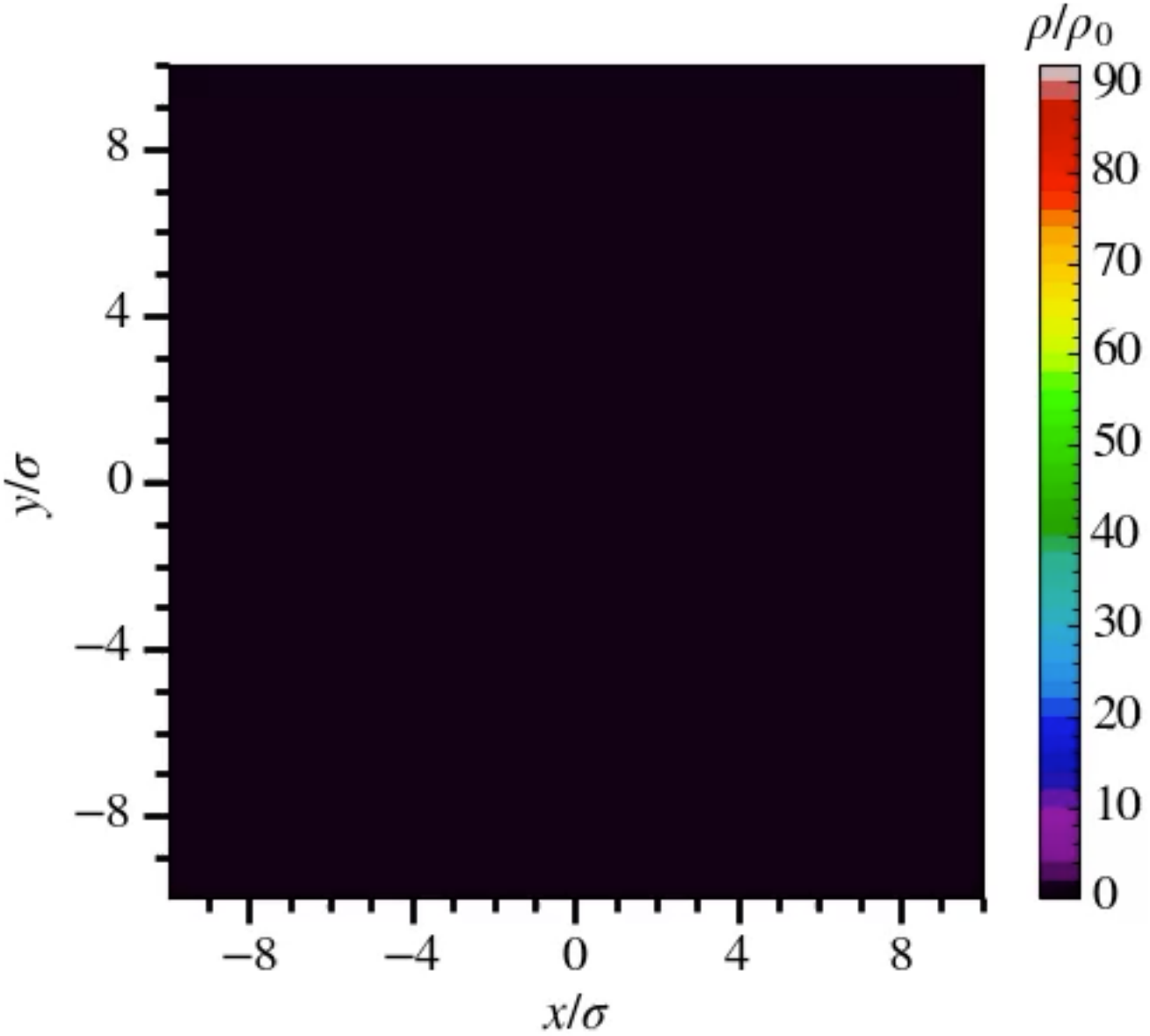
Molecules with $T/T^* = 1E\text{-}5$ (cold)

Radial Vacuum Density Evolution

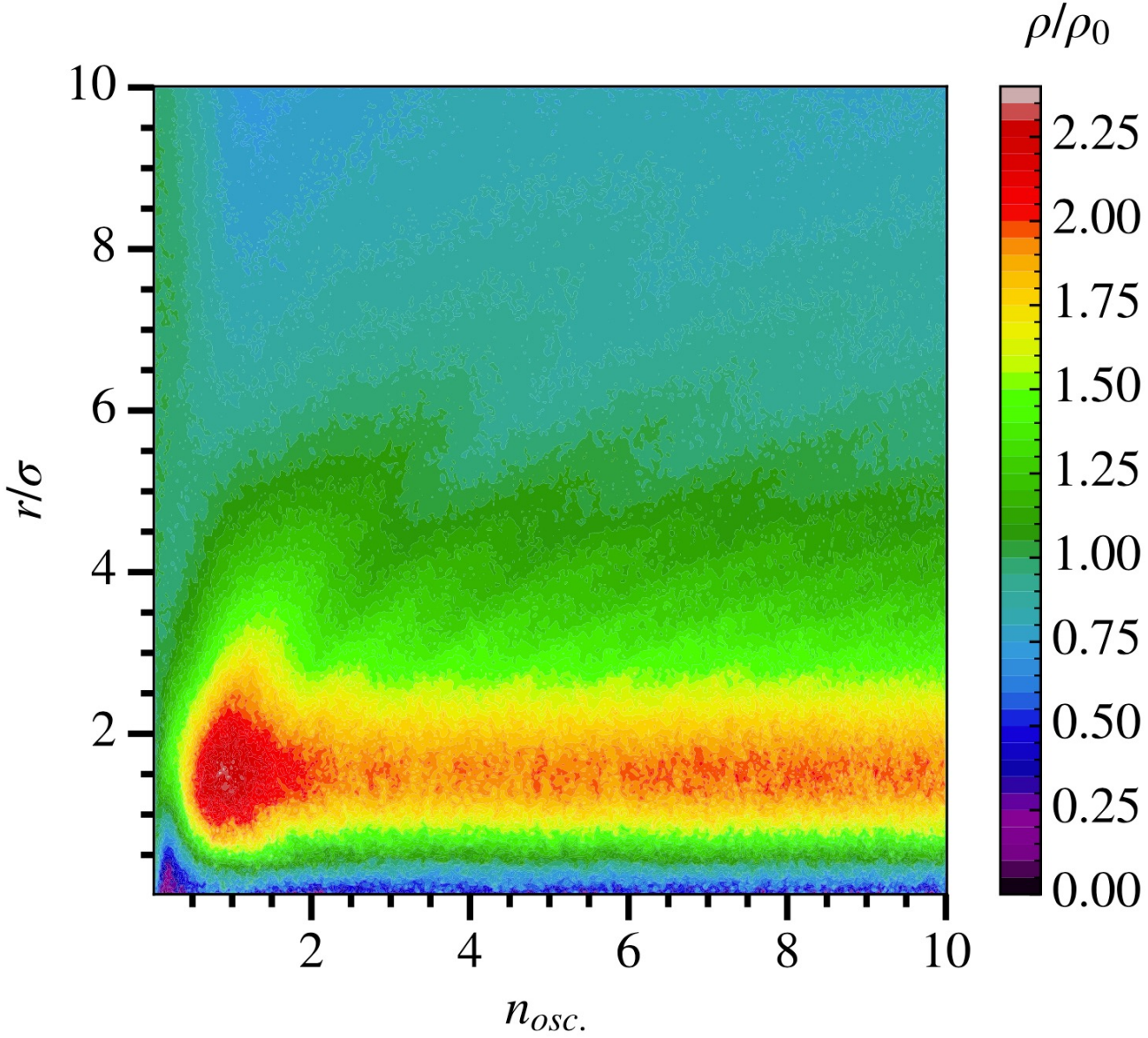
Initial Distribution:
x-y Uniform
v_x-v_y Gaussian



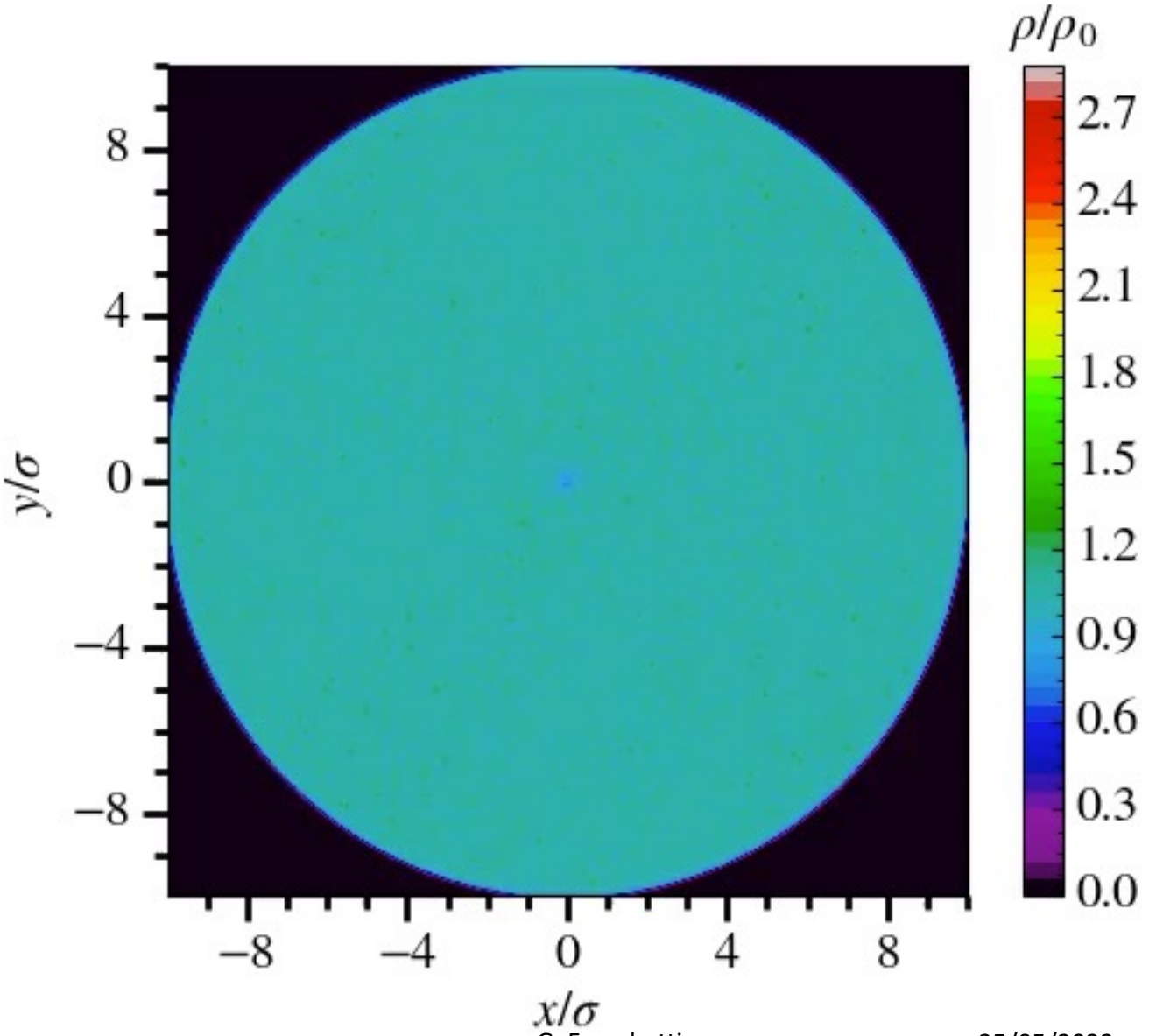
Time evolution $T/T^* = 1E\text{-}5$



Molecules with $T/T^*_p = 0.1$



Time evolution $T/T_p = 0.1$



Model of a bi-atomic molecule

Model of a bi-atomic “classical” molecule:
Two hard spheres bounded by a linear force

$$\frac{d^2\vec{r}_n}{d\tau^2} = \pi^2 \frac{L^2}{\sigma^2} (\vec{p}_n \cdot \nabla_{r_n}) \vec{E}_n(\vec{r}_n)$$

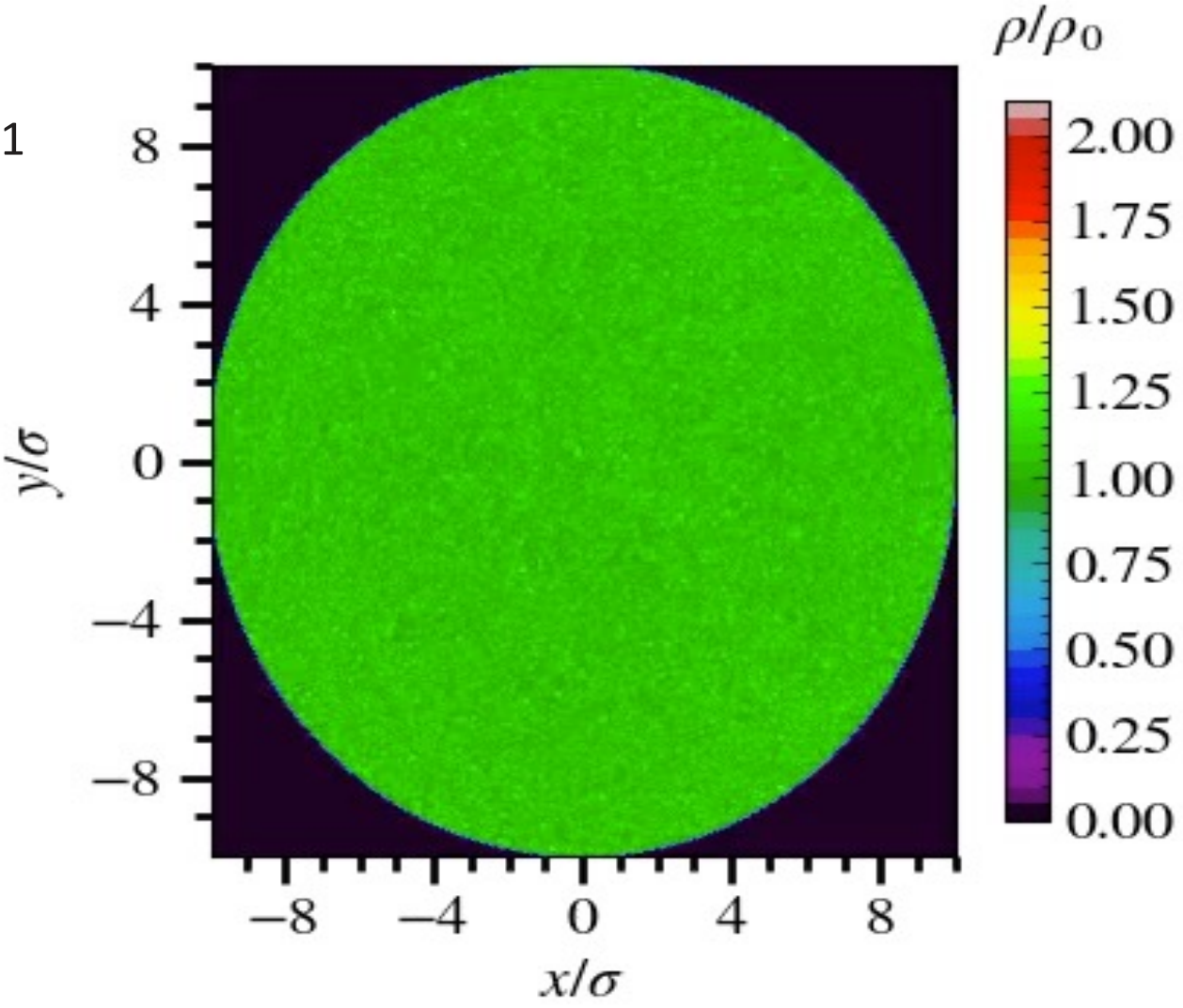
$$\frac{d^2\vec{p}_n}{d\tau^2} = (2\pi)^2 [\hat{p}_n \times \vec{E}_n(\vec{r}_n)] \times \hat{p}_n$$

$$- (2\pi)^2 \frac{k}{QE_0} \left(1 - \frac{1}{p_n}\right) \vec{p}_n .$$

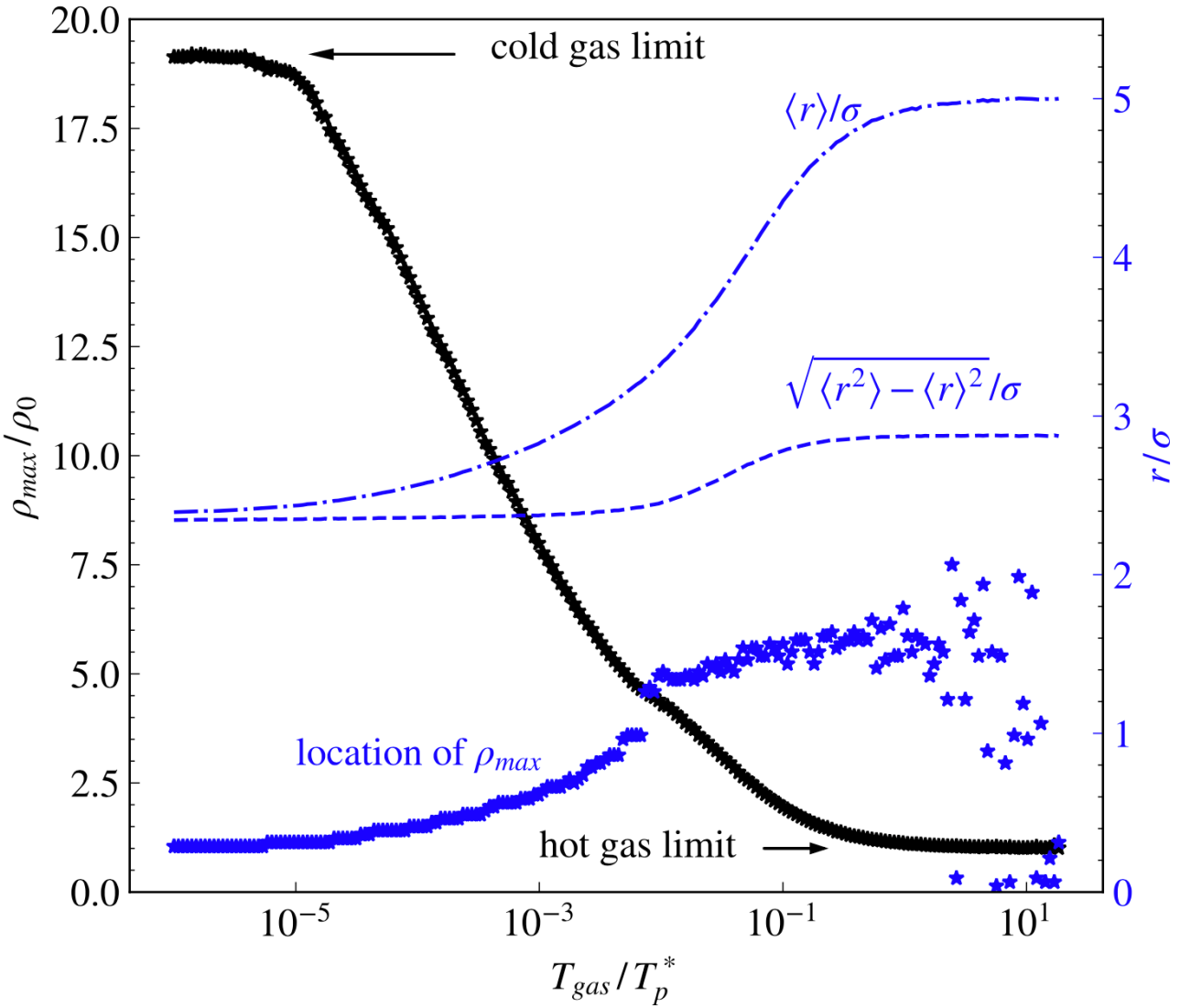
Full dynamics is very hard !! → rigid bi-atomic model is easier to simulate

Benchmarking with a rigid model

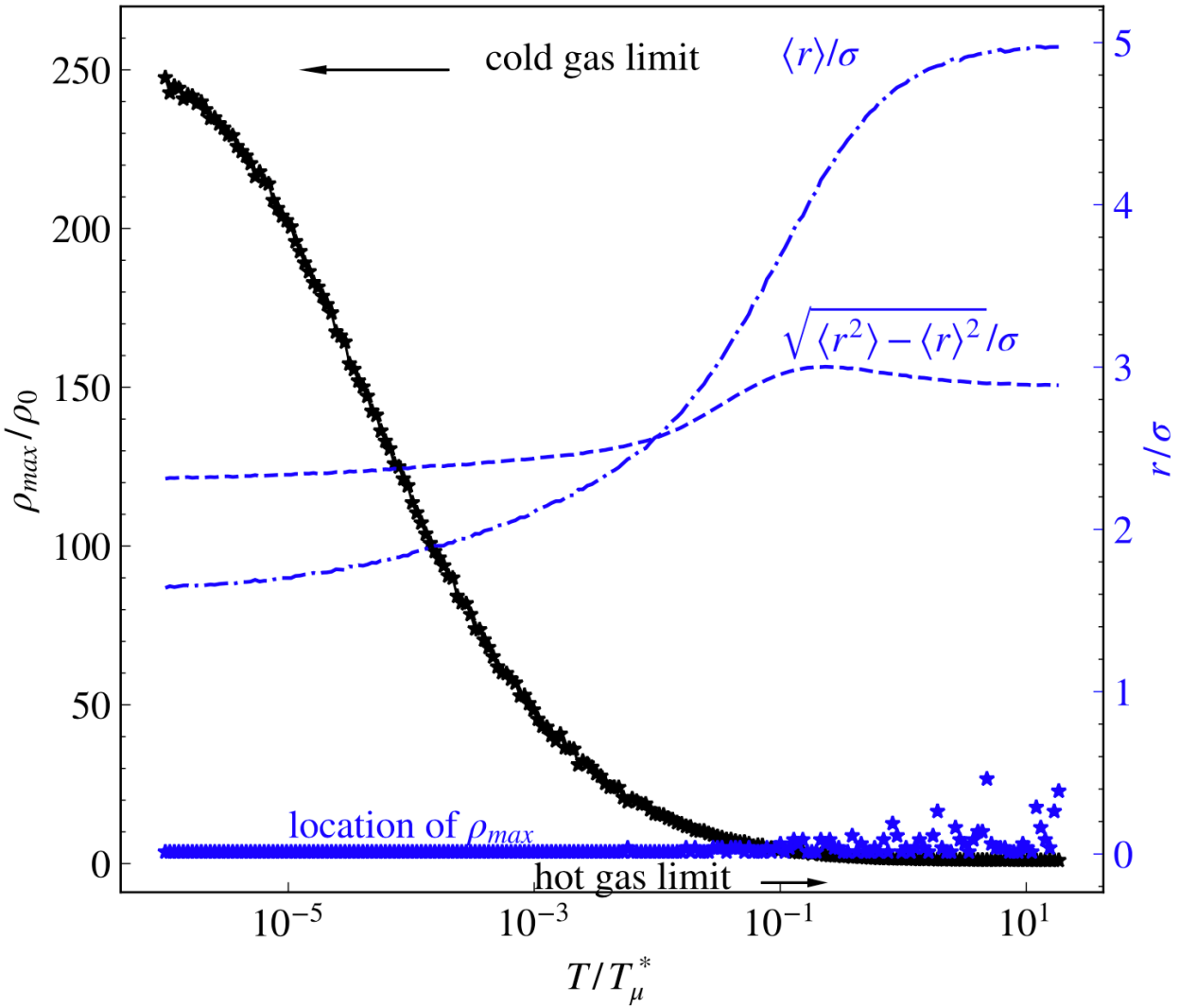
$T/T^*_p = 0.1$



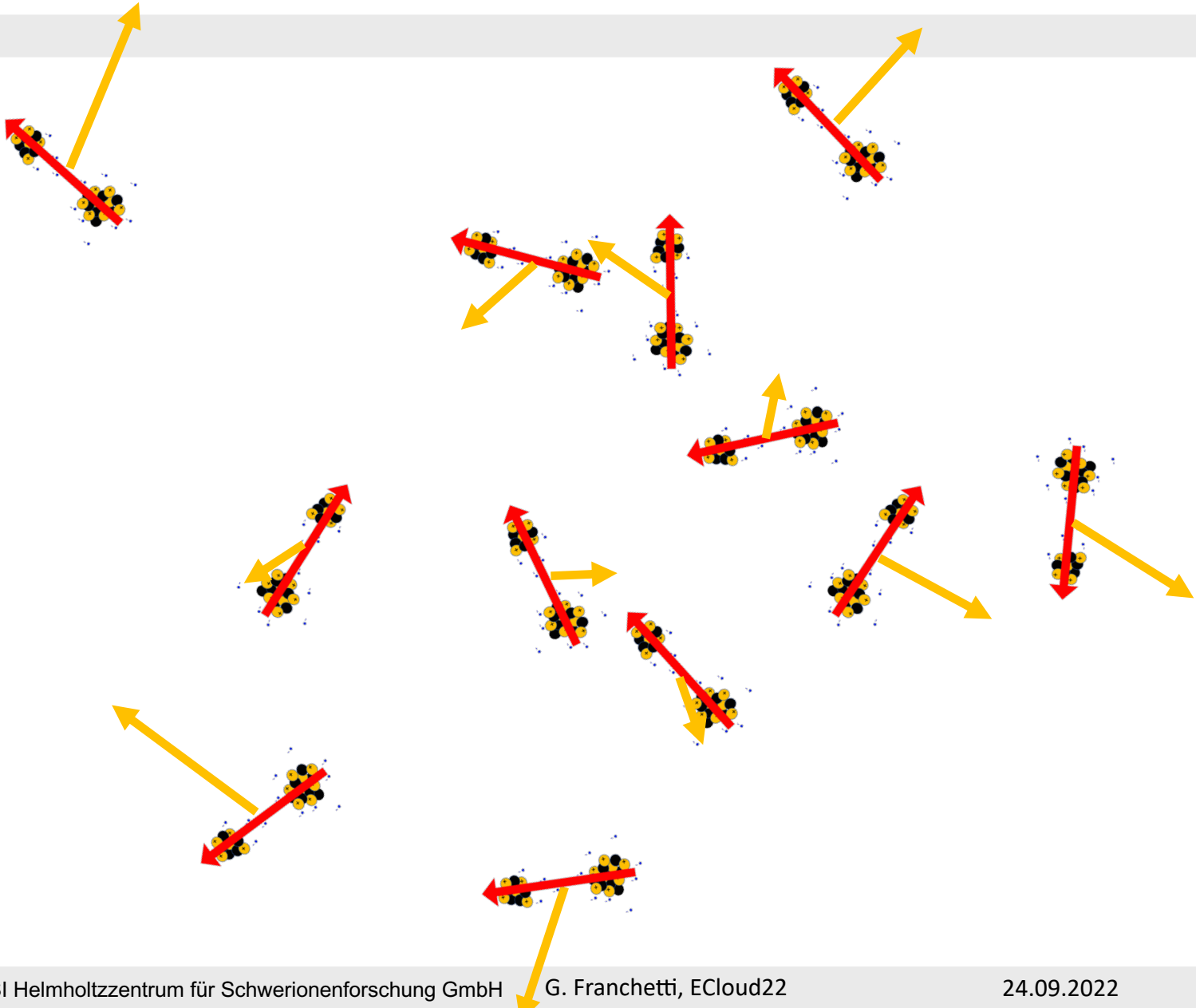
Density enhancement depends critically from T/T^*_p



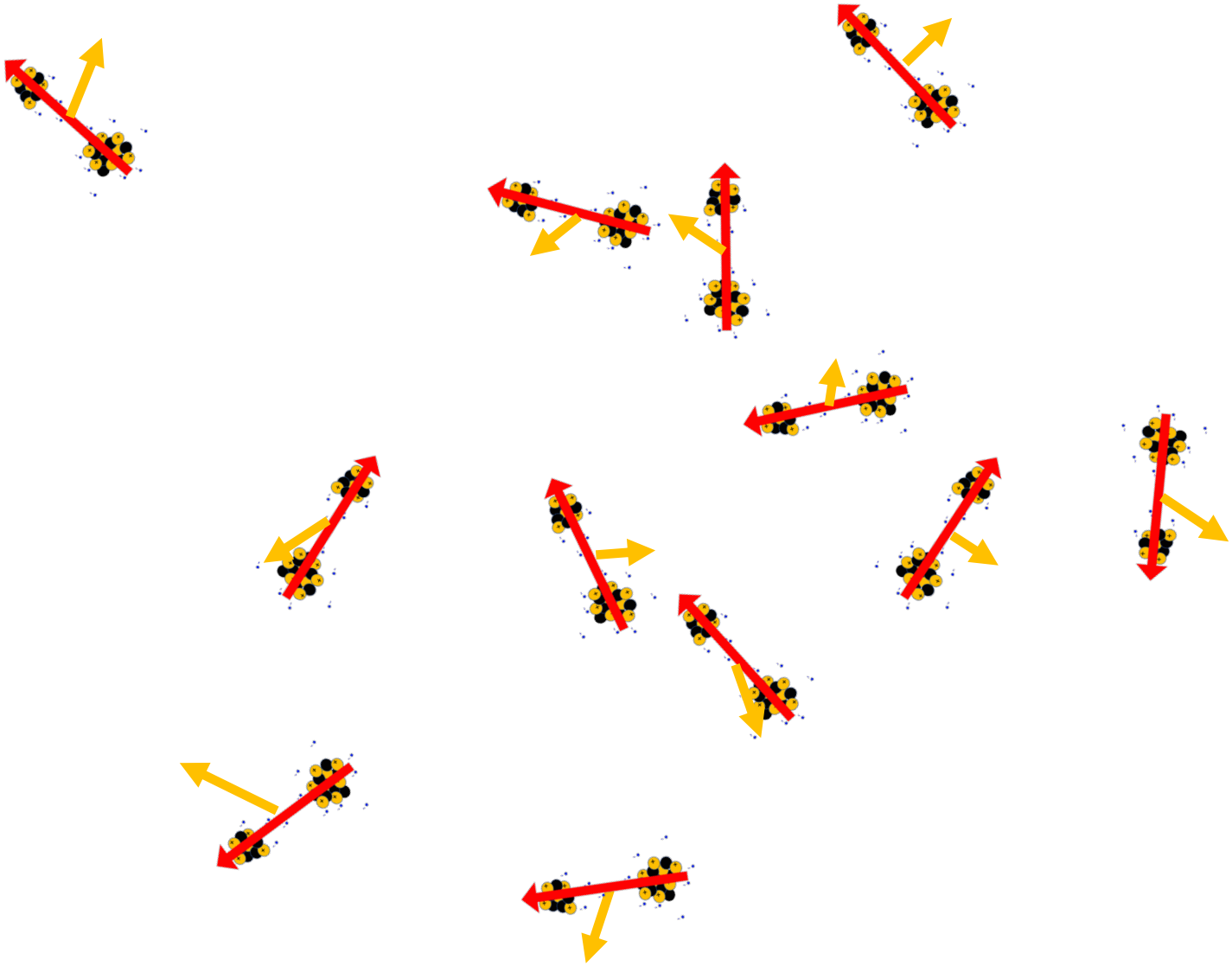
Density enhancement depends critically from T/T^*_μ



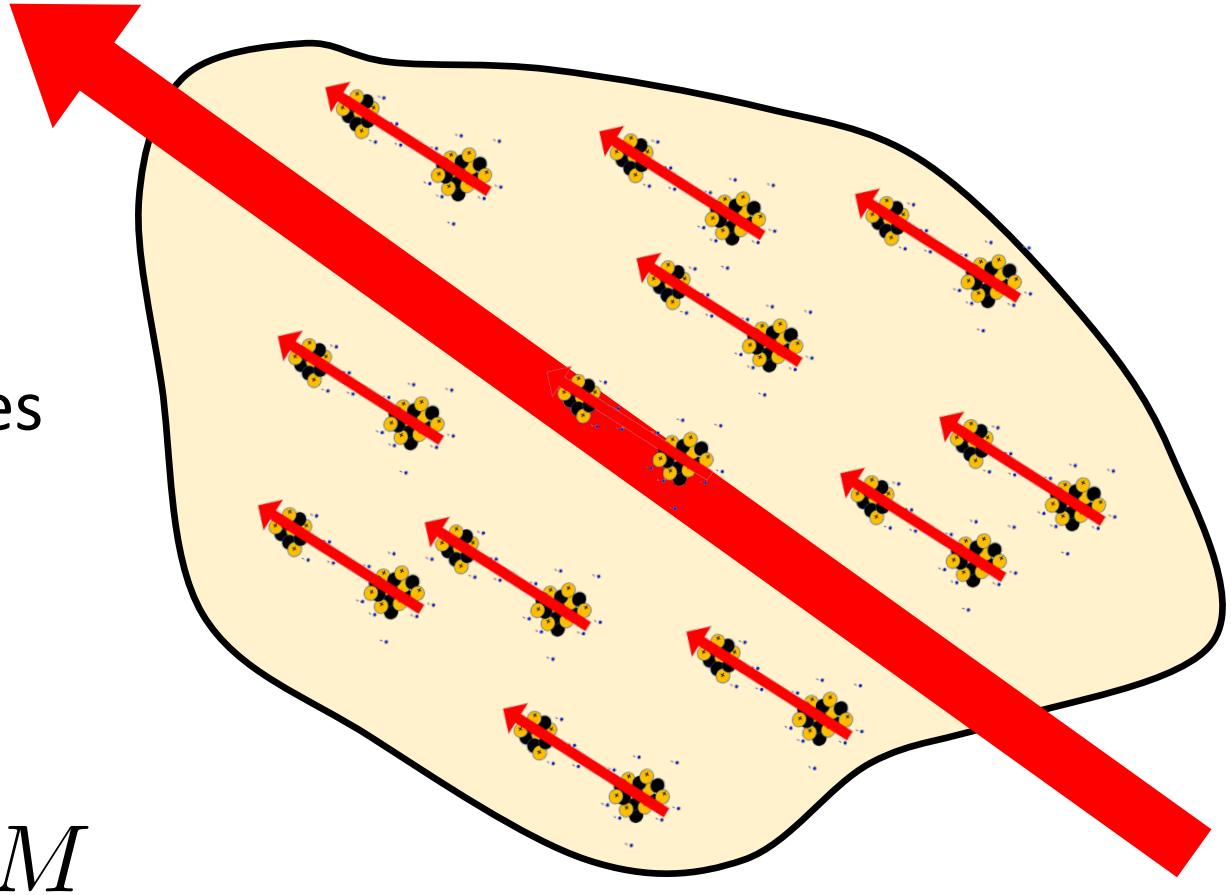
A tantalizing prespective



A tantalizing prespective



Agglomeration or clustering

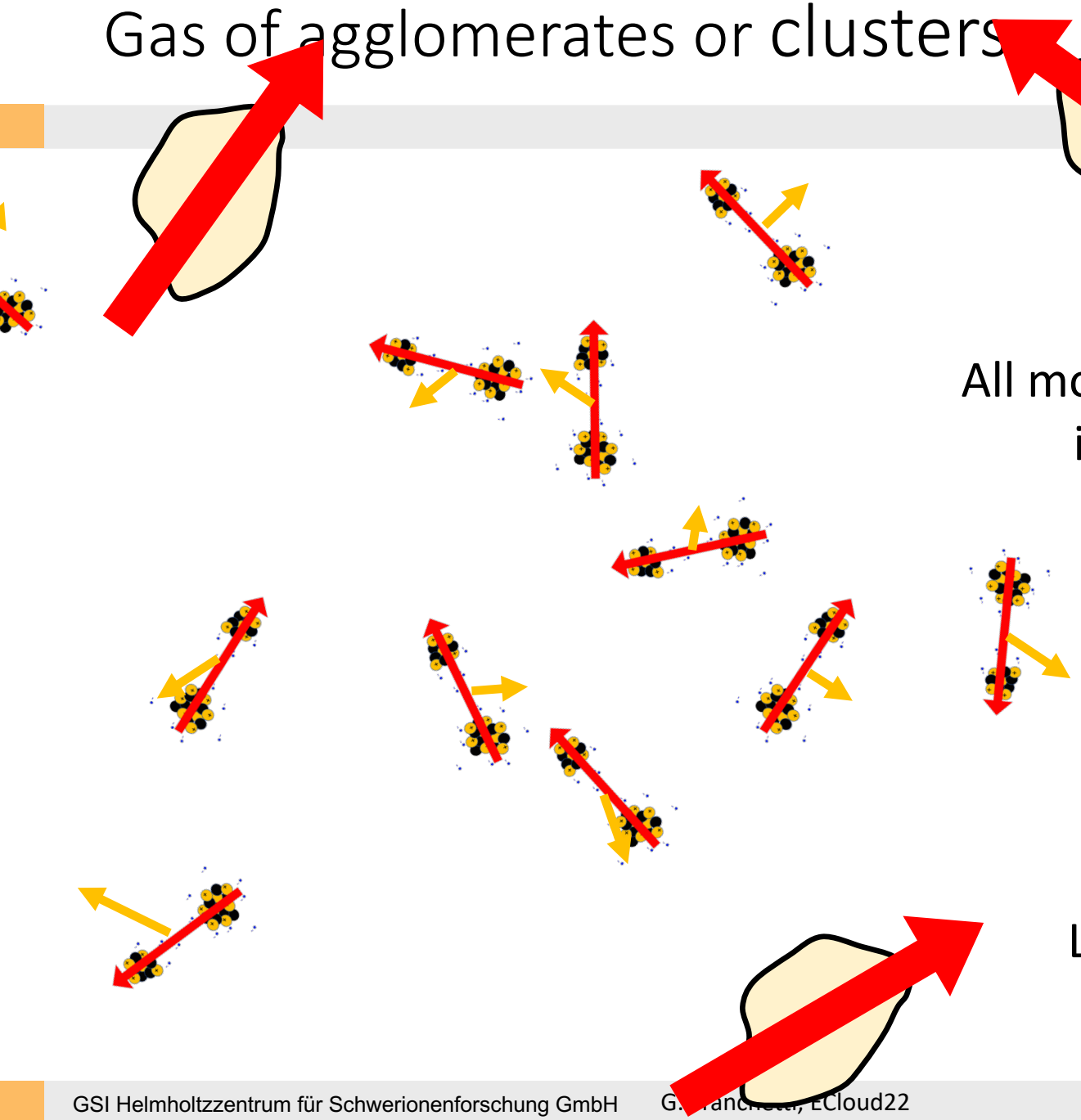


N molecules clusters

$$M_f = NM$$

$$|\vec{p}_f| \leq N|\vec{p}| \qquad T_f^* \leq T_p^* N$$

Gas of agglomerates or clusters

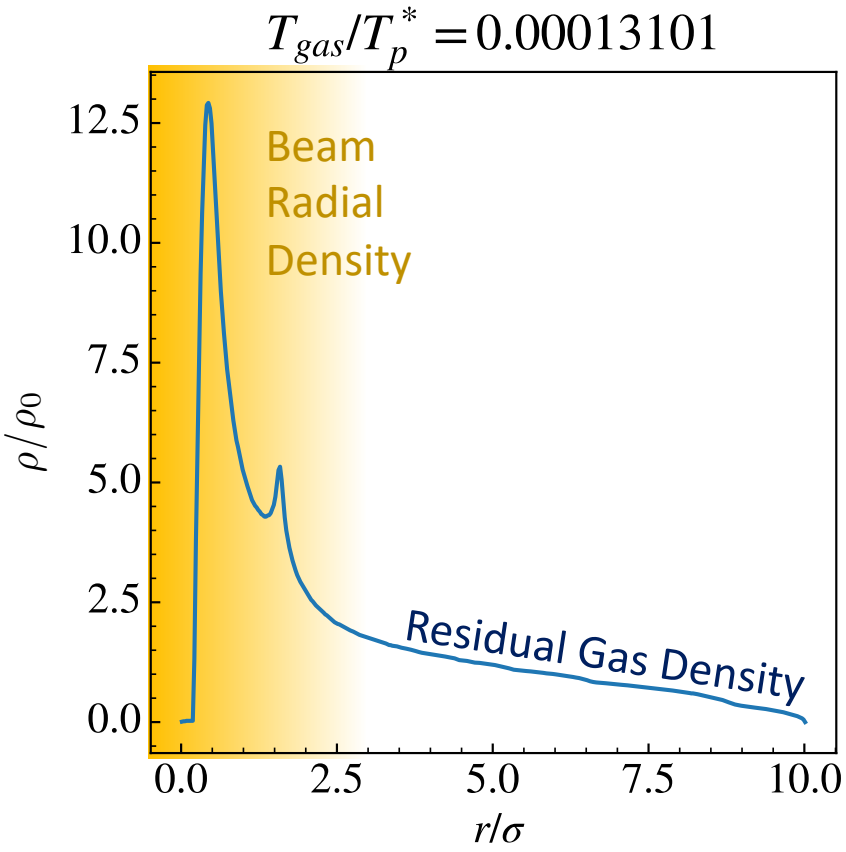


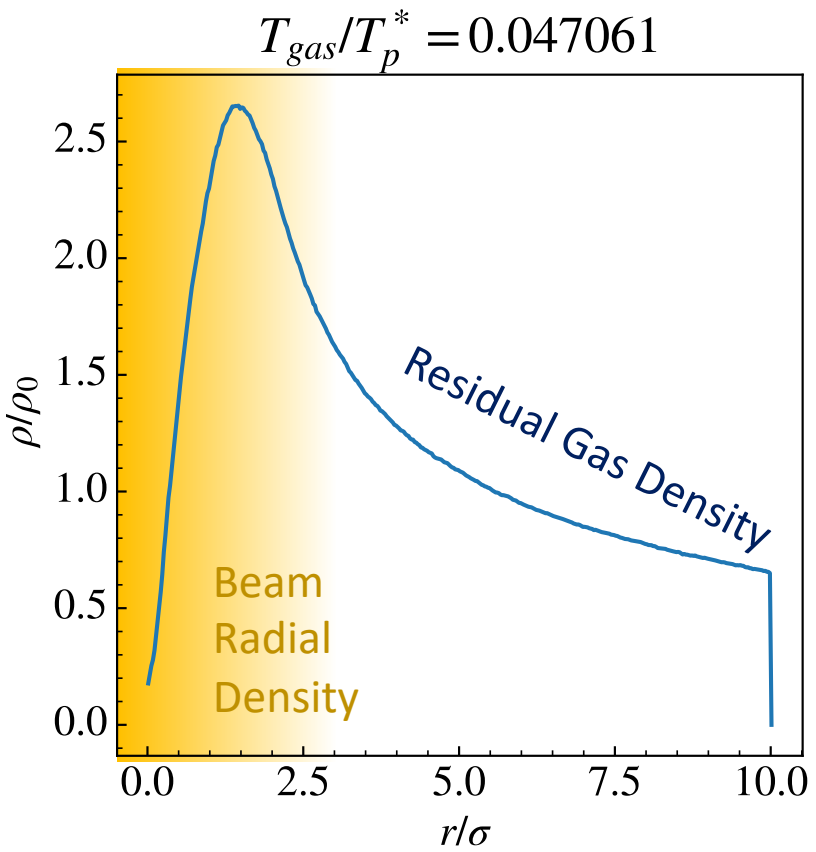
All molecules and flakes are in thermal equilibrium at the temperature T

$$\frac{T}{T_f^*} \gtrsim \frac{T}{T^*}\frac{1}{N}$$

Lowered towards the ``cold gas limit''

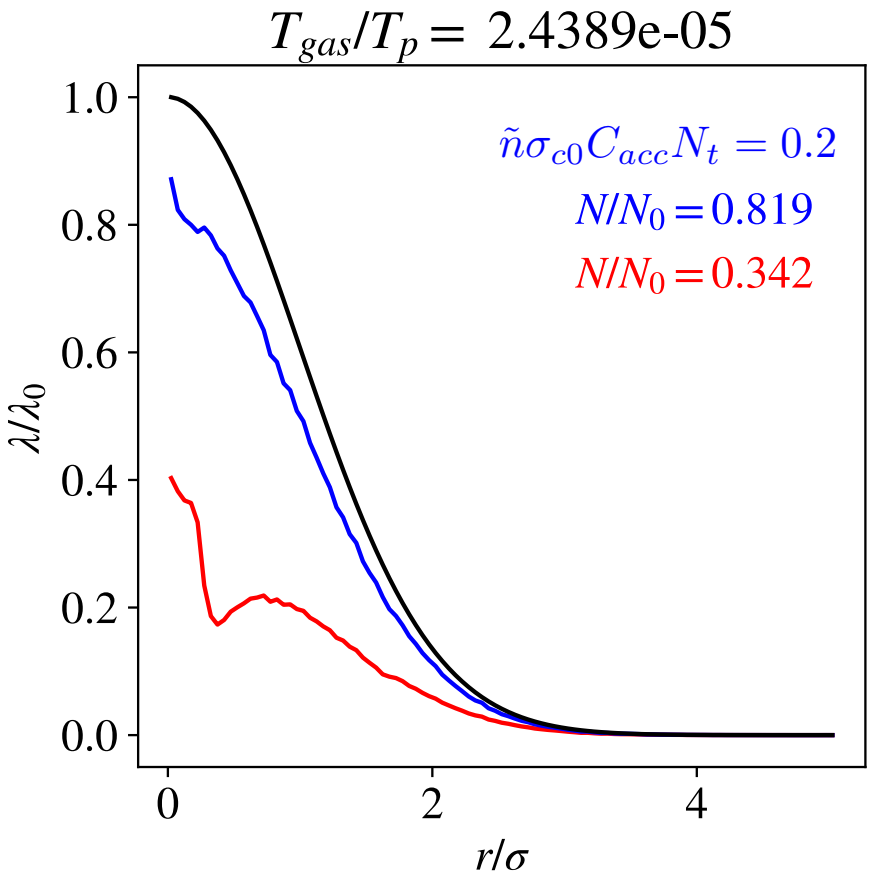
Estimate of the impact on the beam lifetime

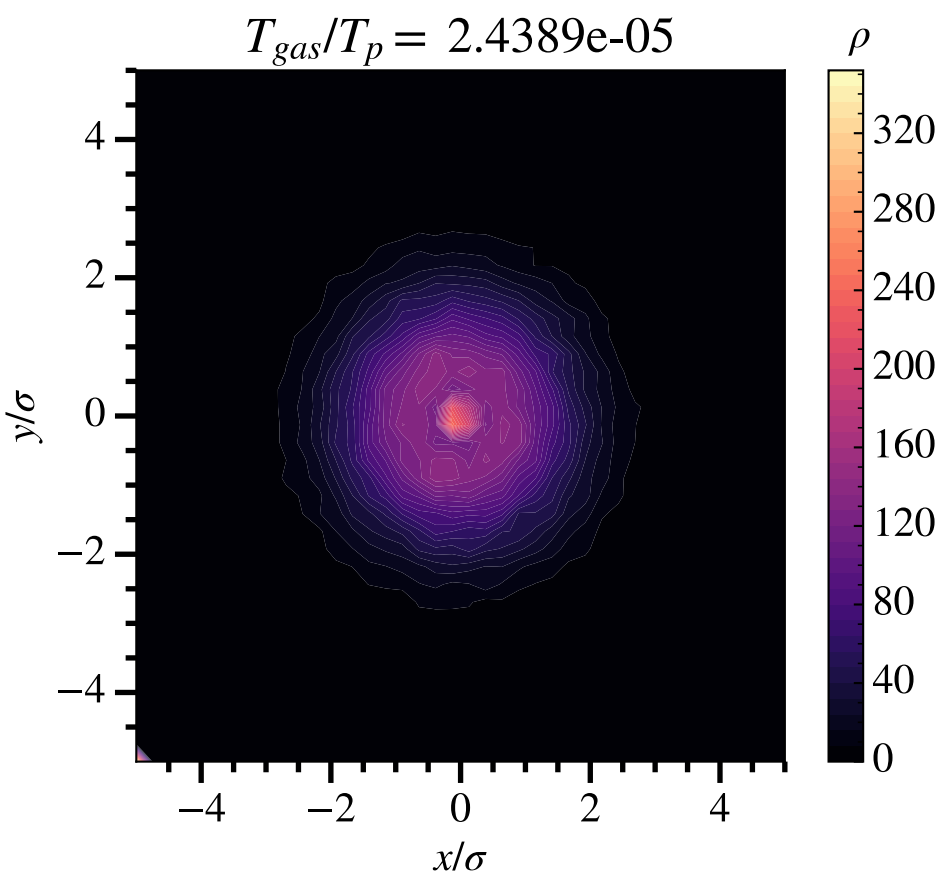




Lifetime is obtained integrating the density of the local molecules with betatron motion

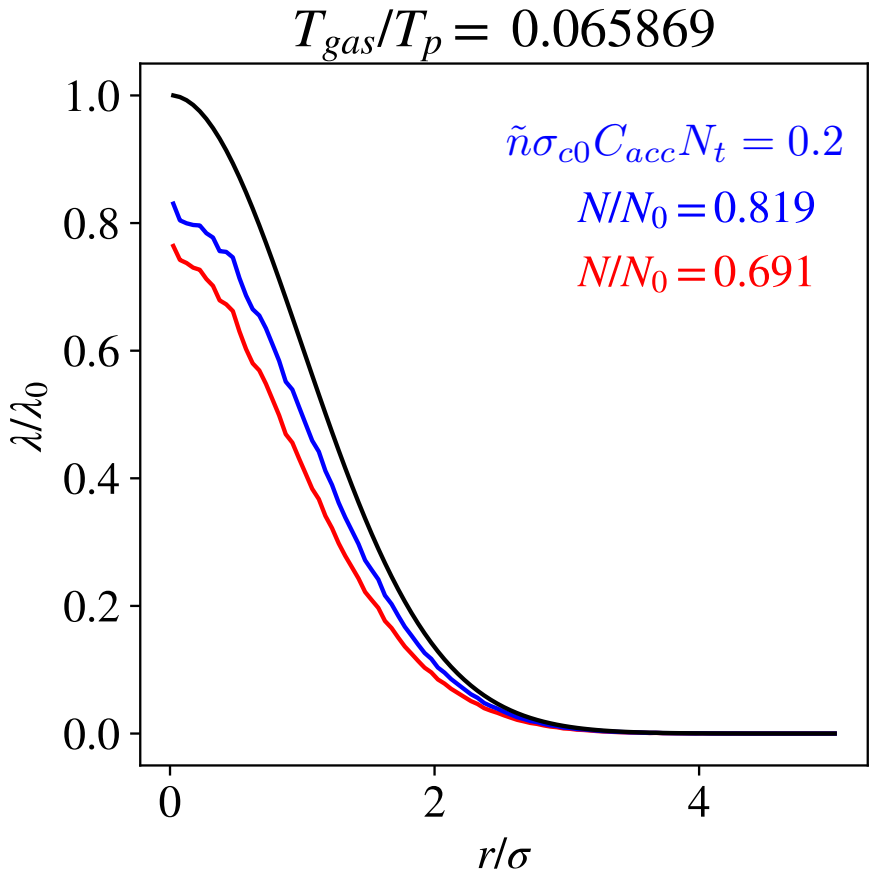
Comparison of beam loss / lifetime

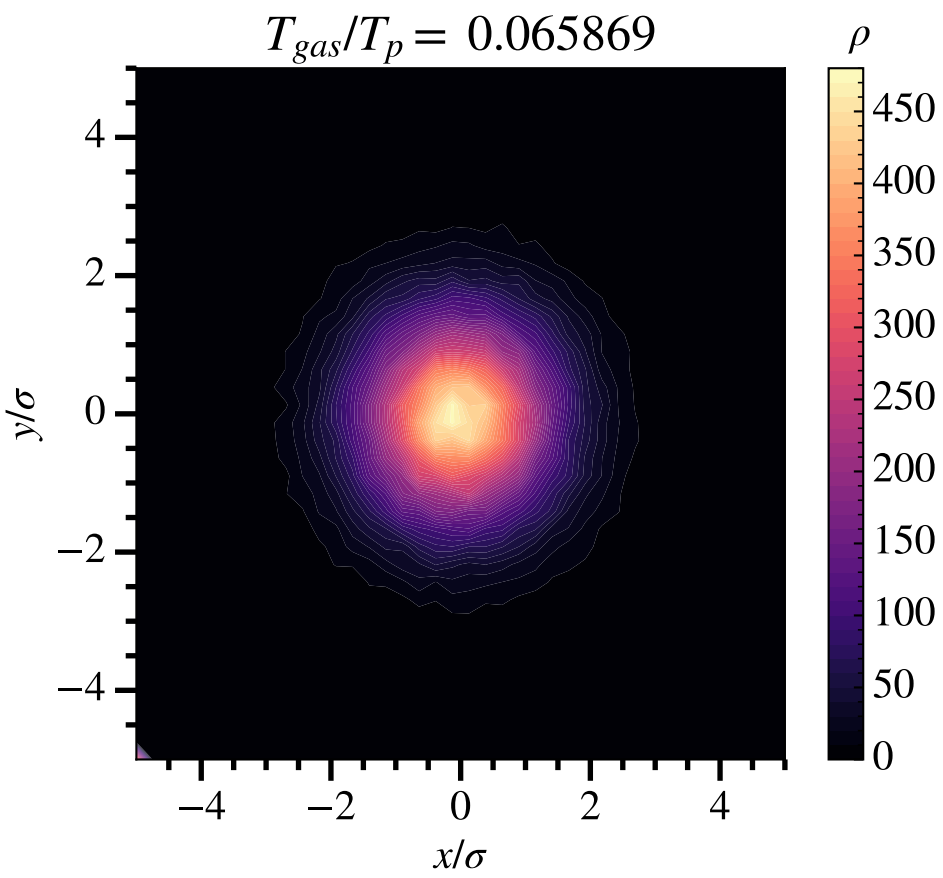




Same flake density as original residual gas density

Comparison of beam loss / lifetime





Same flake density as original residual gas density

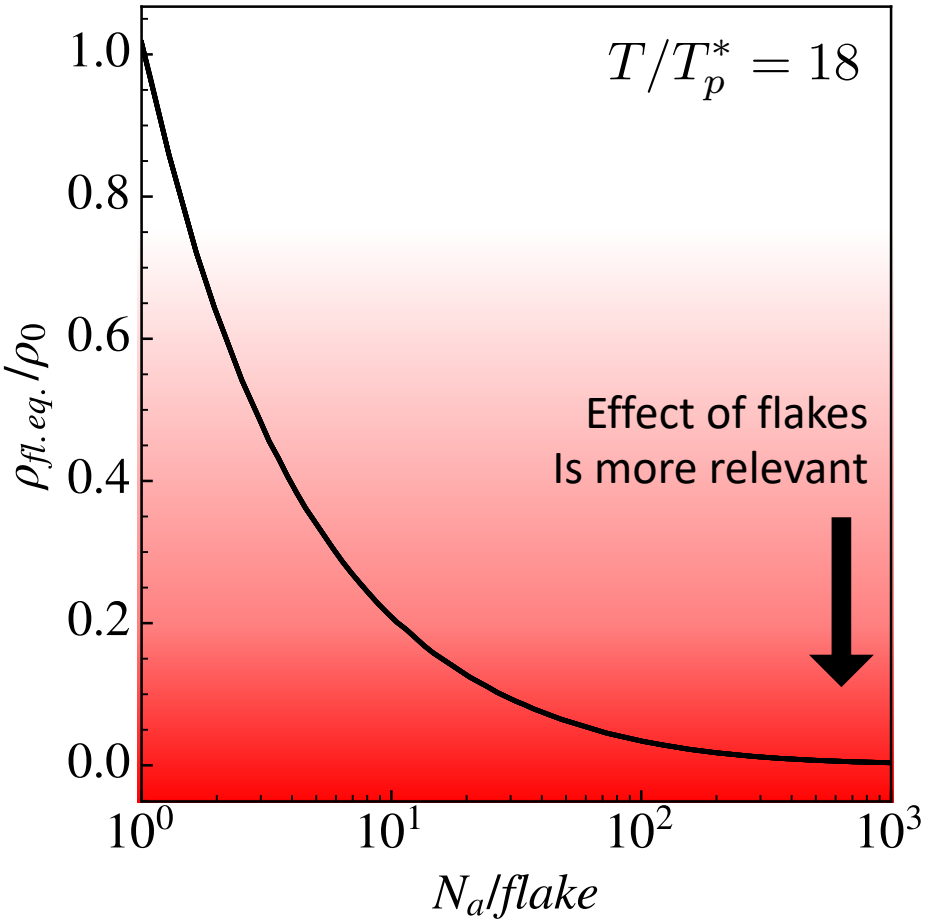
Lifetime equivalent flake density

Cross section ansatz (geometrical)

$$\sigma_C = (N_a/flake)^{2/3}\sigma_{C0}$$

Equivalent flake density

the density of flakes that generate the same beam lifetime as generated by the original residual gas



Of course, this is a figure of merit, full dynamics is more complex

Summary

- Molecules with: a magnetic dipole moment oscillate “around” the transverse center of the particle beam; with an electric dipole moment oscillate “around” a radial equilibrium at the beam “edge”.

- The features of the dynamics & trapping and density enhancement are a function of a trapping temperature T^*, and $T \rightarrow T/T^*$

- It is possible to derive the fraction of molecules, with either electric or magnetic dipole moment, trapped by the beam field, as a function of T/T^*

- Density enhancement may be important in cryogenic vacuum systems, high beam currents or small beam sizes → for future generations of accelerators.

- An estimate of the beam lifetime allows for the establishment of an equivalent flake density according to the number of components of the flake. Hence it allows the assessment of how dangerous the flakes can be..

Thank you for the attention