Trapping of neutral molecules by the beam electromagnetic field

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Topics

- Motivation
- Forces and torques on molecules with dipole moments
- Dynamics of molecules and trapping
- Enhancement of vacuum density
- Phenomenology
- Summary

Motivation

Density of vacuum atoms or molecules → Beamlifetime

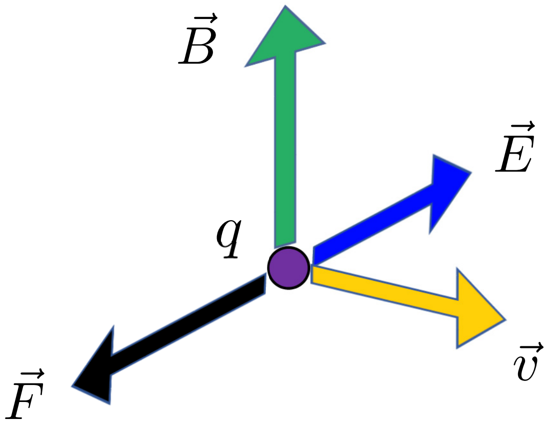
Collision Beam - vacuum molecules

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

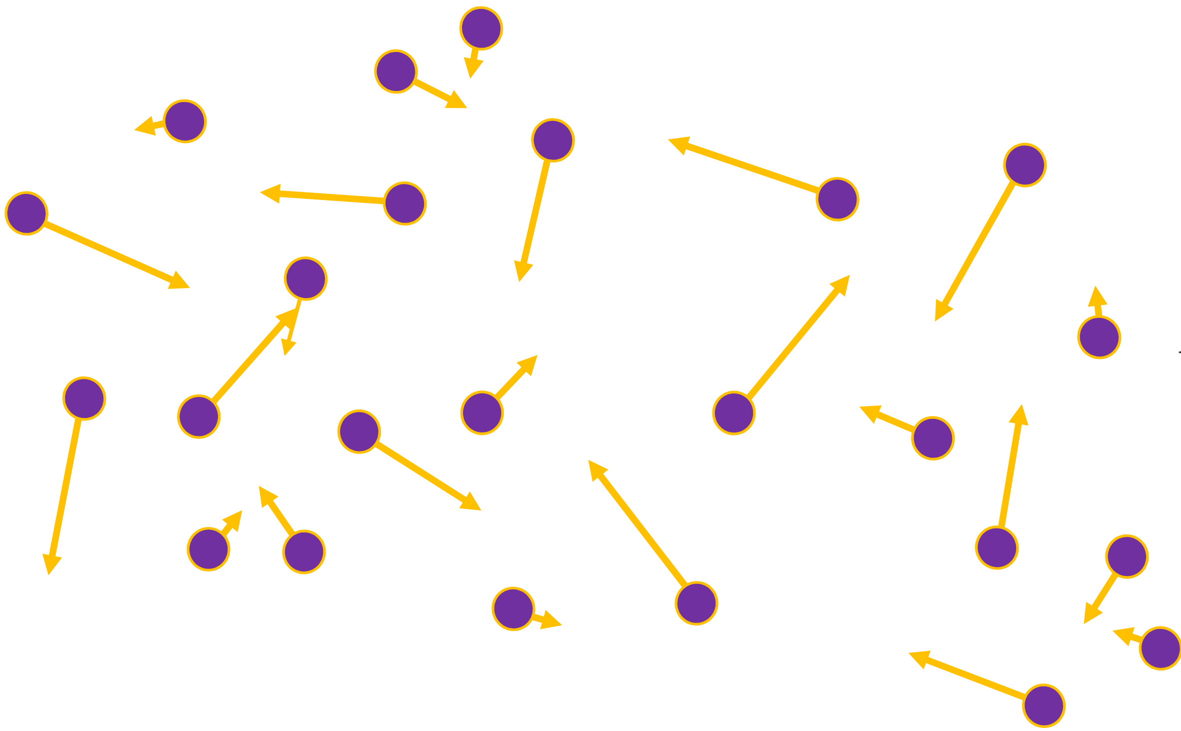
Dynamics of charged particles

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



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

Dynamics of neutral molecules



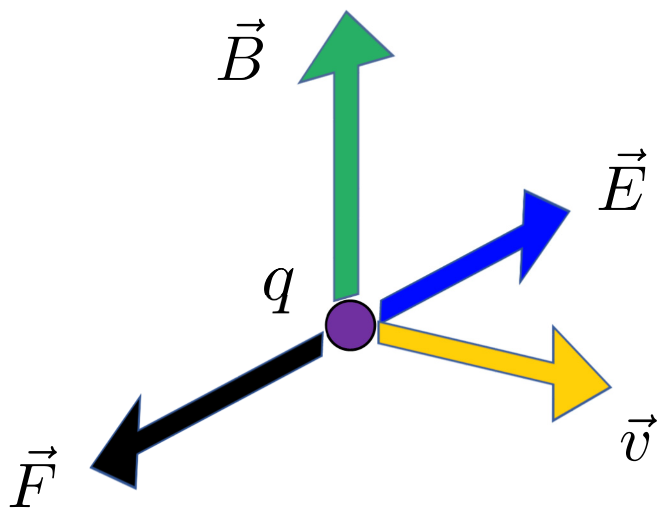
$$v_{rms} = \sqrt{\frac{k_b T}{M}}$$

Thermodynamics → Maxwell-Boltzmann velocity distribution
→ Temperature

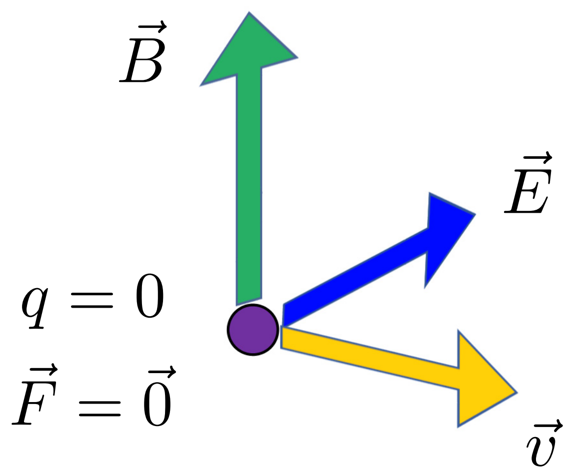
Properties → Collisions, Mean free path, Impingement rate, Pressure

Charged particles vs neutral at first sight

Charged molecule/particle

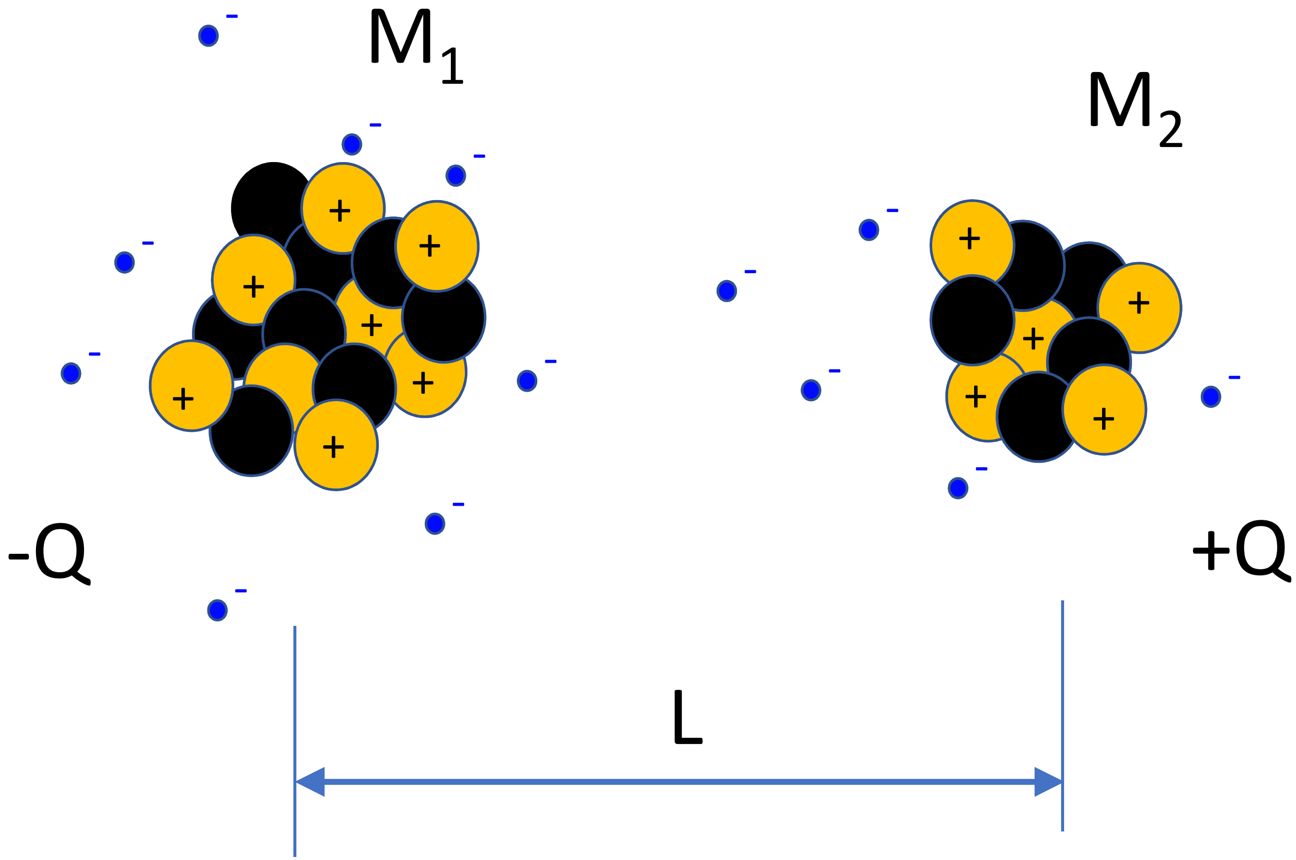


Neutral molecule

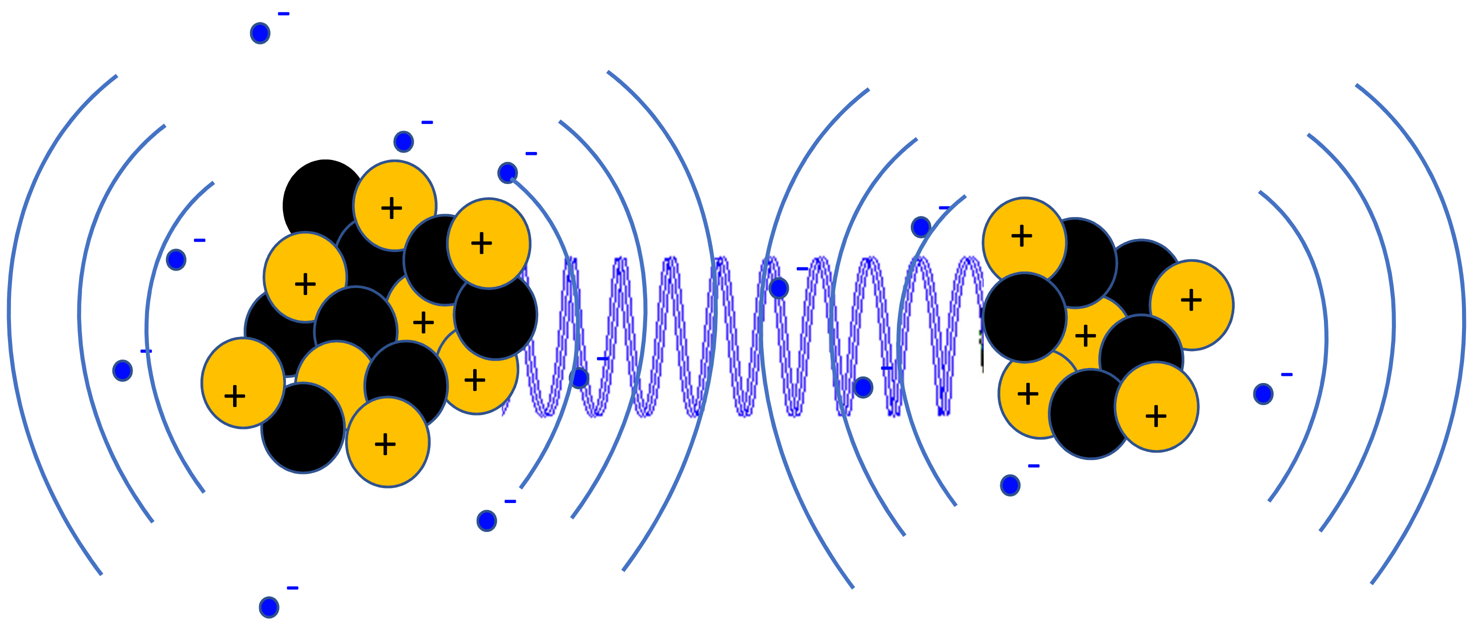


Apparently →
no forces on the molecule

Structure of molecules

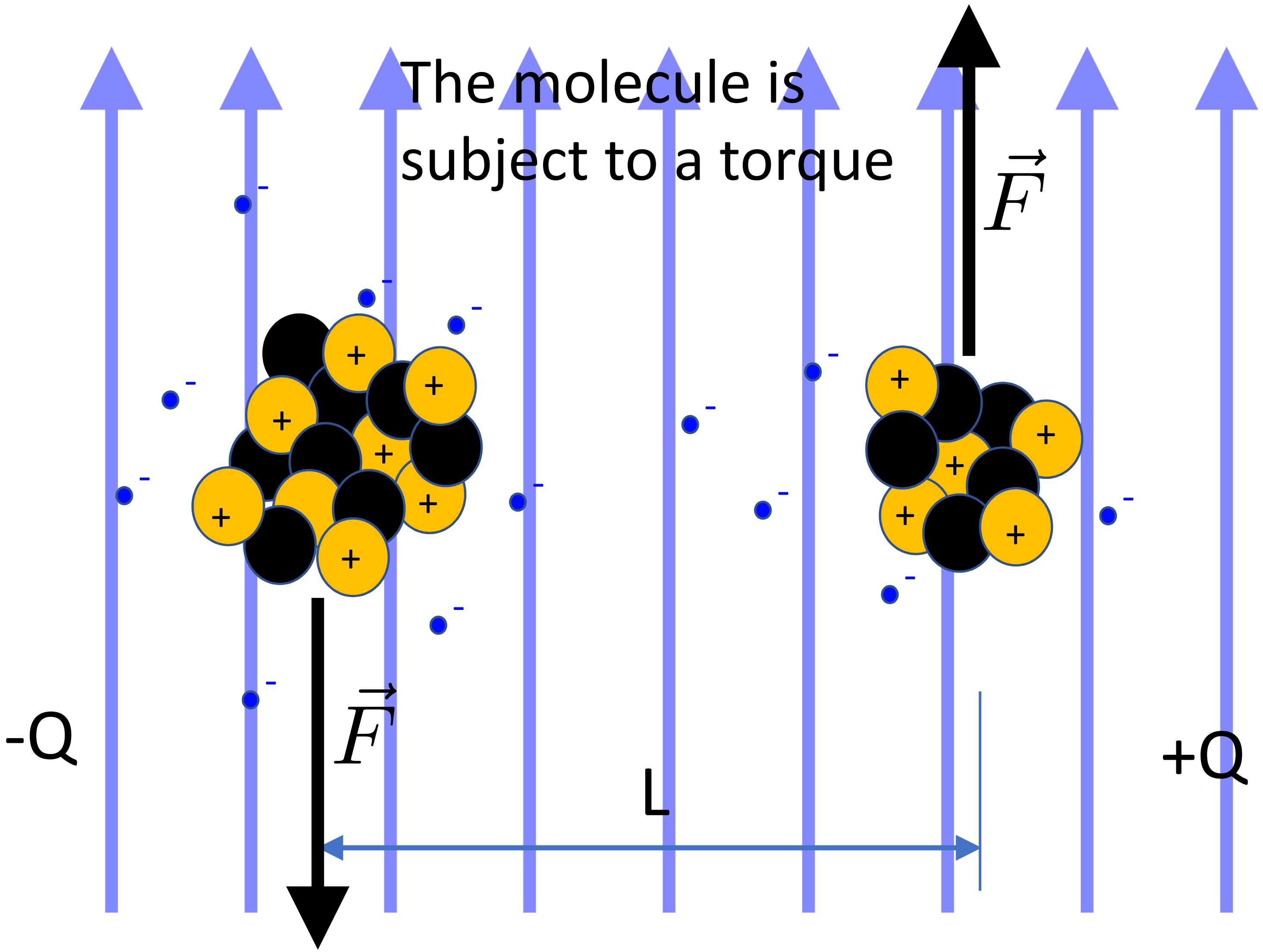


Vibrational state

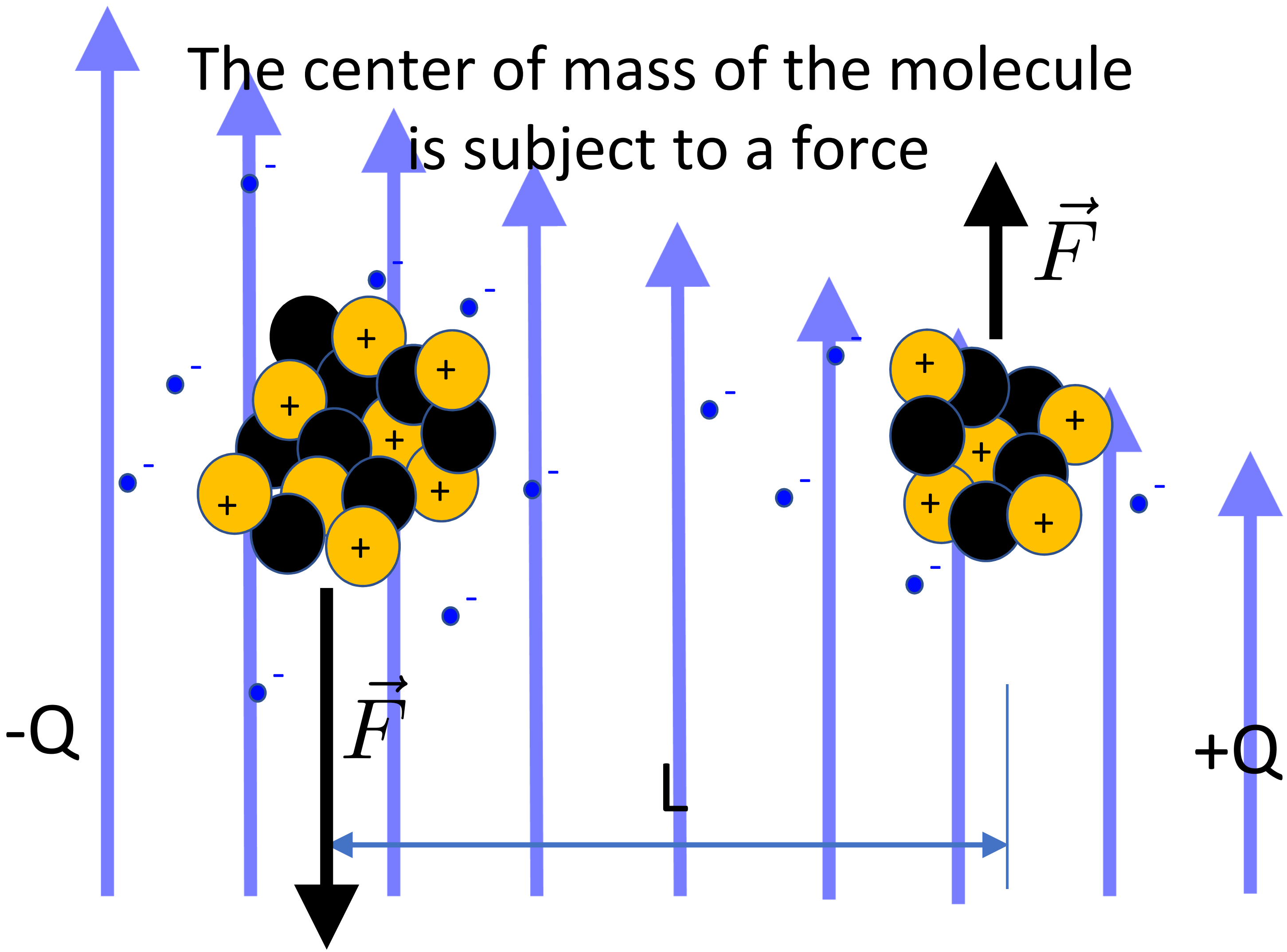


Characteristic molecular vibrational frequency → very large

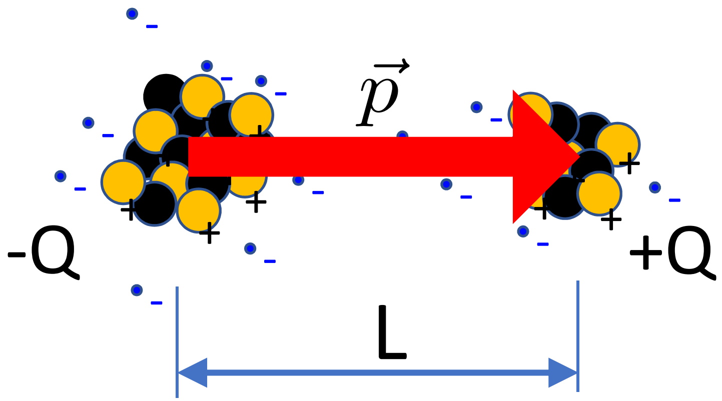
Molecules and electric fields



Molecules and electric fields



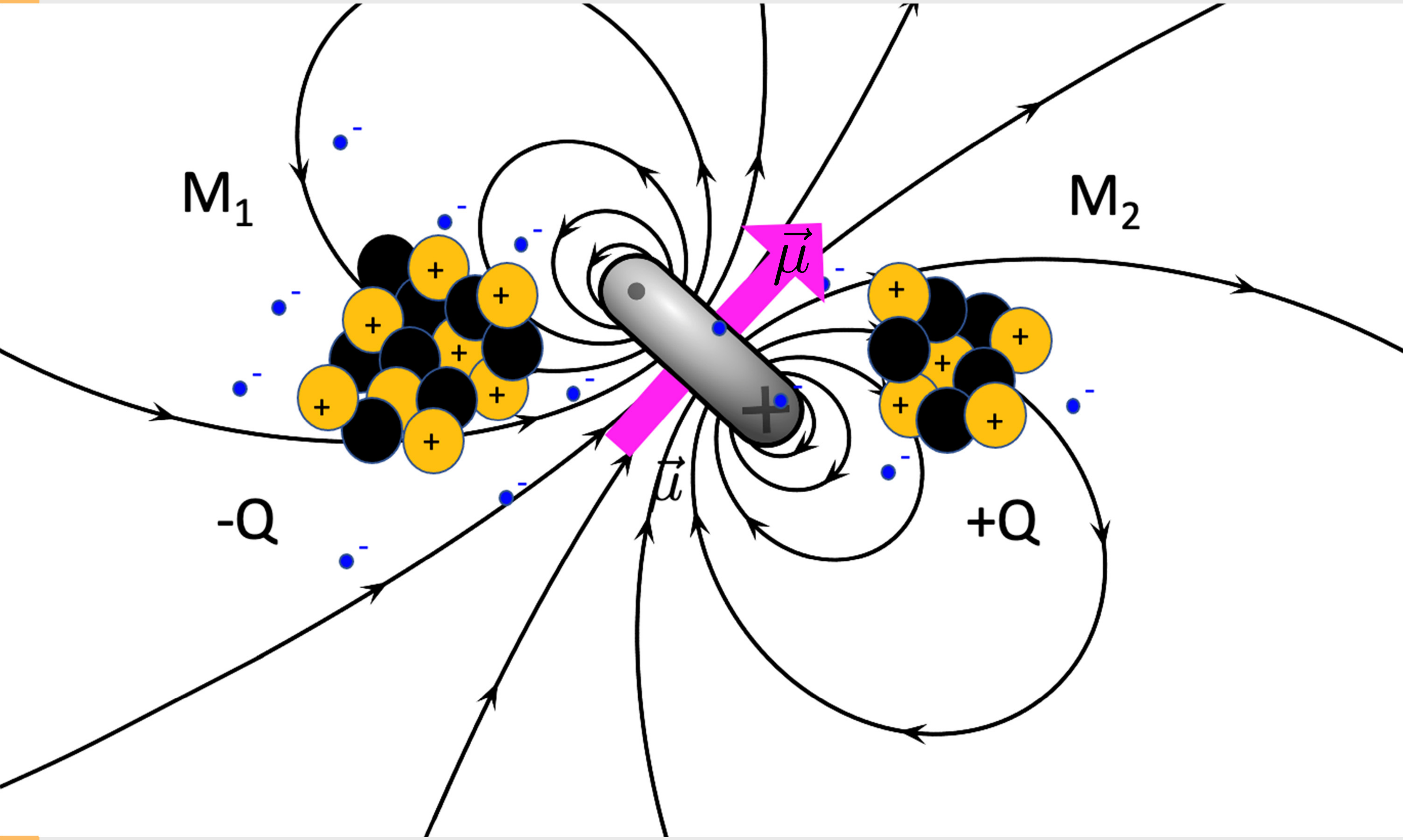
Electric dipole moment



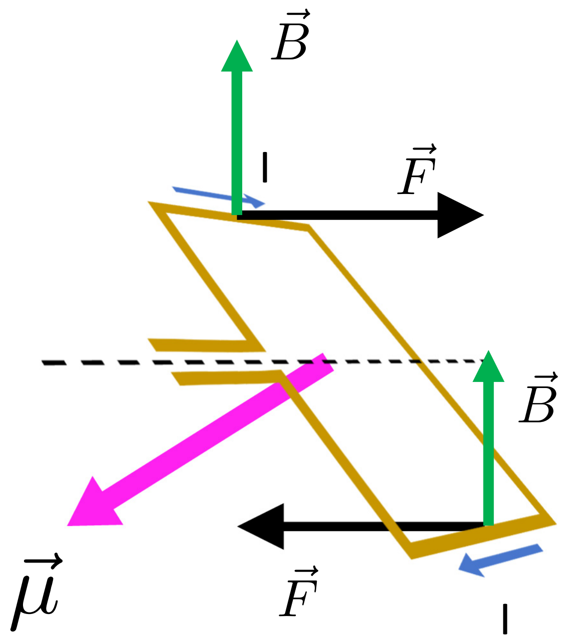
$$\vec{p} = Q\vec{L}$$

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

Molecules and magnetic fields



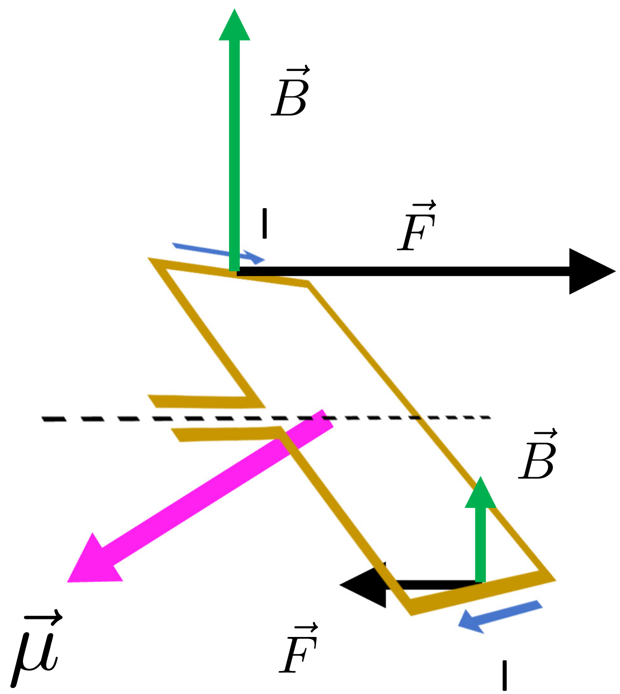
Molecules and magnetic fields



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

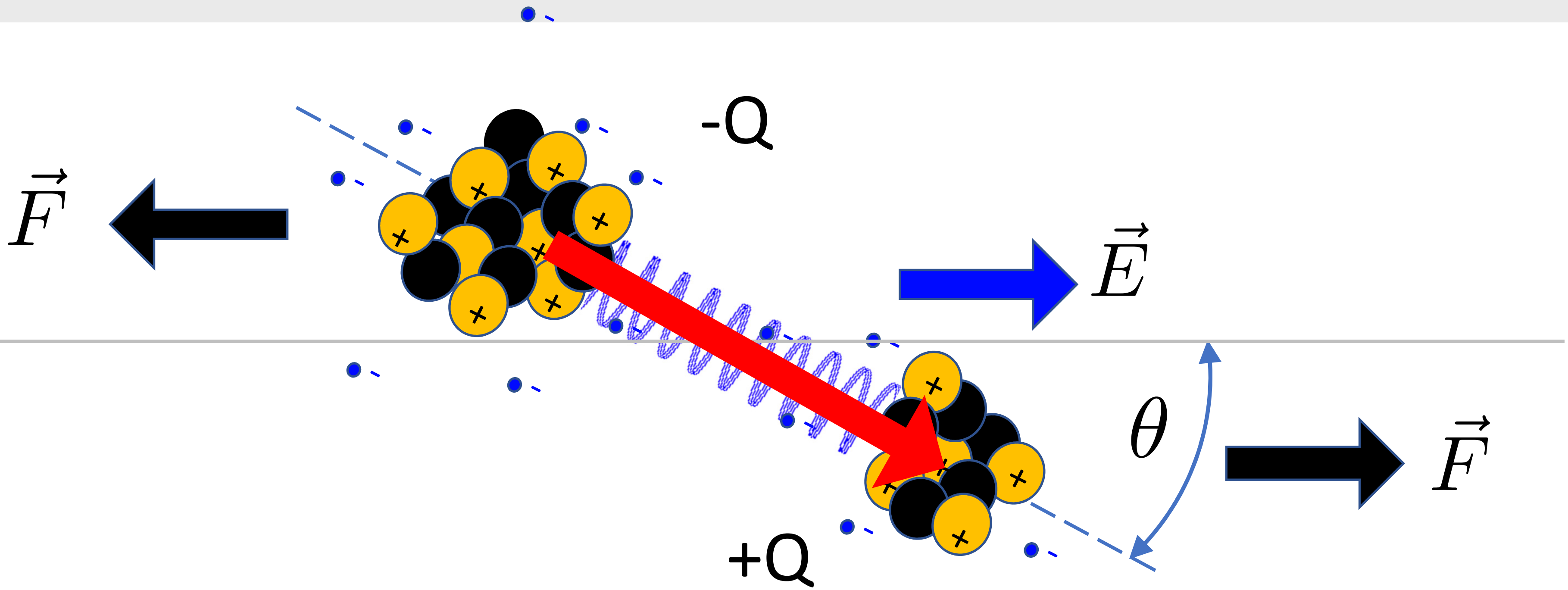
Molecules of interest

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 eÅ with e the electron charge, 1 Å = 0.1 nm

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

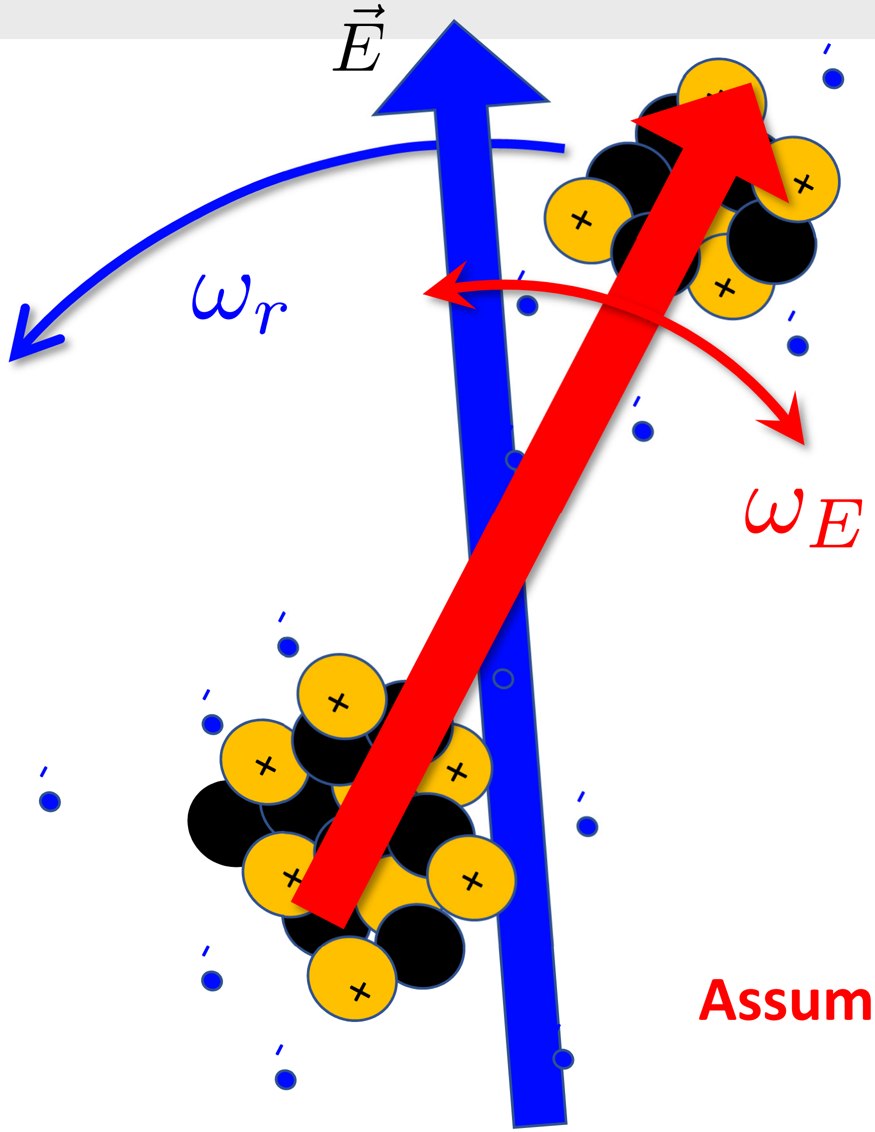
Dipole moment alignment and intrinsic time scale



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



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

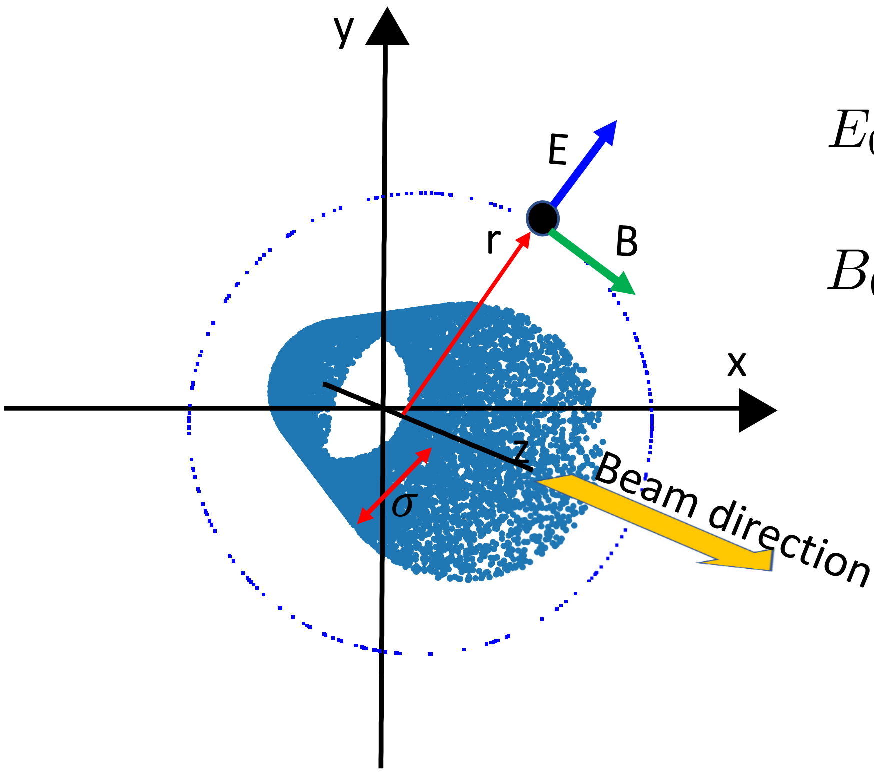
$$\omega_r = \frac{v_{cm}}{r_c}$$

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

Assumption: the dipole is aligned to the local field

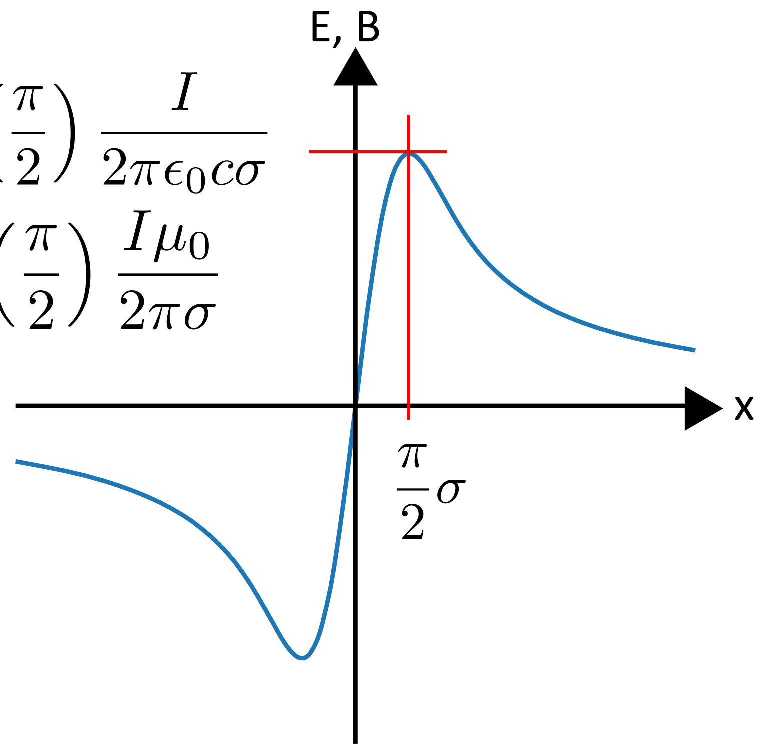
Electromagnetic beam field

Transverse Gaussian beam distribution



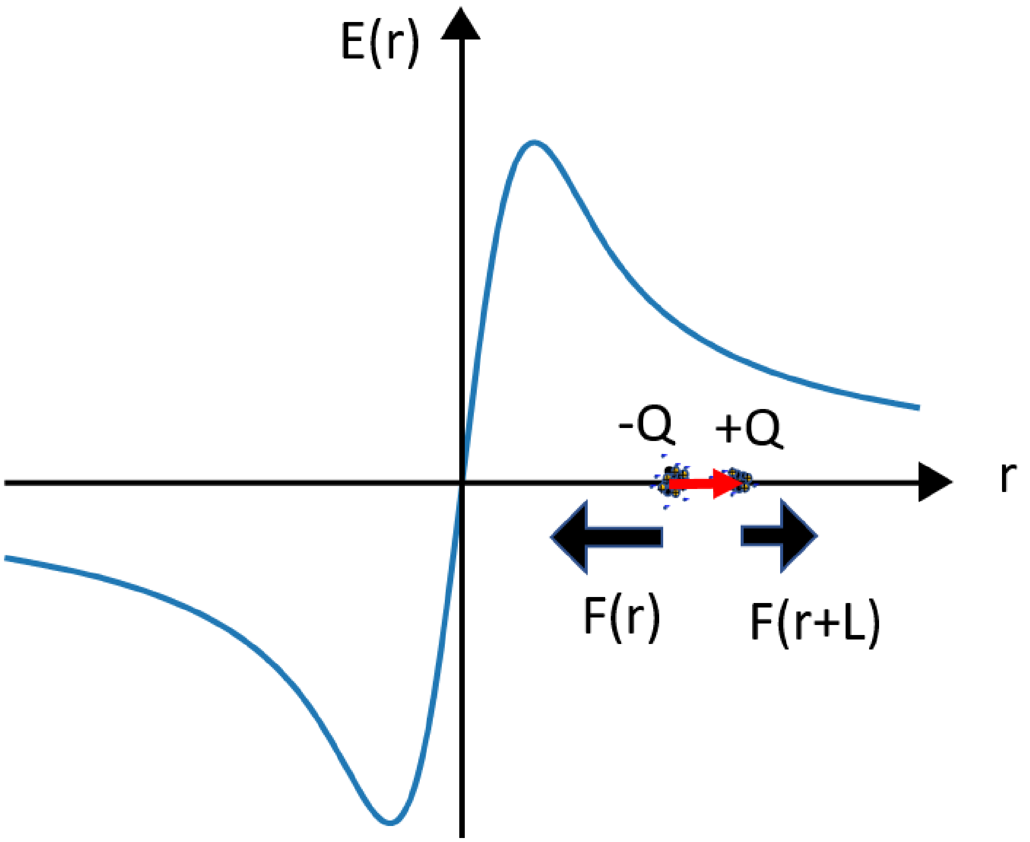
$$E_0 = \ln\left(\frac{\pi}{2}\right)\frac{I}{2\pi\epsilon_0 c\sigma}$$

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



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

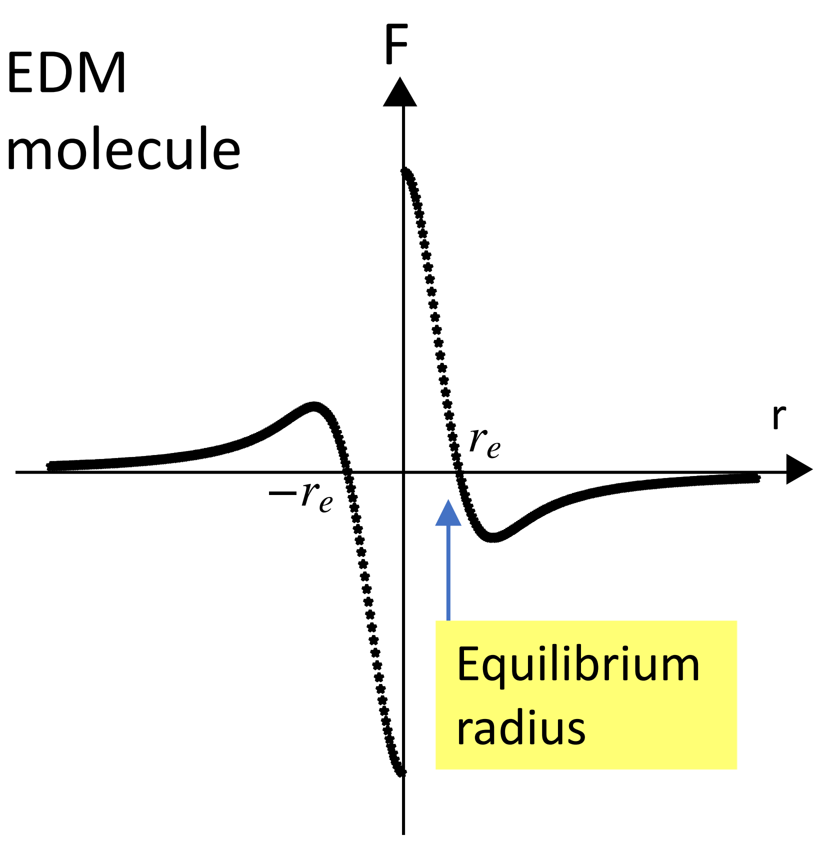
Force on a molecule from $\vec{E}$

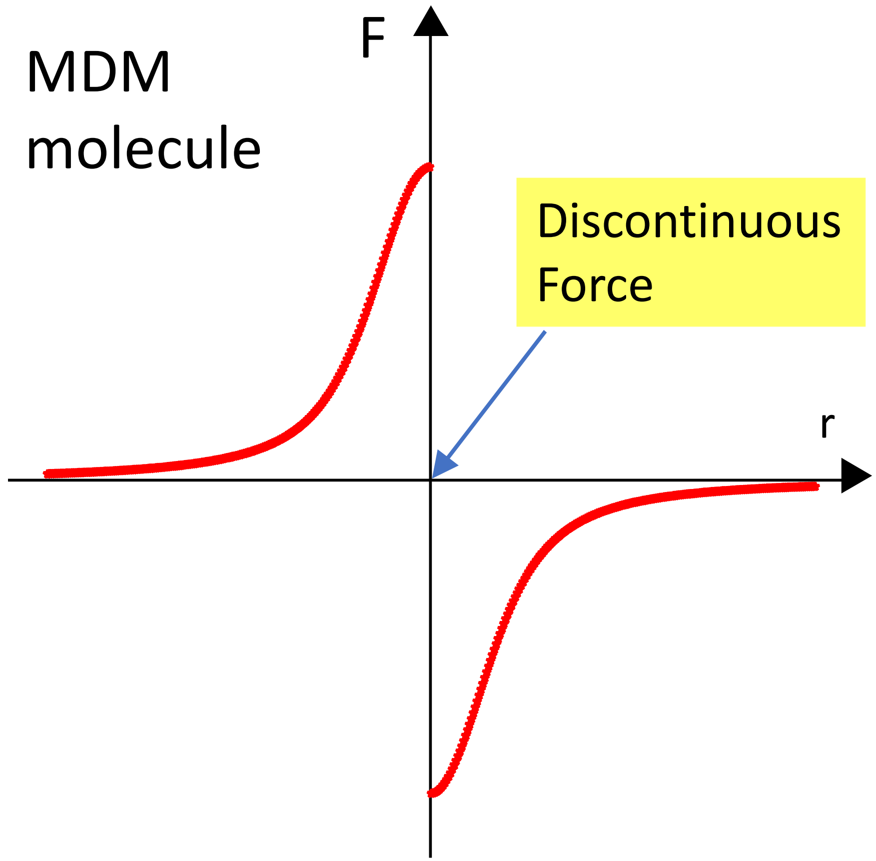


$$F = +QE(r+L) - QE(r) = QLE'(r) = pE'(r)$$

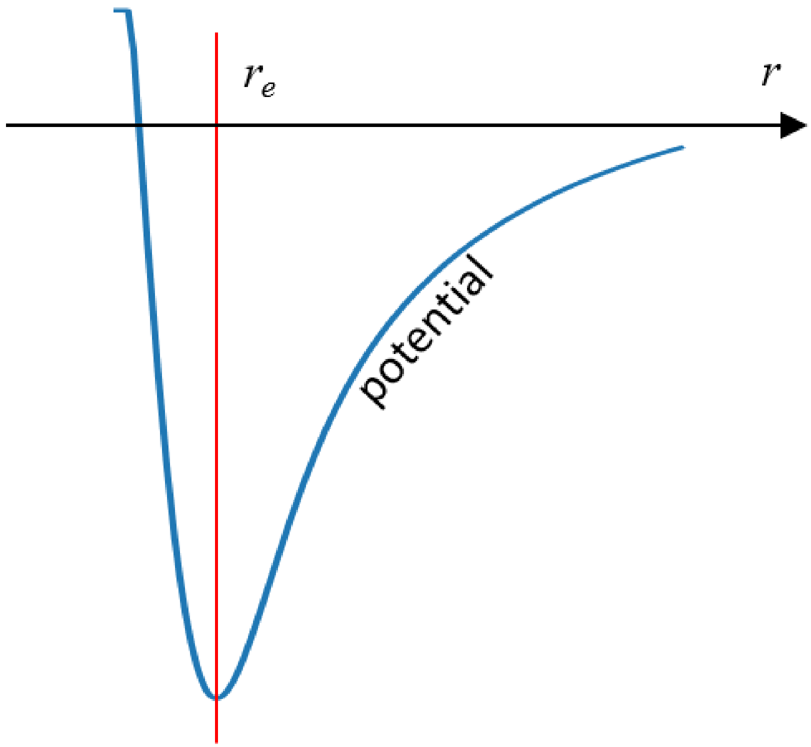
For molecules with dipole moment aligned, the Force on the center of mass is:

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





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^*

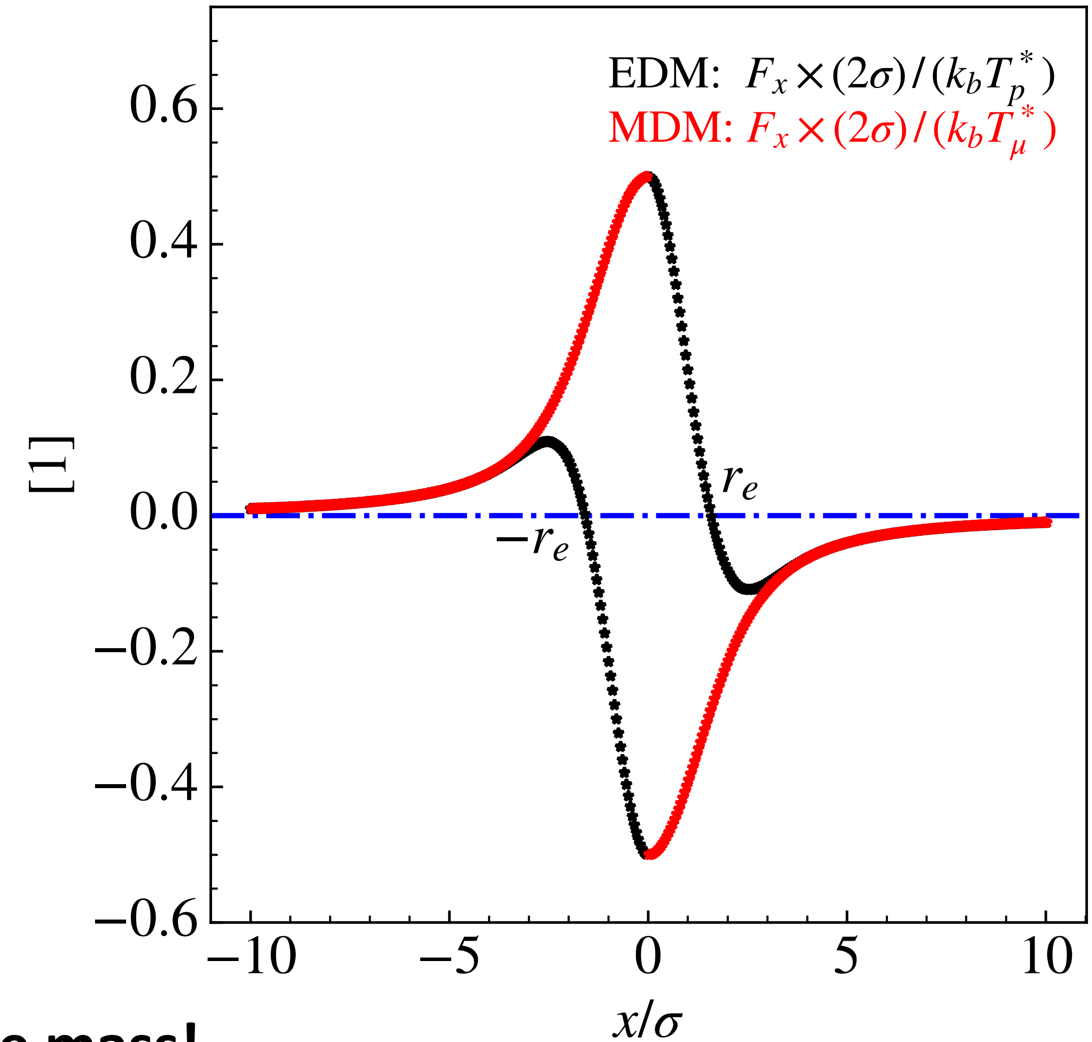
The amount of trapping depends on T/T^*

Trapping temperature and Forces

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

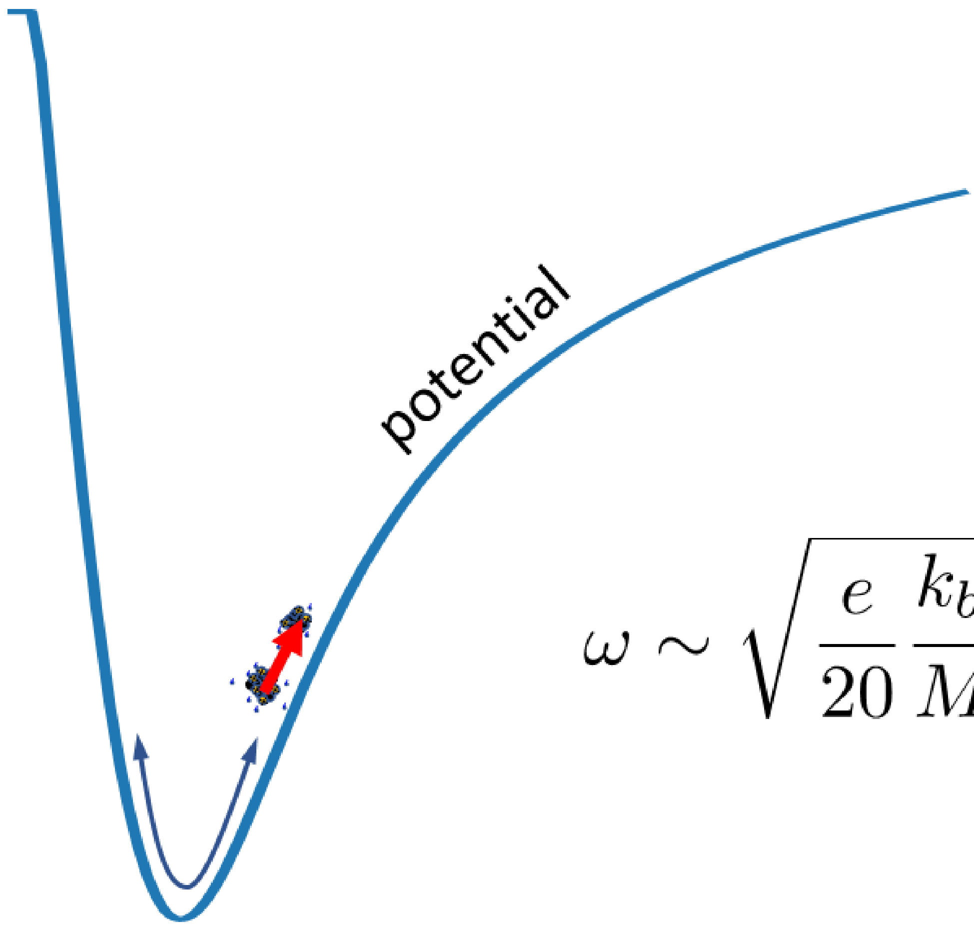
$$T_\mu^* = \frac{1}{\pi \epsilon_0 k_b c} \frac{I}{\sigma} \frac{\mu}{c}$$

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



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

23.04.21

Time scales

Vibrational	Very fast
Oscillation around E-field	$\omega_E = \sqrt{\frac{pE}{I}}$ $\omega_E^2 \simeq \ln\left(\frac{\pi}{2}\right) \frac{k_b}{mL^2} T_p^*$
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

σ = 3 x 10^{-4} m

I = 1 A

E_0 = 9 x 10^4 V/m

B_0 = 3 × 10^{-4} T = 3 Gauss

Bunched beam

σ = 2 × 10^{-4} m

σ_z = 0.076 m

N_b = 1.2 × 10^{11} protons

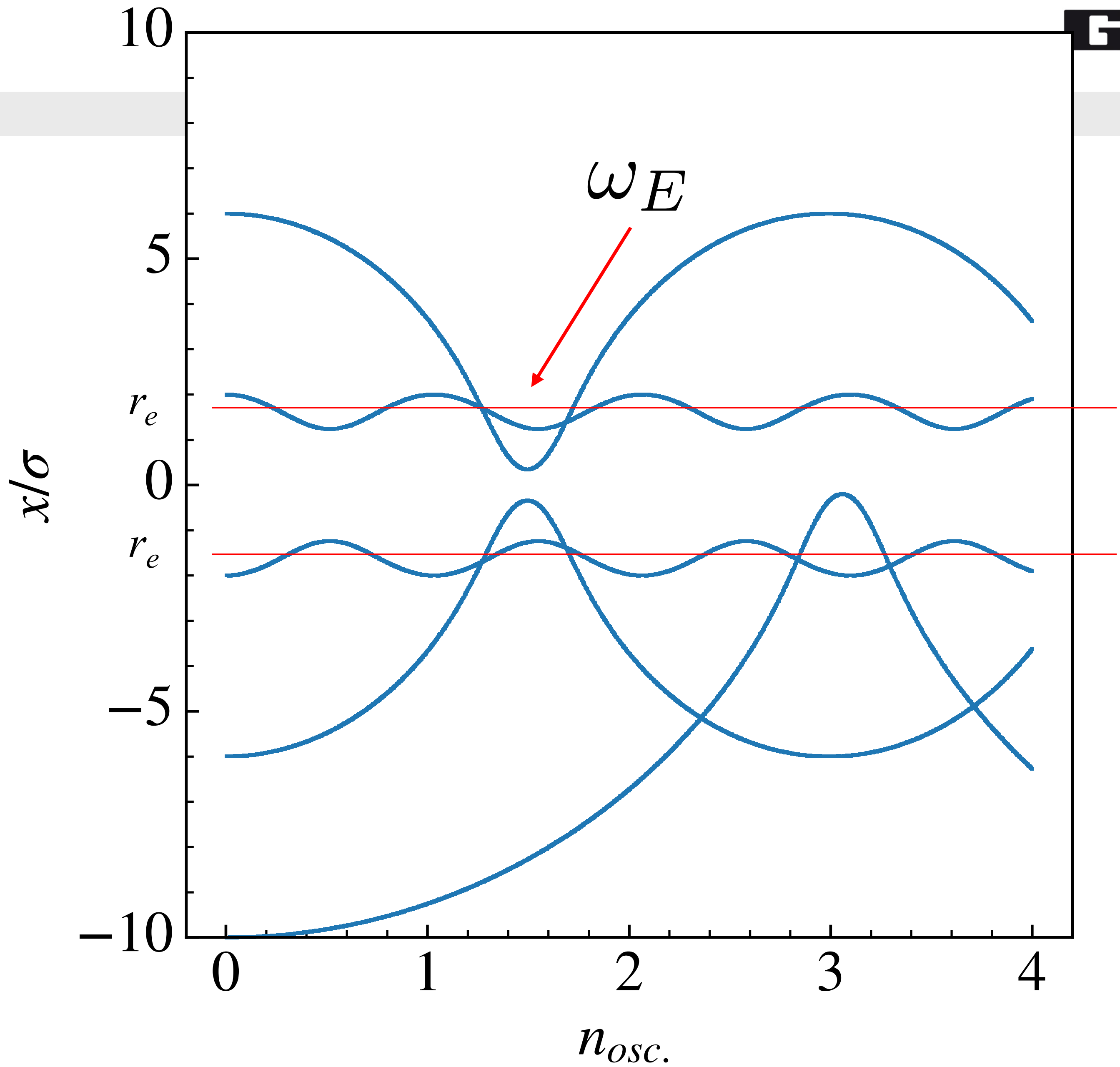
E_0 = 4 × 10^6 V/m

B_0 = 137 × 10^{-4} T = 137 Gauss

Vaccum temperature

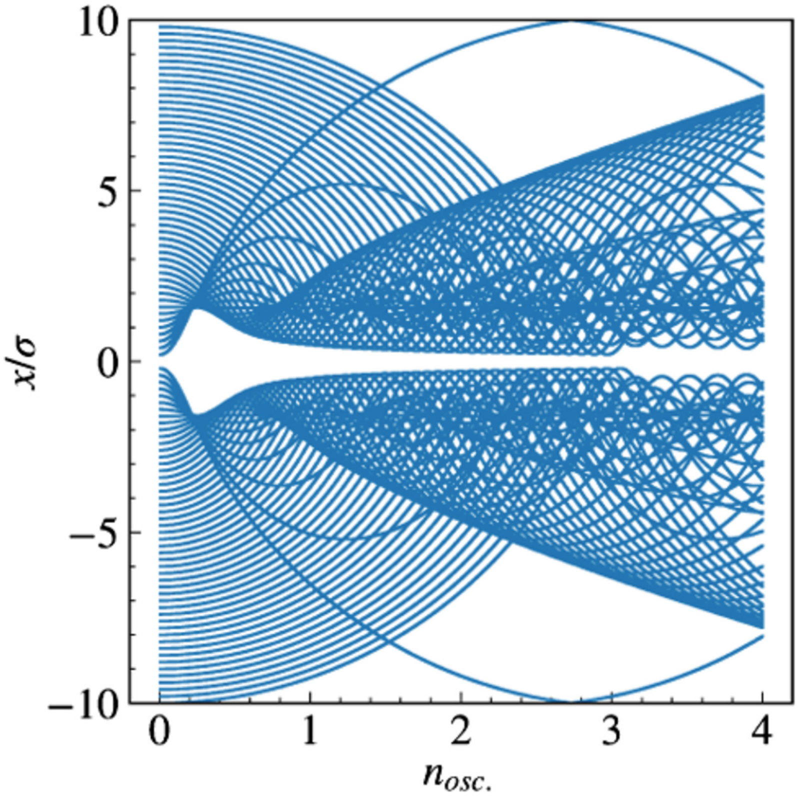
T = 2 K

H_2O	O_2
p = 6.2 x 10^{-30} Cm	μ = 2.8 BM = 2.6 x 10^{-23} J/K
M = 3 x 10^{-26} Kg	M = 5.3 x 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^*_μ = 2.5 mK
ω = 11189 rad/s	
f = 1780 Hz	

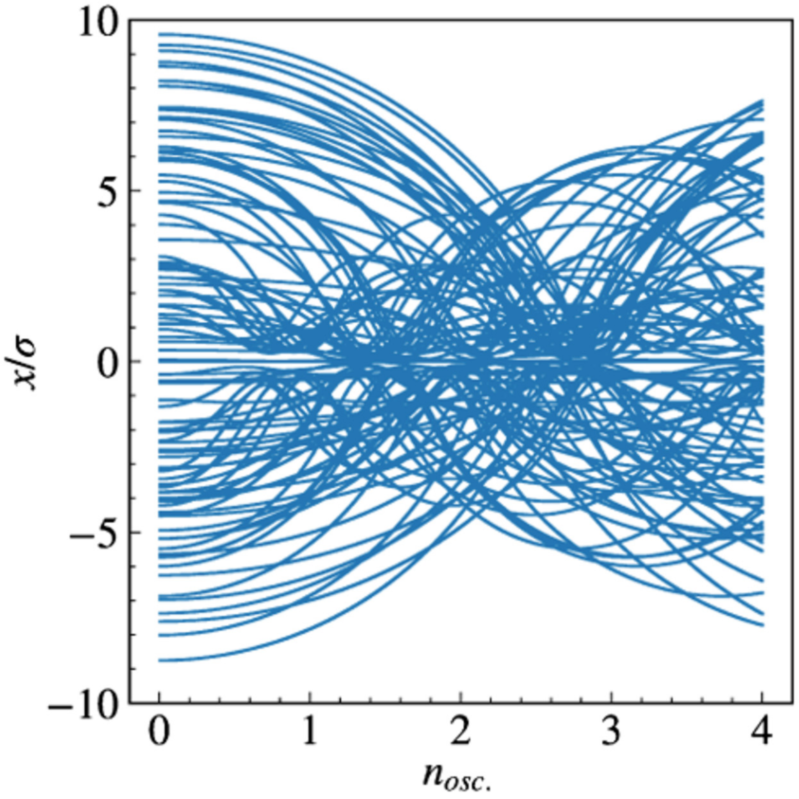


10
5
0
−5
−10
r_e
r_e
x/σ
ω_E
0
1
2
3
4
$n_{osc.}$

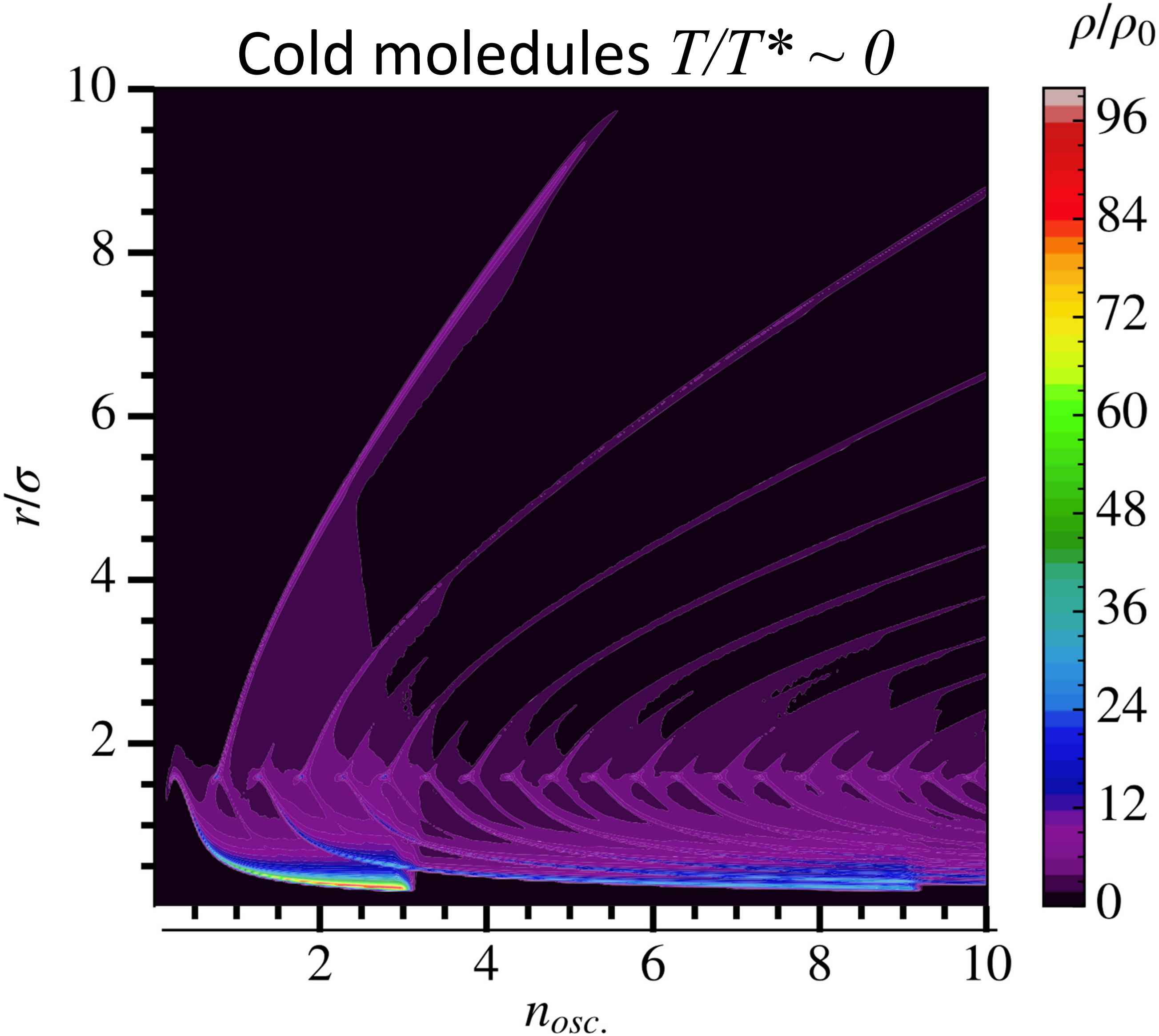
Cold molecules only in x



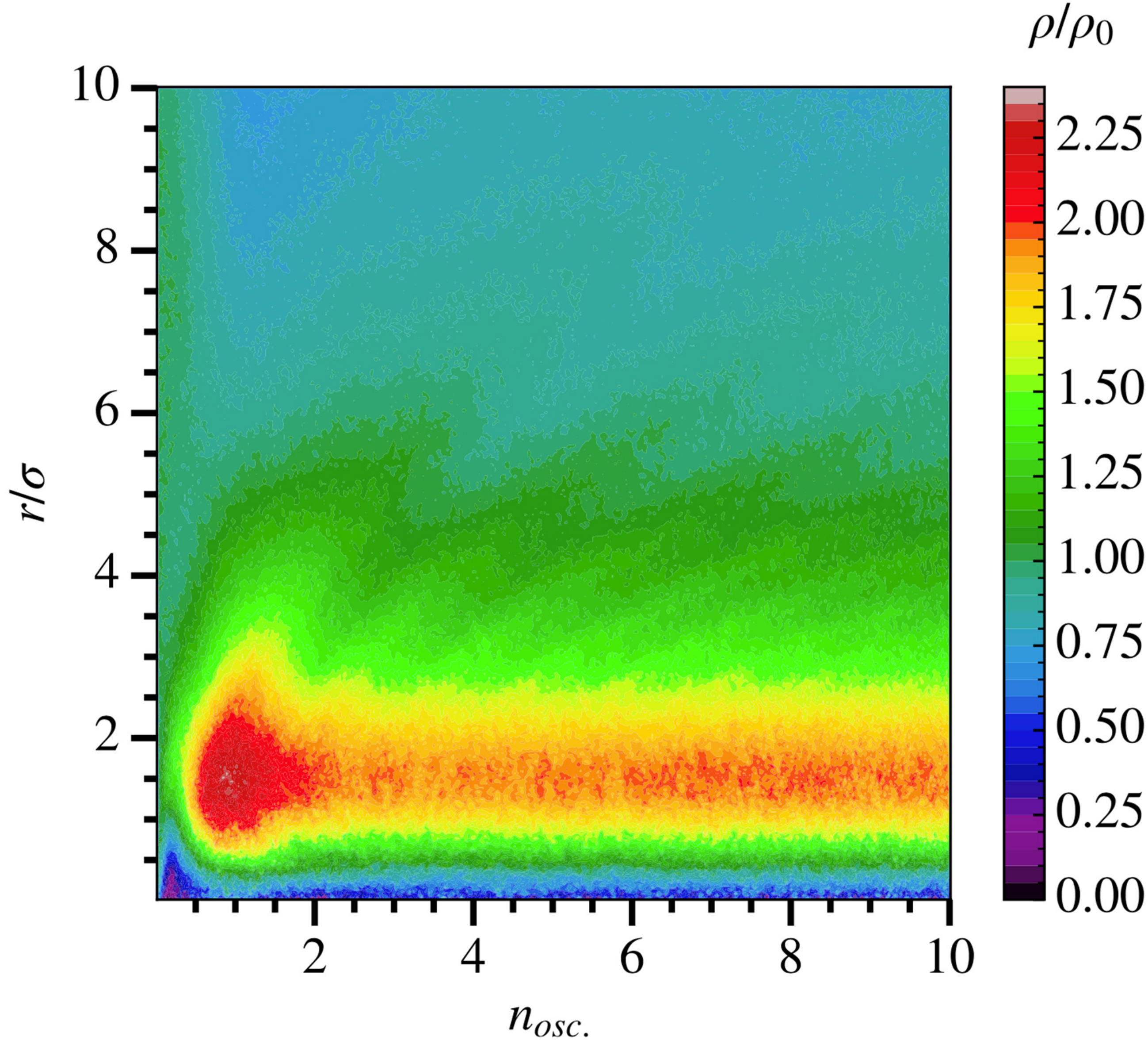
Cold molecules in xy



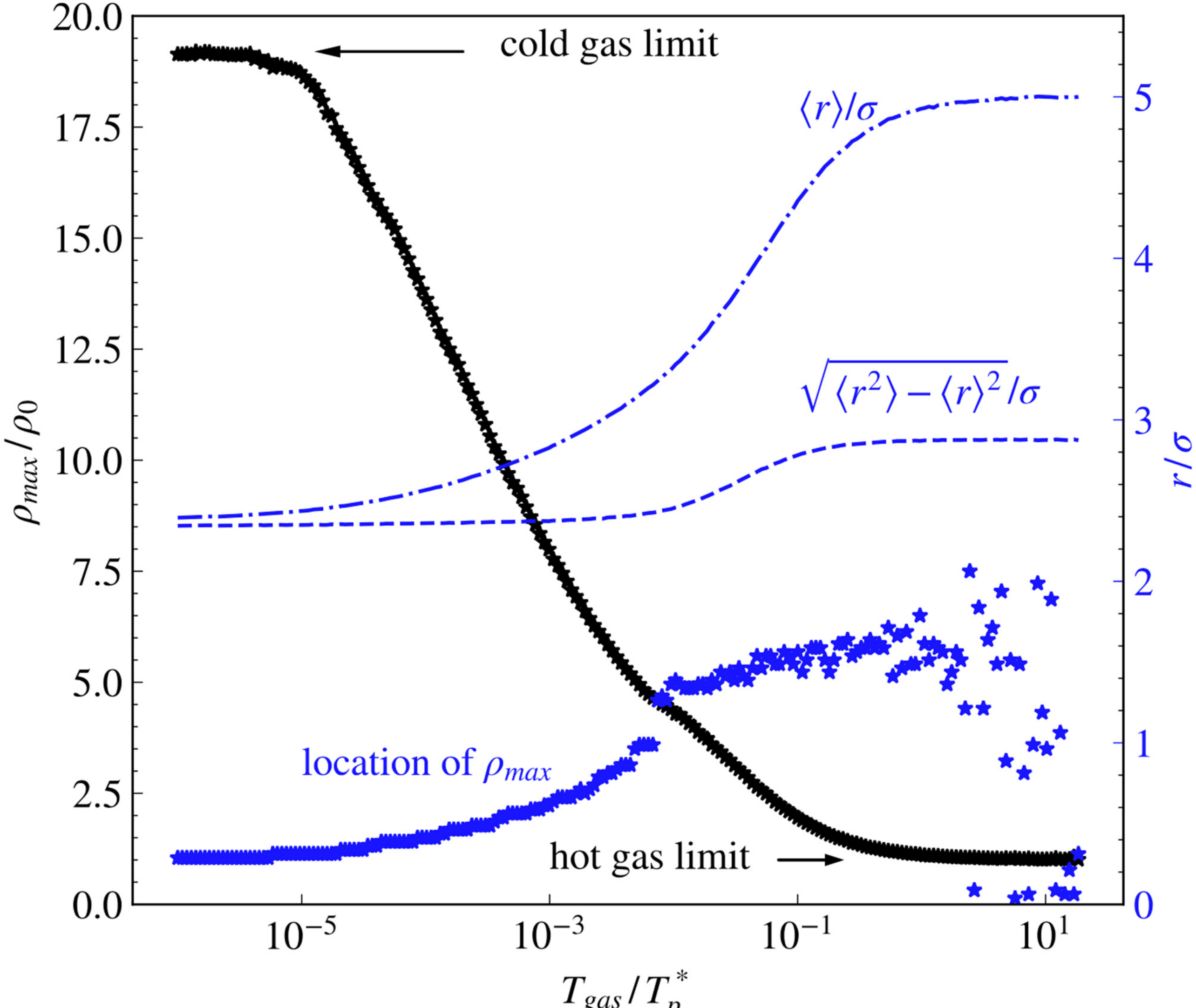
Radial density evolution



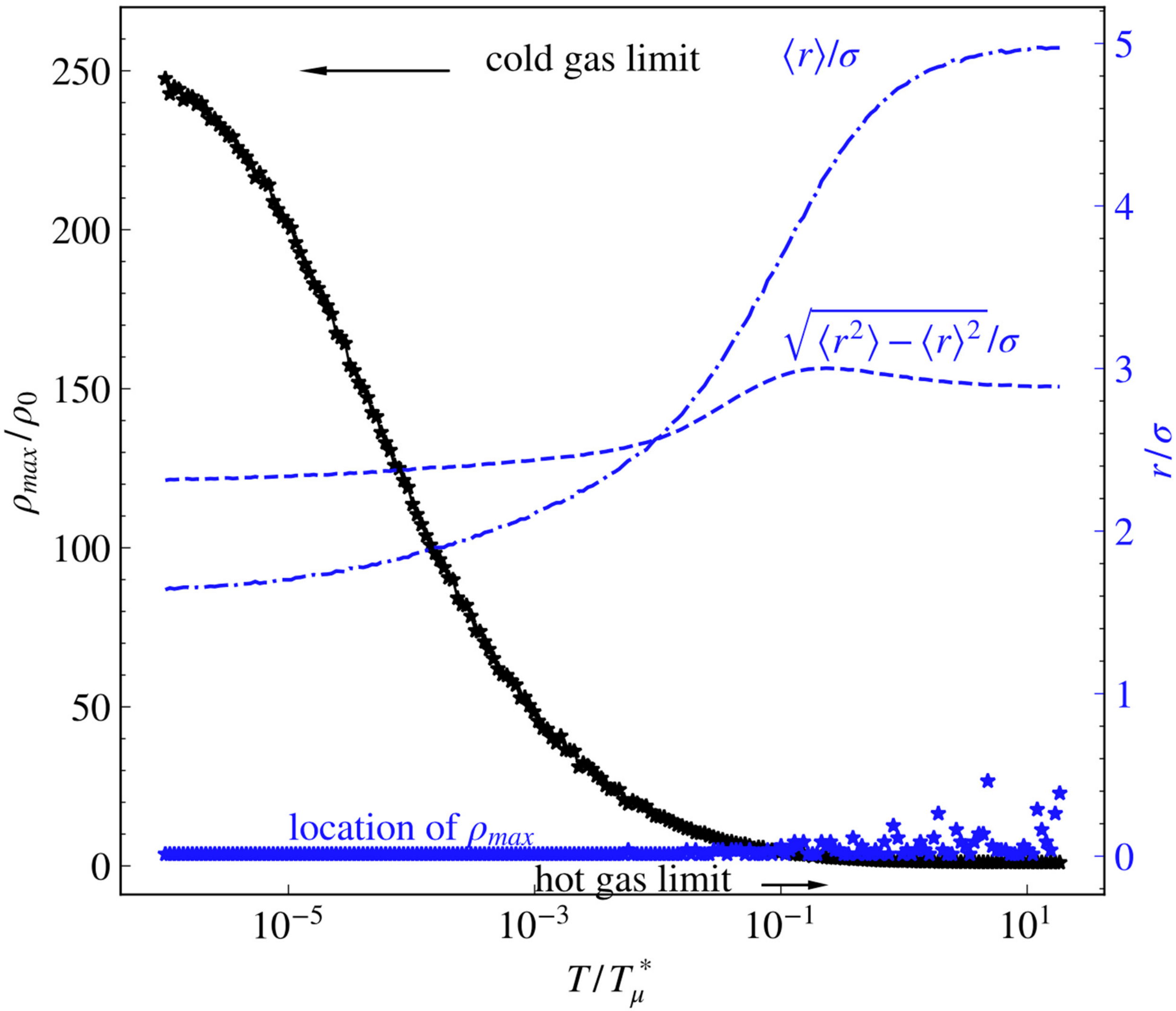
Molecules with $T/T^*_p = 0.1$



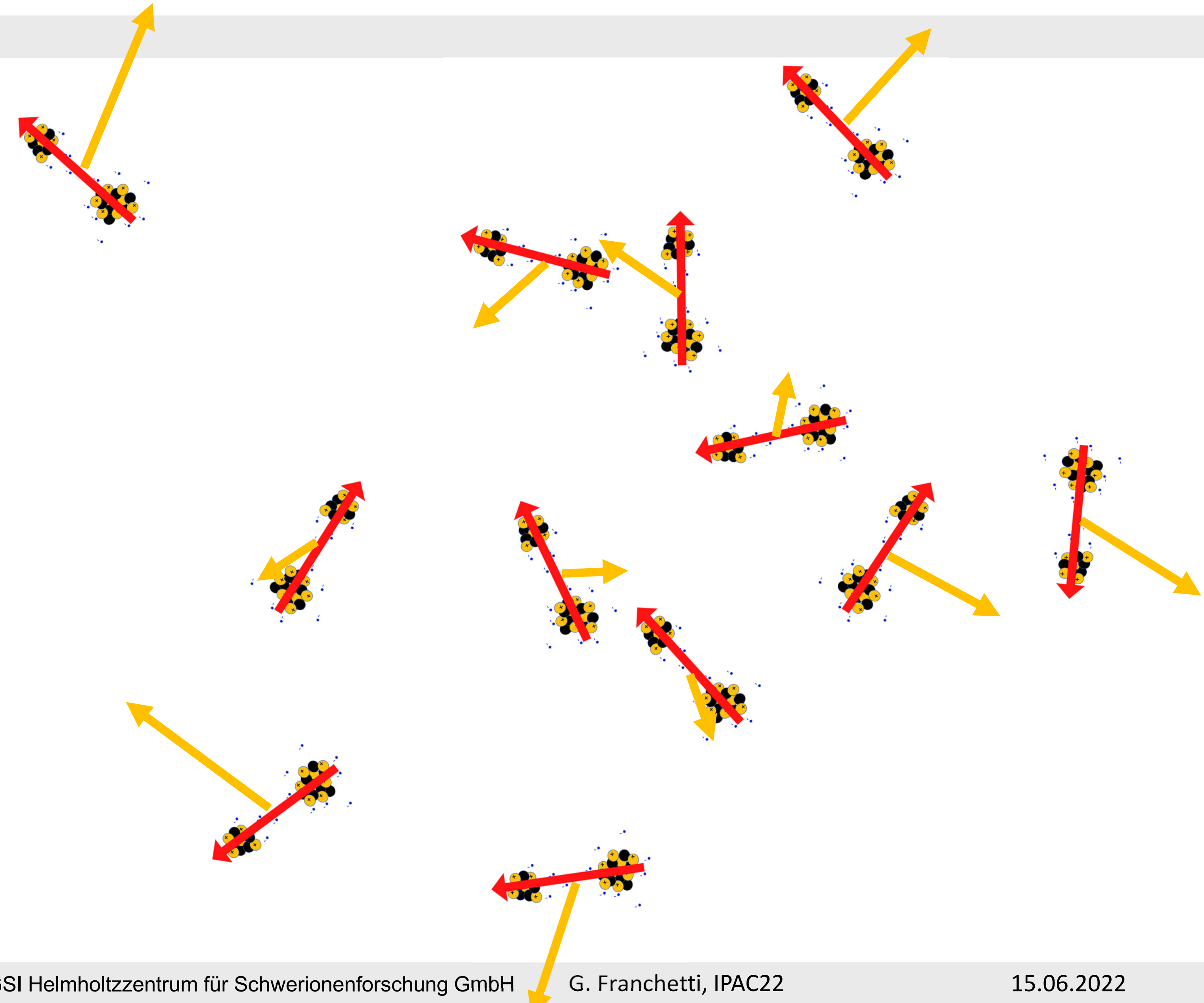
Density enhancement depends critically from T/T^*_p



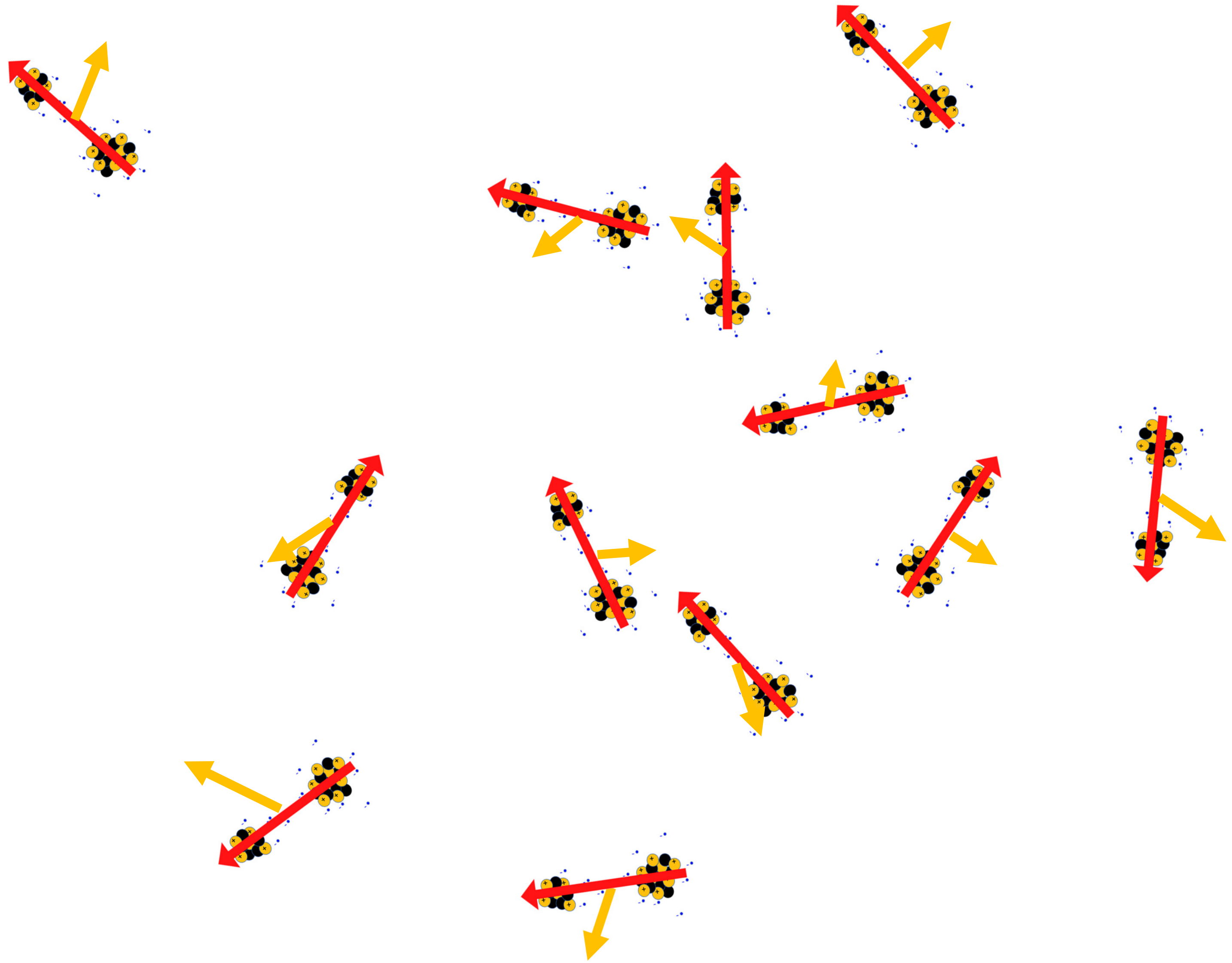
Density enhancement depends critically from T/T^*_μ



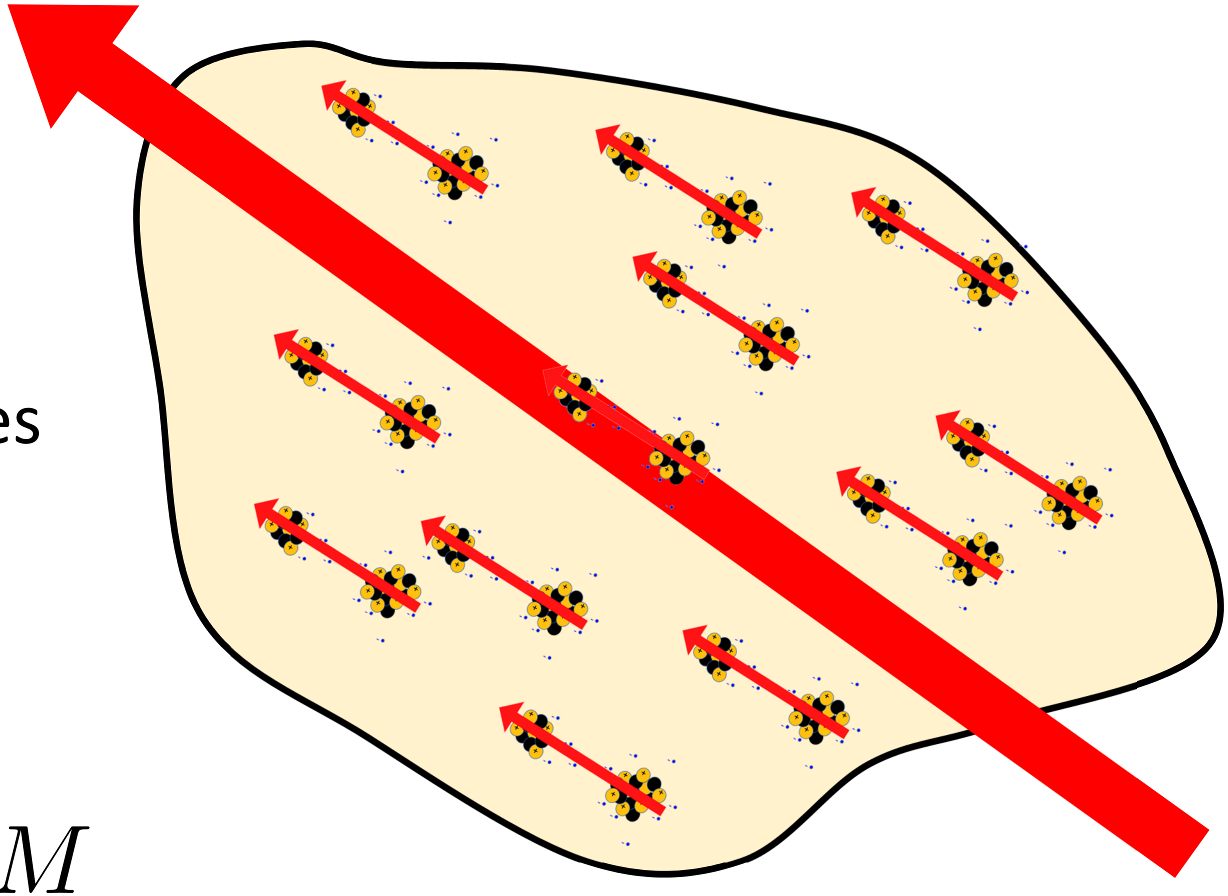
A tantalizing prespective



A tantalizing prespective



Agglomeration or clustering



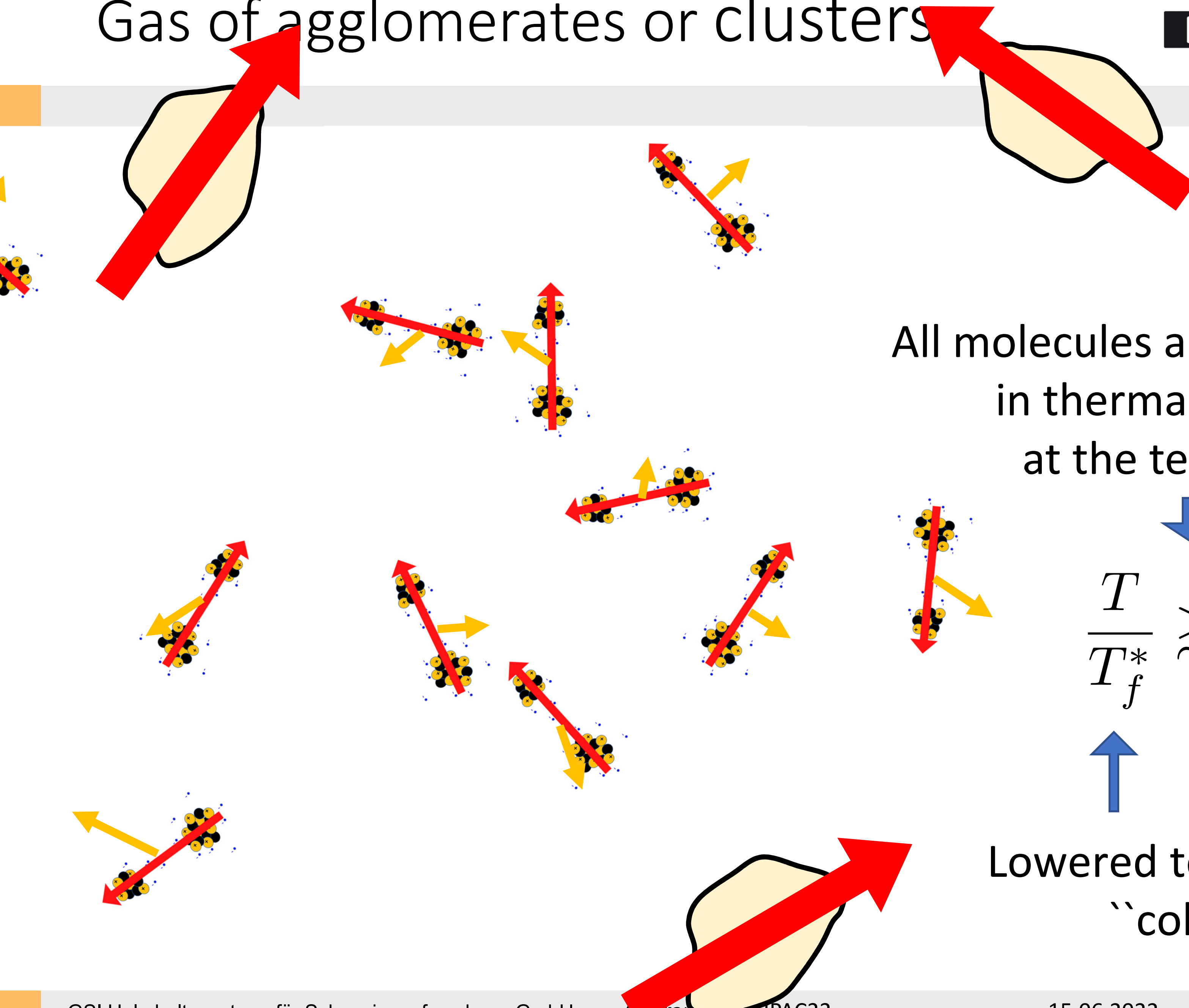
N molecules clusters

$$M_f = NM$$

$$|\vec{p}_f| \leq N|\vec{p}|$$

$$T_f^* \leq T_p^* N$$

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''

Phenomenology ?

- Observations of beam loss and beam instabilities in the 2017 and 2018 LHC runs cannot be explained by the motion of single neutral molecules, which, at a temperature of 5 K, would mostly not be trapped by the field of the beam.

- The trapping of larger neutral flakes, or agglomerates of a large number of polar water or paramagnetic oxygen molecules, is possible.

- **If flakes had been formed in the LHC, this could well have contributed to the magnitude of the observed phenomena.**

- **Flakes formation?** The degraded situation encountered after a beam screen warm-up from about 5 to 80-90 K (“regeneration”) around the LHC location 16L2 was executed in August 2017, since the higher temperature during the warm-up **could** have facilitated the formation of flakes. **Hypothesis open to investigation**.

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^*
- Missing: studies of the effect on multi-bunches → very hard because of small-large system time scale is problematic for simulations
- Density enhancement may be important in cryogenic vacuum systems, high beam currents or small beam sizes → for future generations of accelerators.

Thank you for the attention