Trapping of neutral molecules by the beam electromagnetic field

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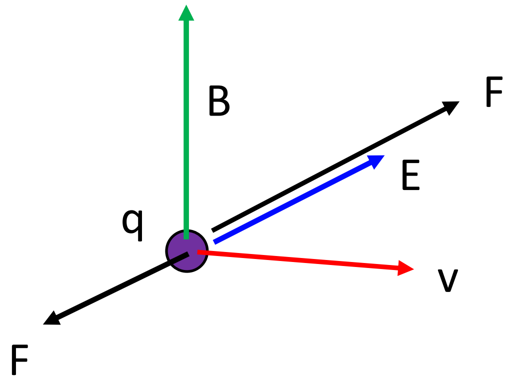
Topics

- Forces and torques on molecules with dipole moments
- Dynamics of molecules - Trapping
- Enhancement of local densities
- Summary
- Outlooks

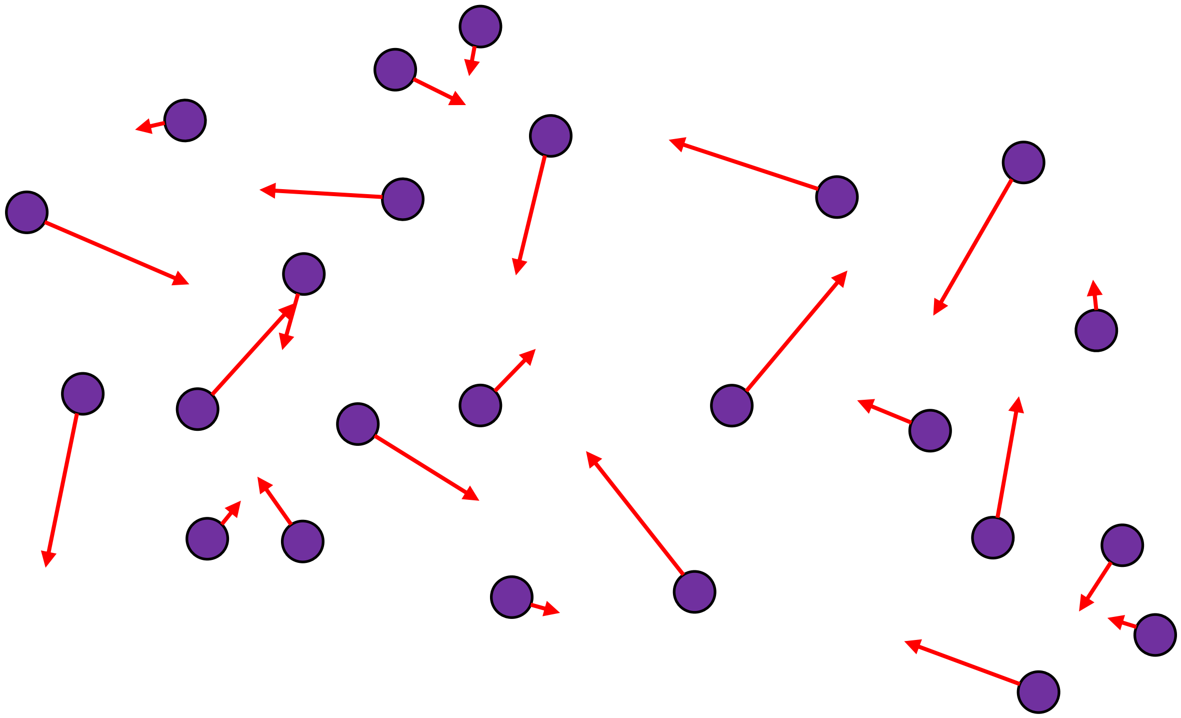
Dynamics of charged particles

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



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

Dynamics of neutral molecules

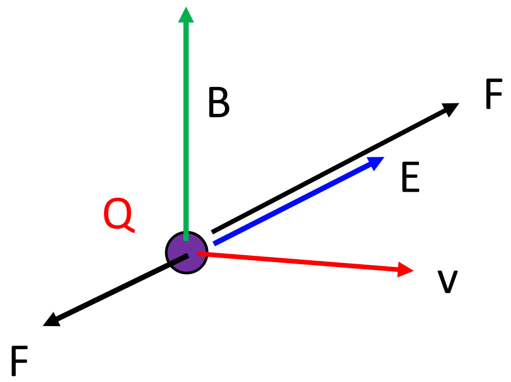


Thermodynamics → Maxwell-Boltzmann velocity distribution → Temperature

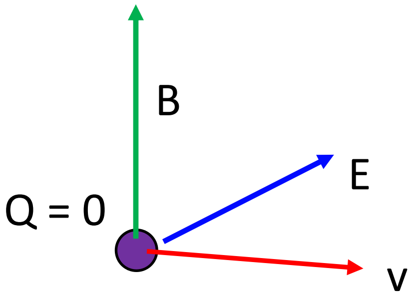
Properties: Collisions, Mean free path, Impingement rate, Pressure

At first sight

Charged molecule/particle

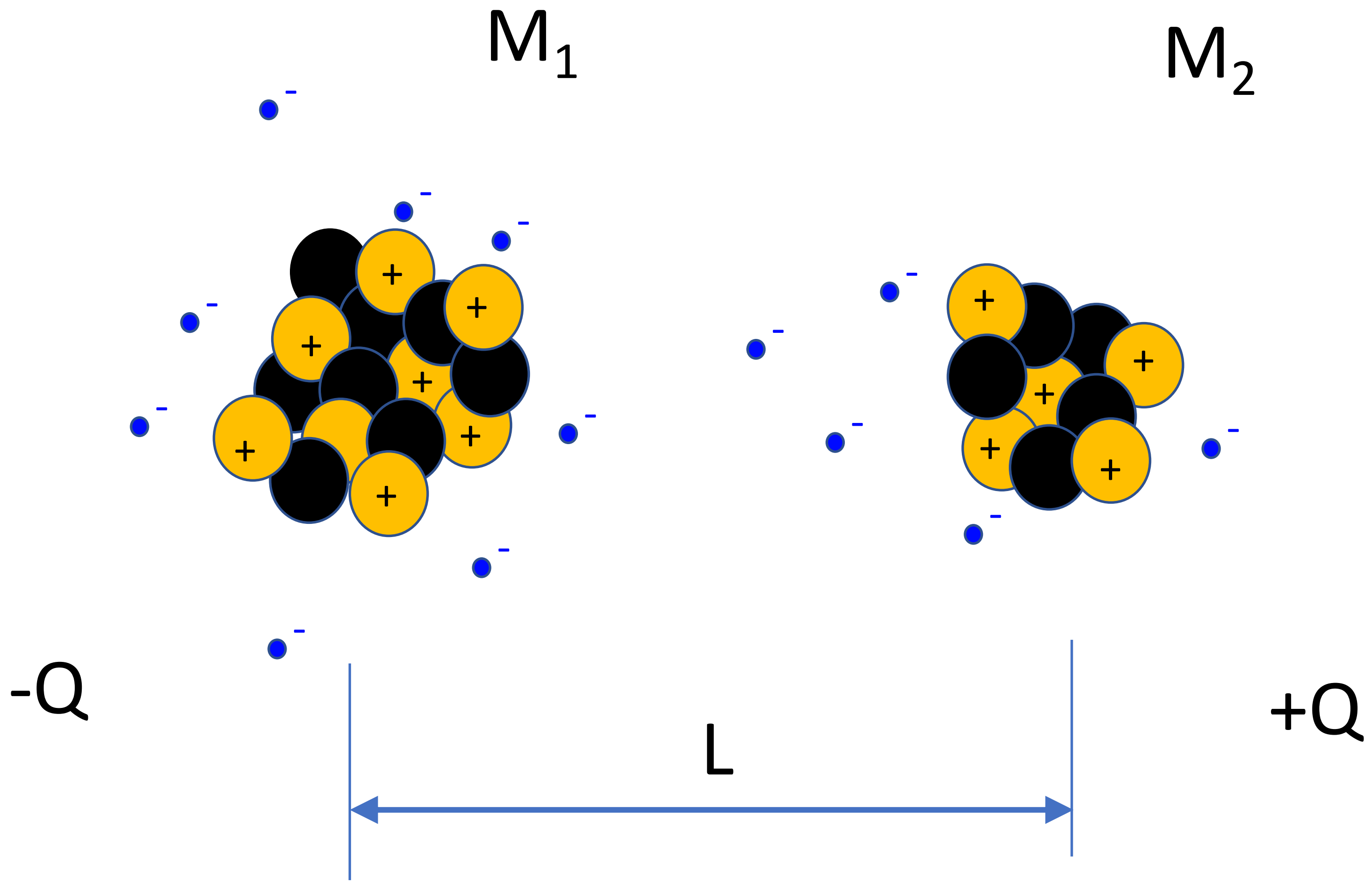


Neutral molecule/particle

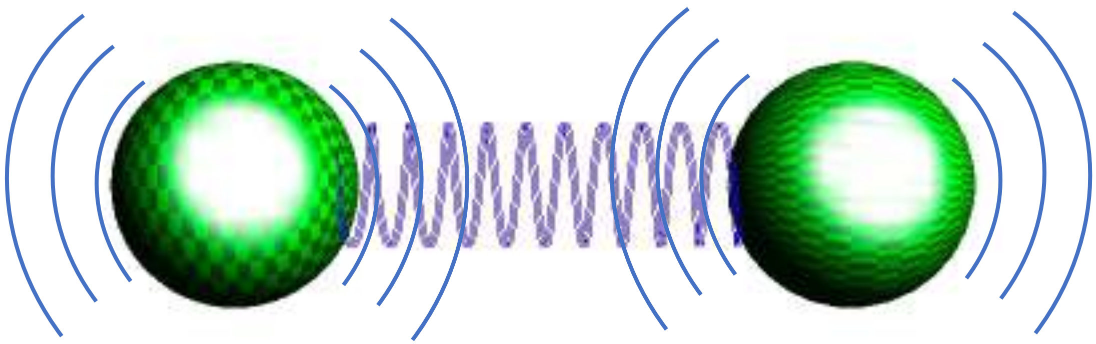


No forces on the molecule/particle

Structure of molecules



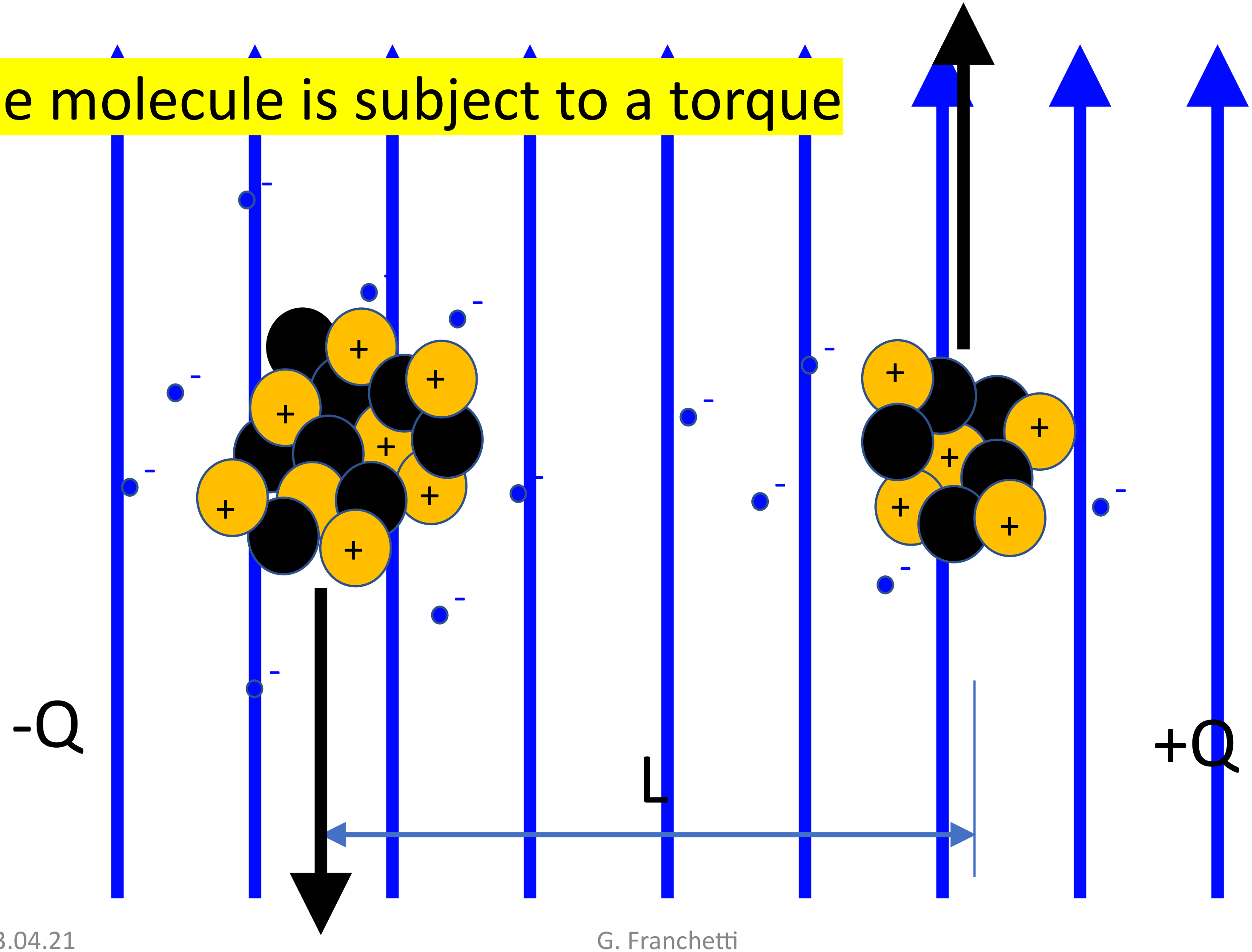
Vibrational state



Characteristic molecular vibrational frequency → very large

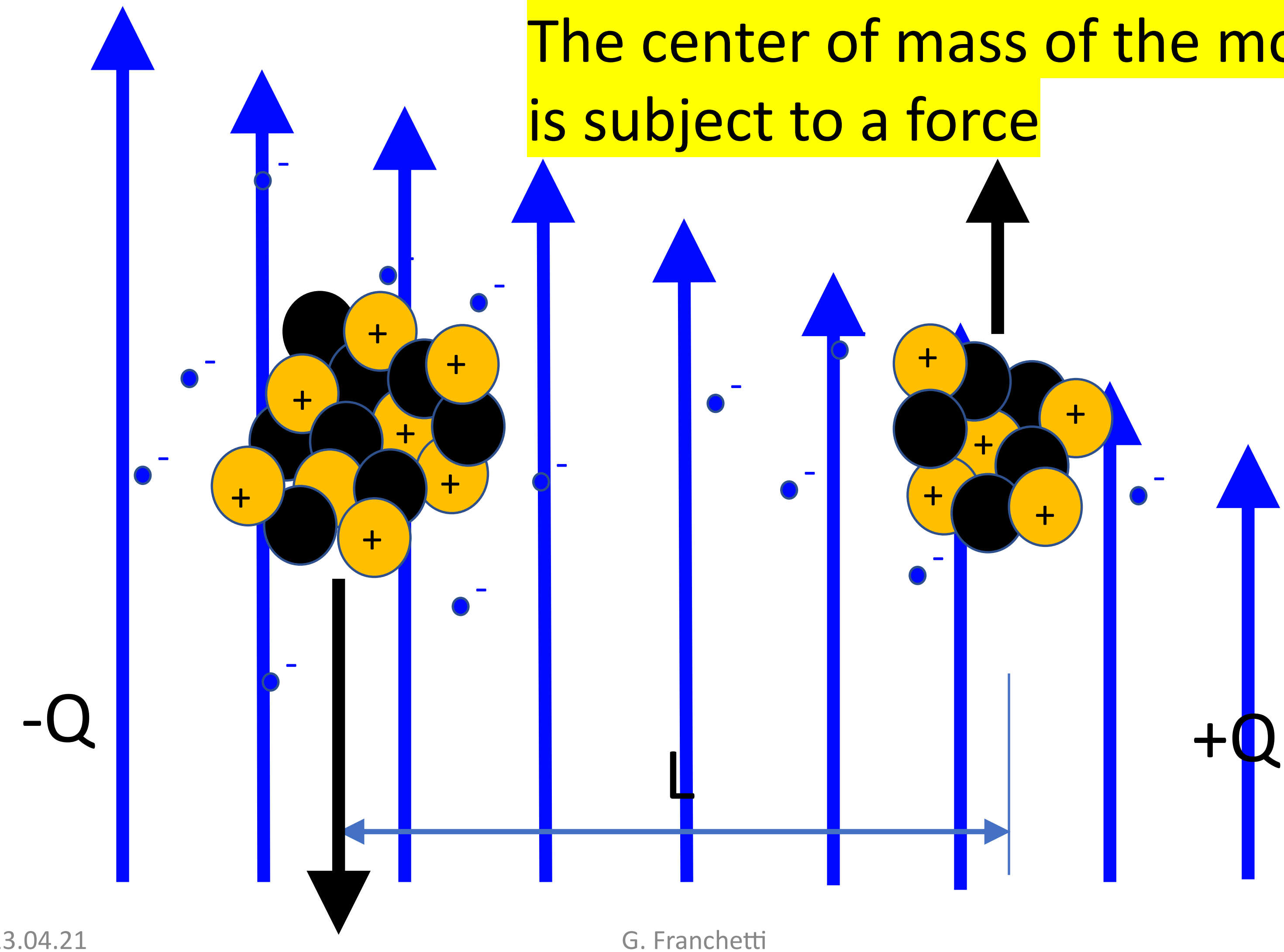
Molecules and electric fields

The molecule is subject to a torque



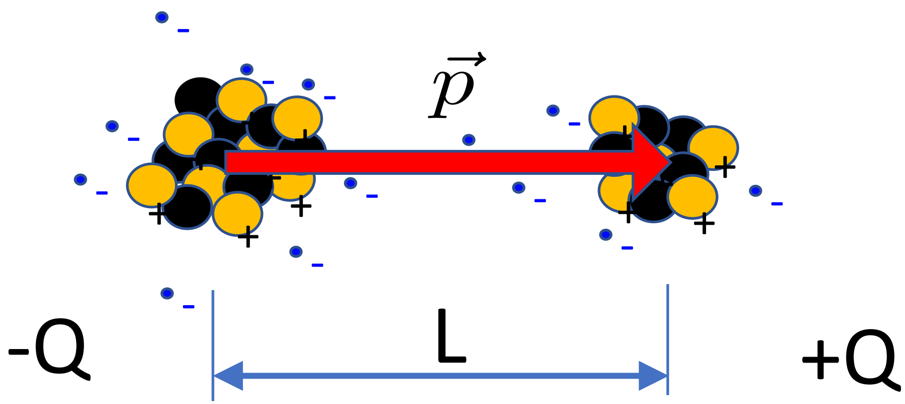
Molecules and electric fields

The center of mass of the molecule is subject to a force



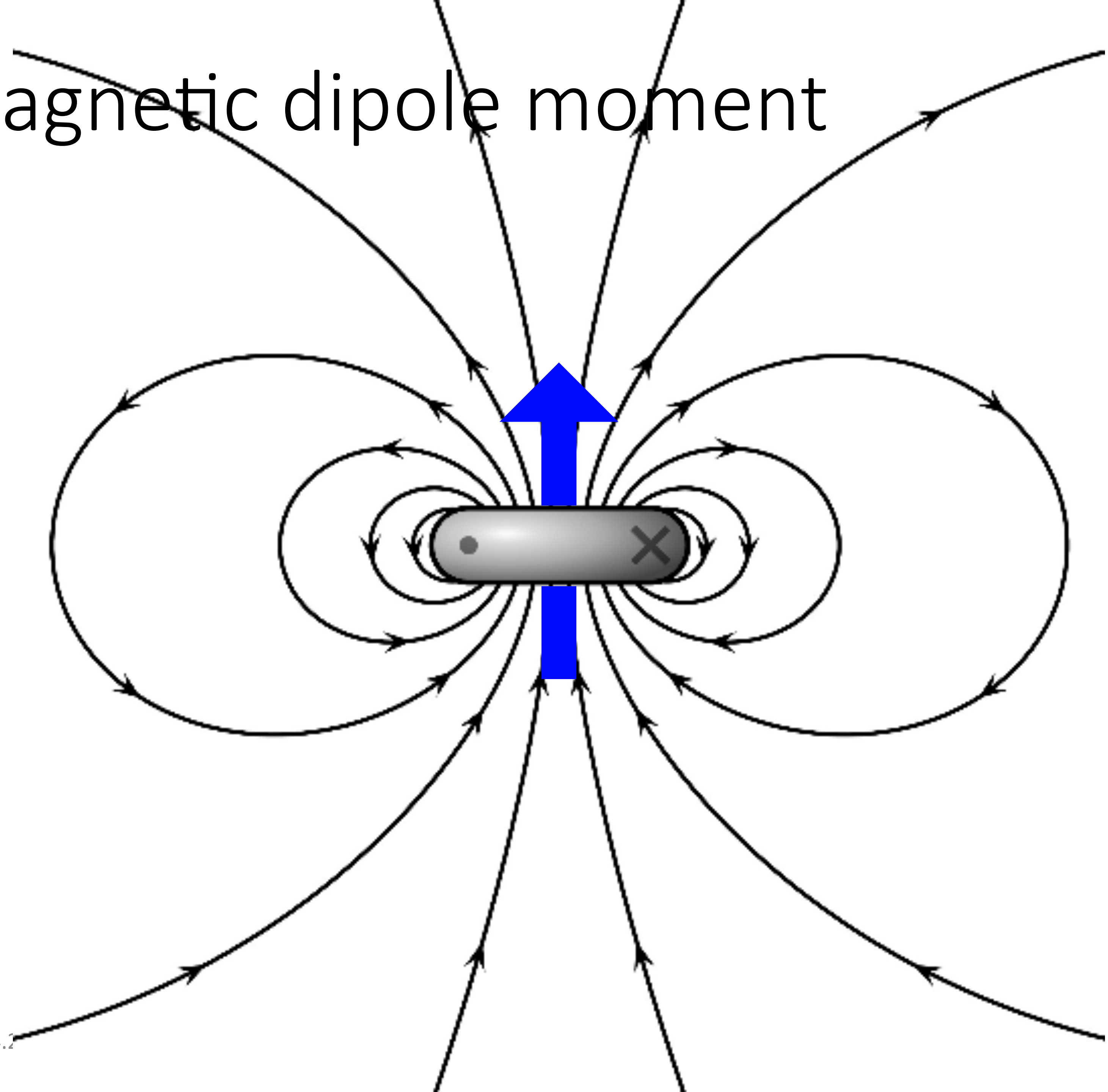
$$
\begin{cases}
\vec{\tau} = \vec{p} \times \vec{E} & \leftarrow \text{Torque} \\
\vec{F}_t = (\vec{p} \cdot \nabla)\vec{E} & \leftarrow \text{Force on the center of mass}
\end{cases}
$$

Electric dipole moment

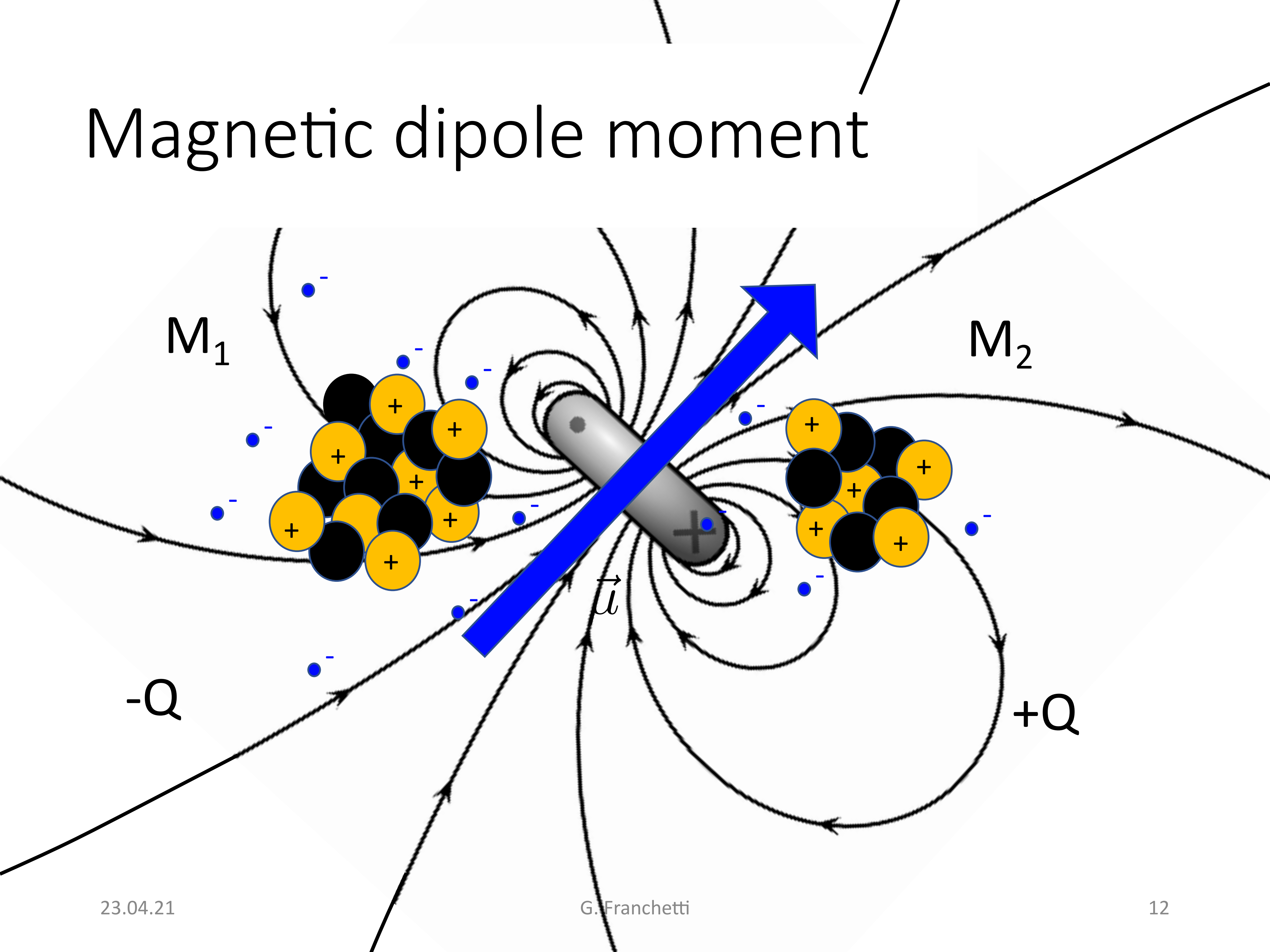


$$\vec{p} = Q\vec{L},$$

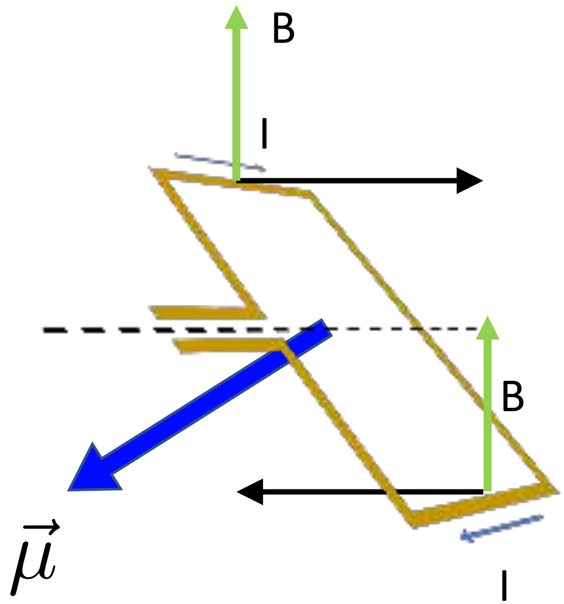
Magnetic dipole moment



Magnetic dipole moment



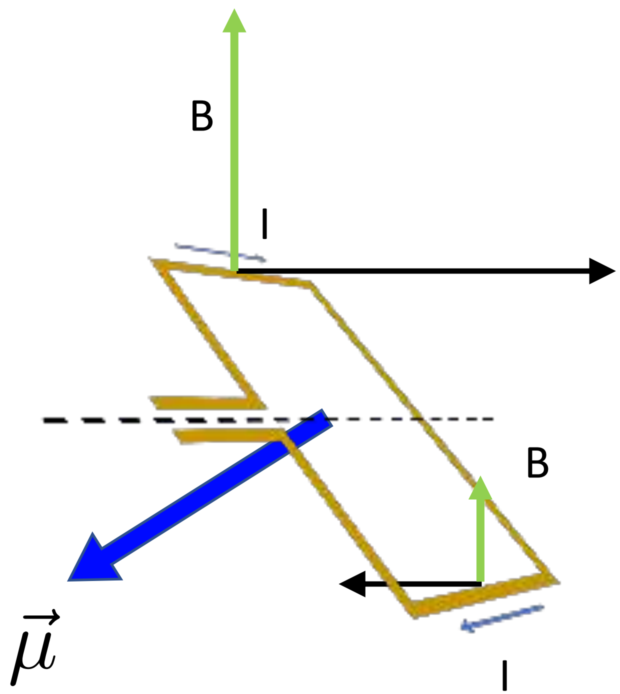
Dipole moment and magnetic fields



Torque

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

Dipole moment and magnetic fields



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

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

Dynamics of neutral molecules

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

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

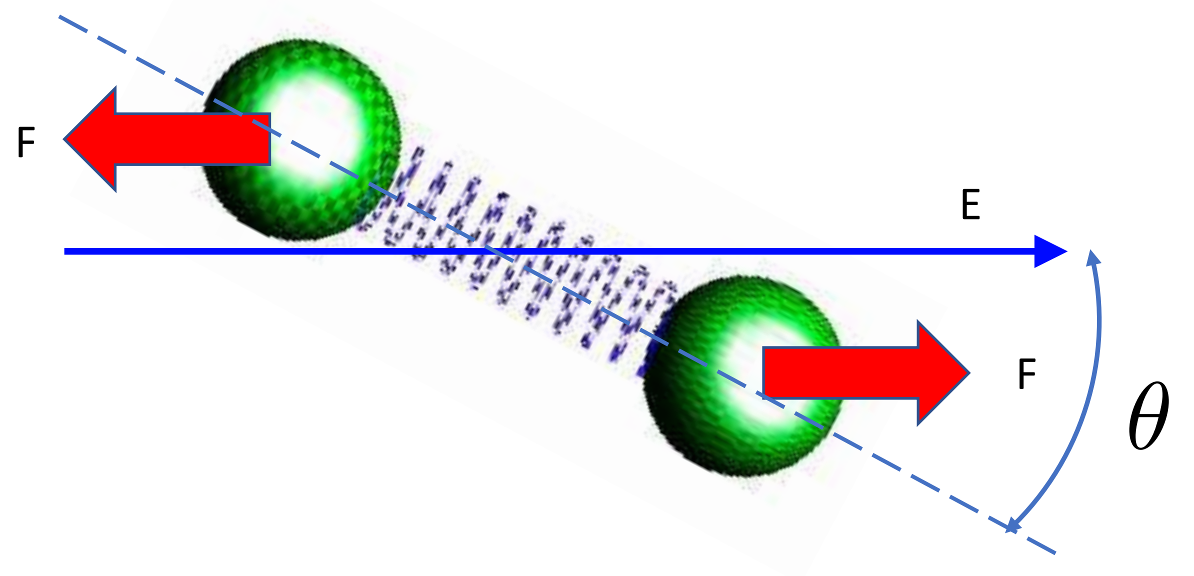
Molecules of interest

Molecule	EDM [D]	MDM [BM]	*M* [amu]
H_2O	0.39	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 and 1 Å = 0.1 nm

[BM] = Bohr magneton, its value is 9.27 × 10E−24 J/T

Dipole alignment and intrinsic time scale

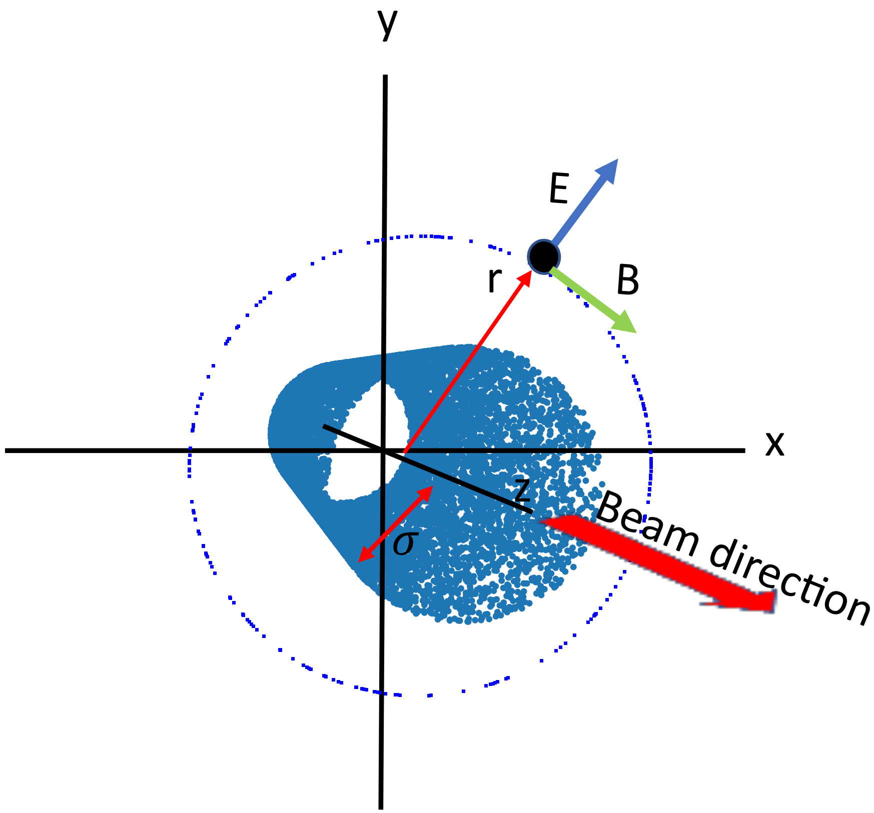


The dipole tends to align to the field, and has a fast frequency of oscillation

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

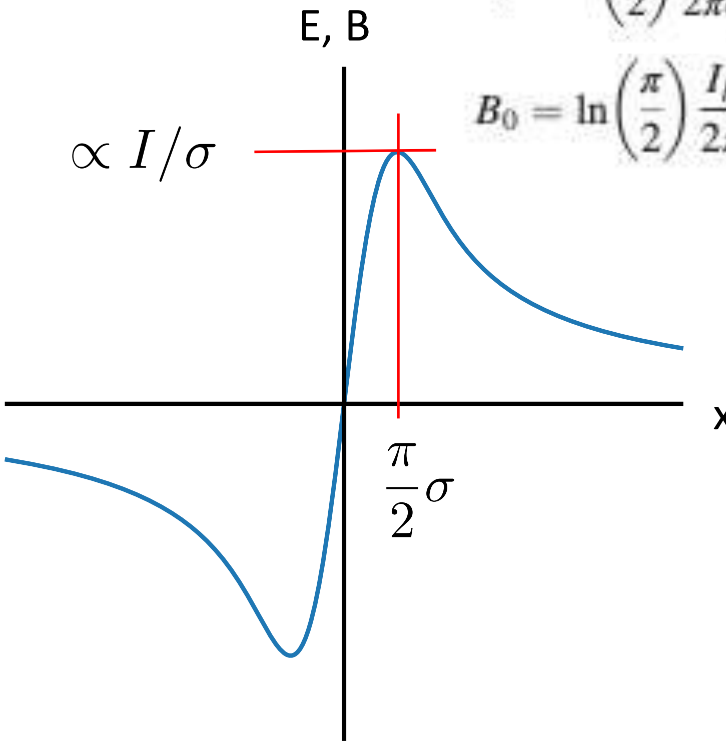
Assumption: the dipole as aligned to the local field

Electromagnetic beam field



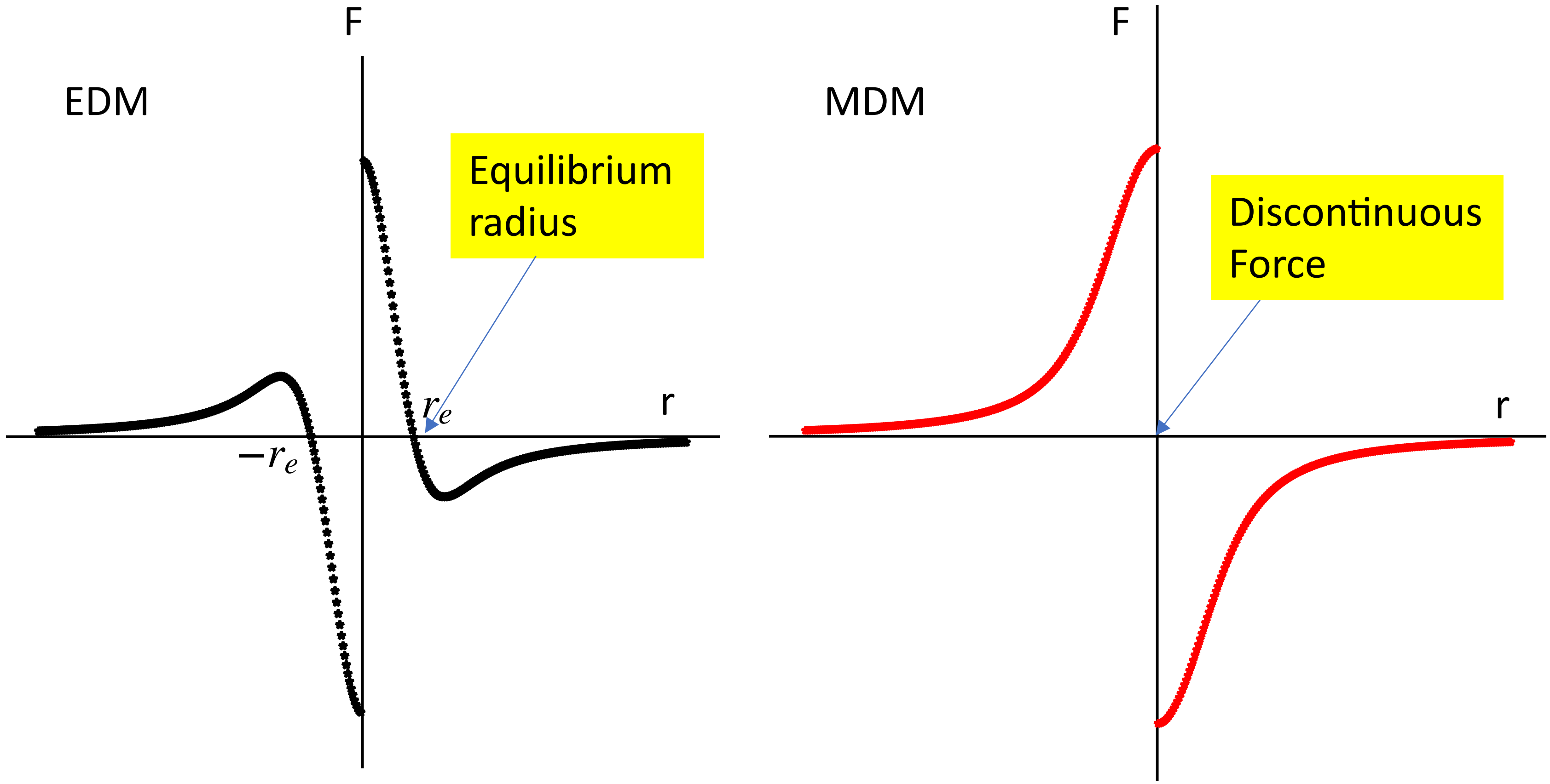
$$E_0 = \ln\left(\frac{\pi}{2}\right)\frac{I}{2\pi\epsilon_0 c\sigma}$$

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

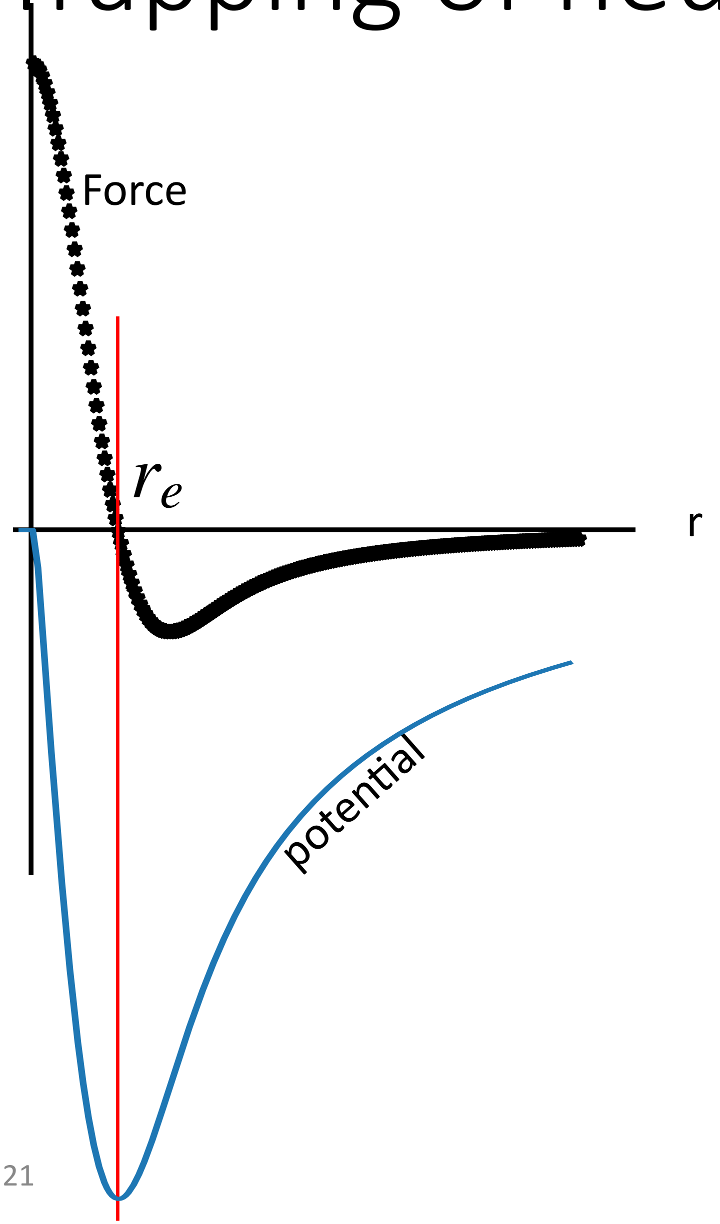


For LHC
- $E_0 \approx 4 \times 10^6$ V/m
- $B_0 = 137 \times 10^{-4}$ T = 137 Gauss

For molecules with dipole alignment the force on the center of mass is the following



Trapping of neutral molecules



This force produces a potential Well

Molecules Trapping

Kinetic energy of molecules small enough to remain inside the potential Well

Initial kinetic energy → Temperature

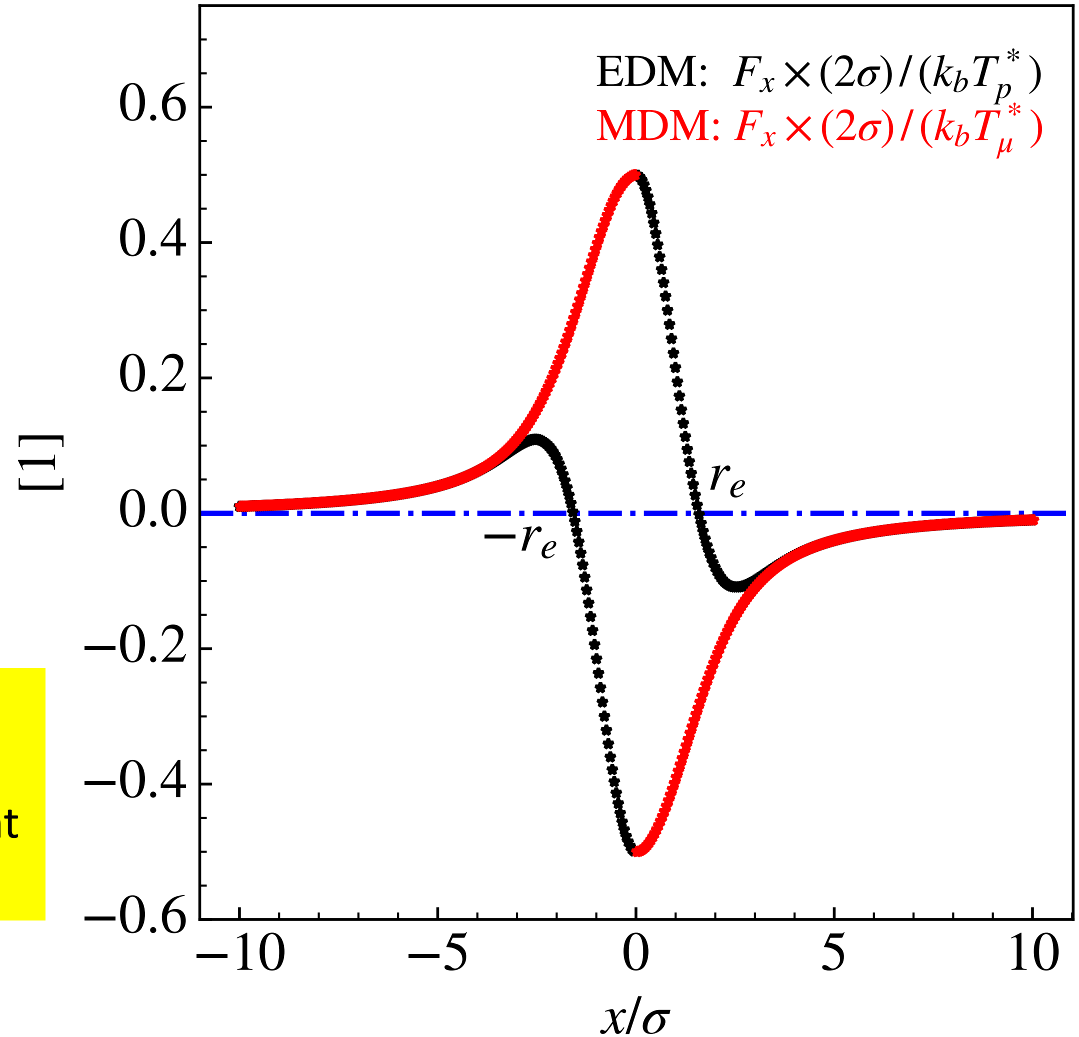
Potential Well → Trapping temperature T^*

Trapping temperature and Forces

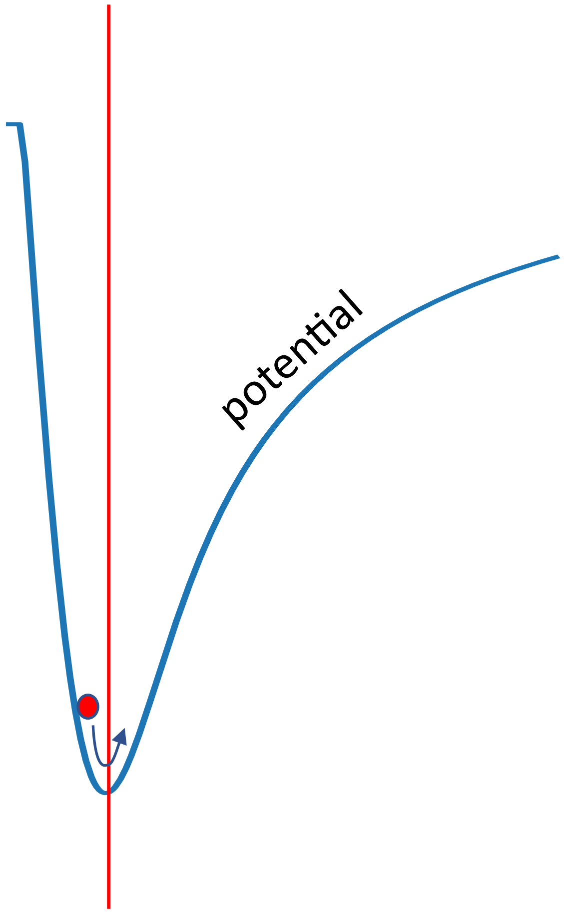
$$T_p^* = \frac{1}{\pi\epsilon_0 k_b c}\frac{I}{\sigma}p$$

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

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



Oscillations around the equilibrium radius

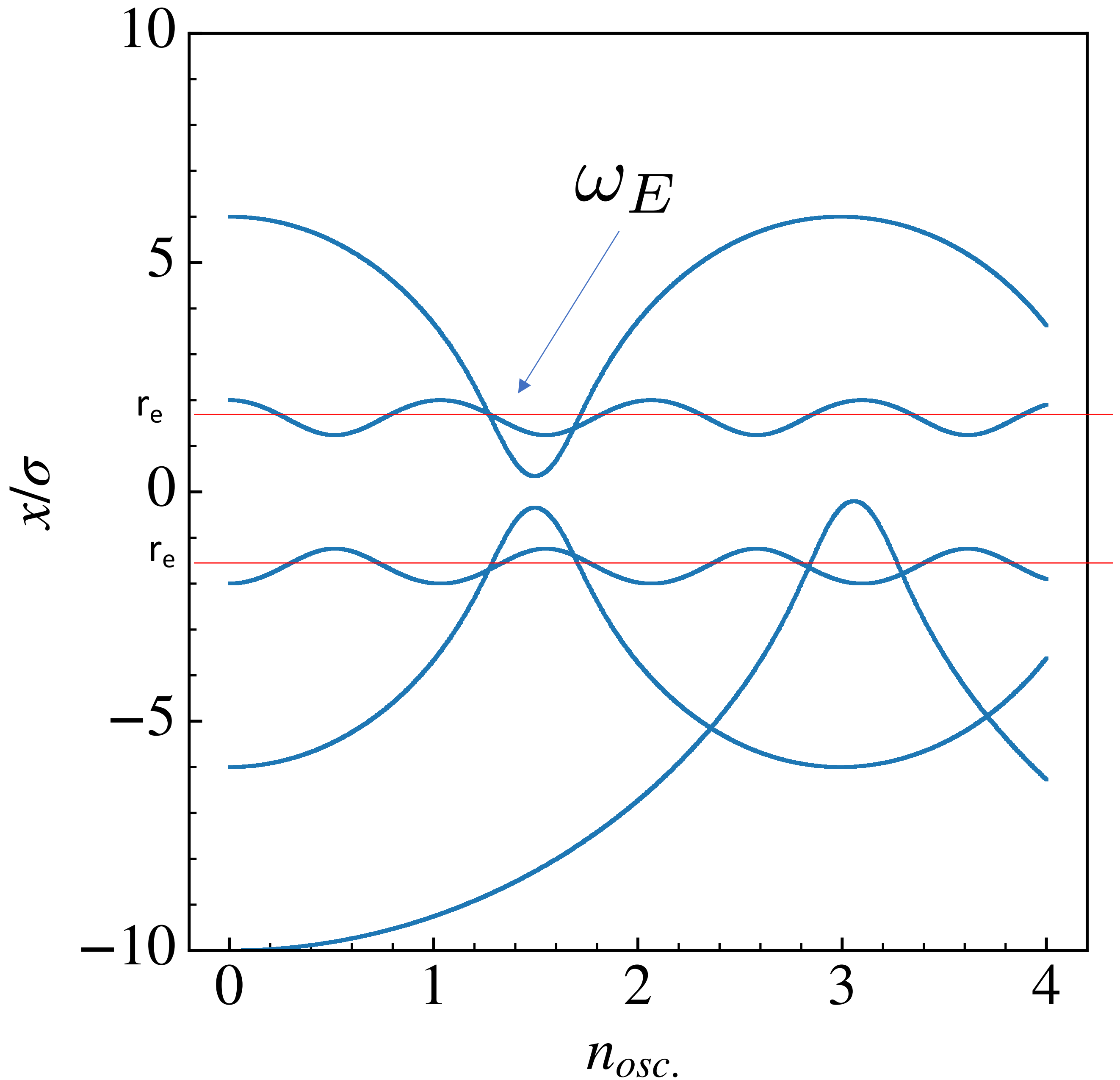


$$\omega \sim \sqrt{\frac{e}{20}\,\frac{k_b T_p^*}{M\sigma^2}}$$

Time scales

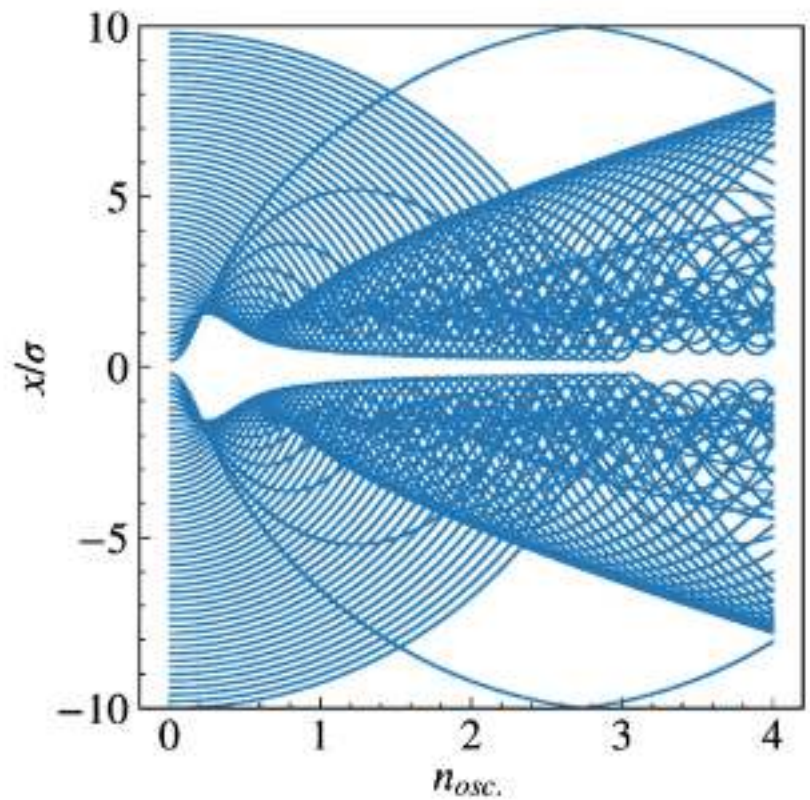
Vibrational	Very fast
Oscillation around field	$\omega_E = \sqrt{\frac{pE}{I}}$ $\omega_E^2 \simeq \ln\left(\frac{\pi}{2}\right)\frac{k_b}{mL^2}T_p^*$
Oscillation around equilibrium radius	$\omega \sim \sqrt{\frac{e}{20}\frac{k_b T_p^*}{M\sigma^2}}$

For a water molecule, H_2O, characterized by $M = 3 \times 10^{-26}$ kg and $p =$ 6.2 x 10^{-30} C m, and a beam with $\sigma = 3 \times 10^{-4}$ m and $I = 1$ A, we find $\omega = 11189$ rad/s. Hence, in this case, the frequency of oscillation around the equilibrium radius r_e is $f = \omega/(2\pi) = 1780$ Hz, which, for the LHC, is of the order of the fractional betatron frequency.

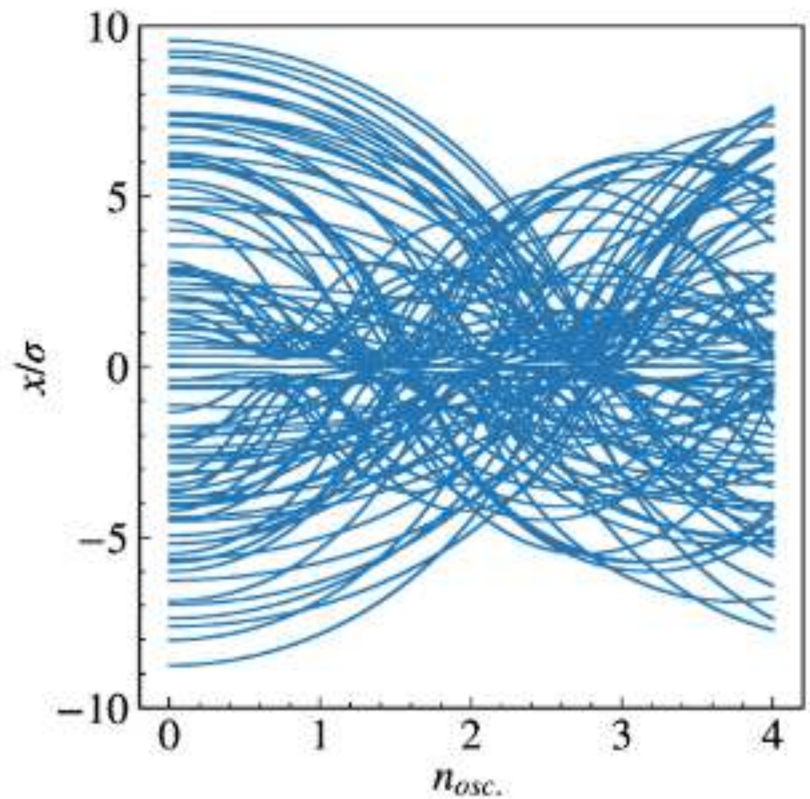


10
5
0
−5
−10
ω_E
r_e
r_e
x/σ
0
1
2
3
4
$n_{osc.}$

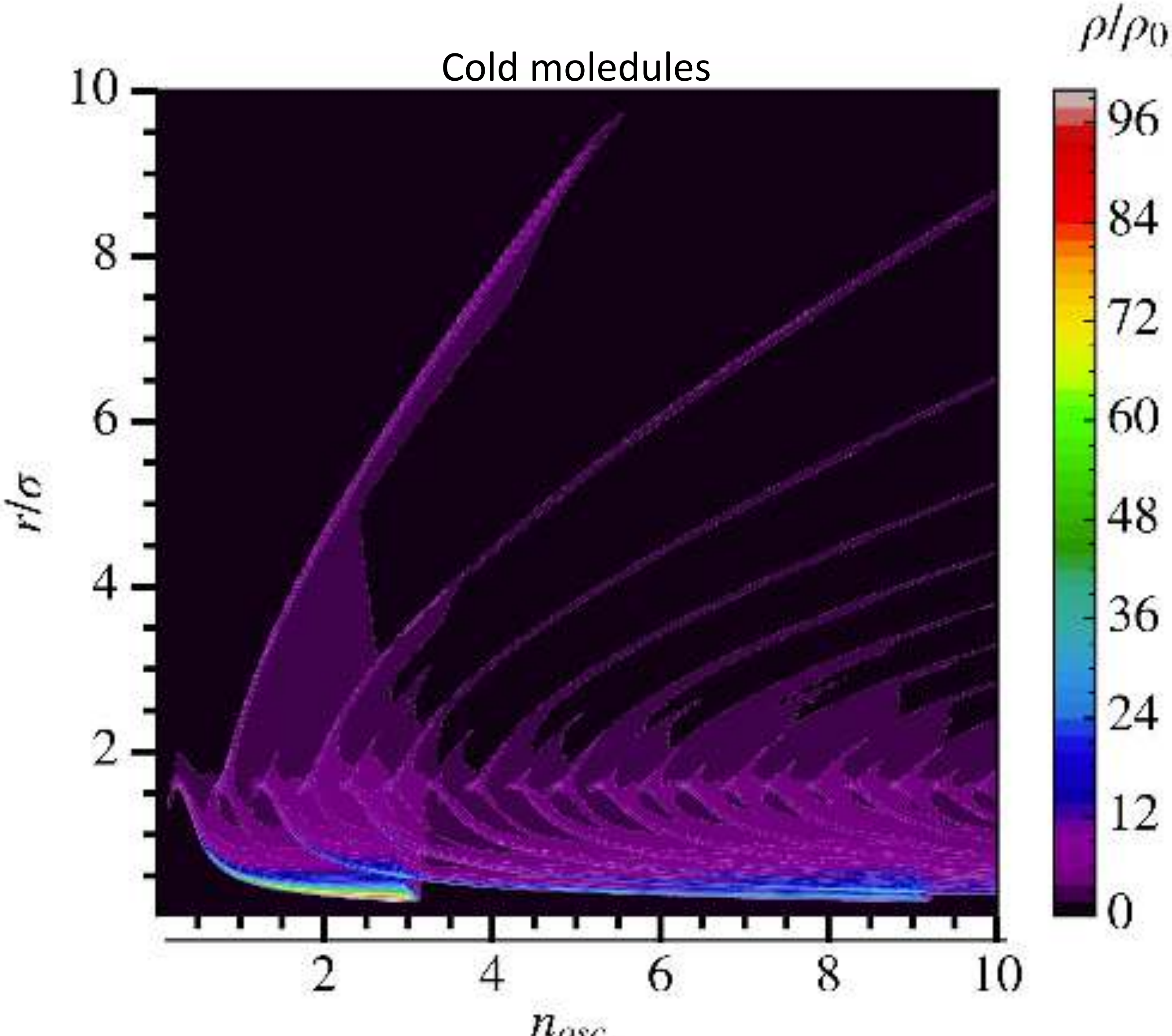
Cold molecules only in x



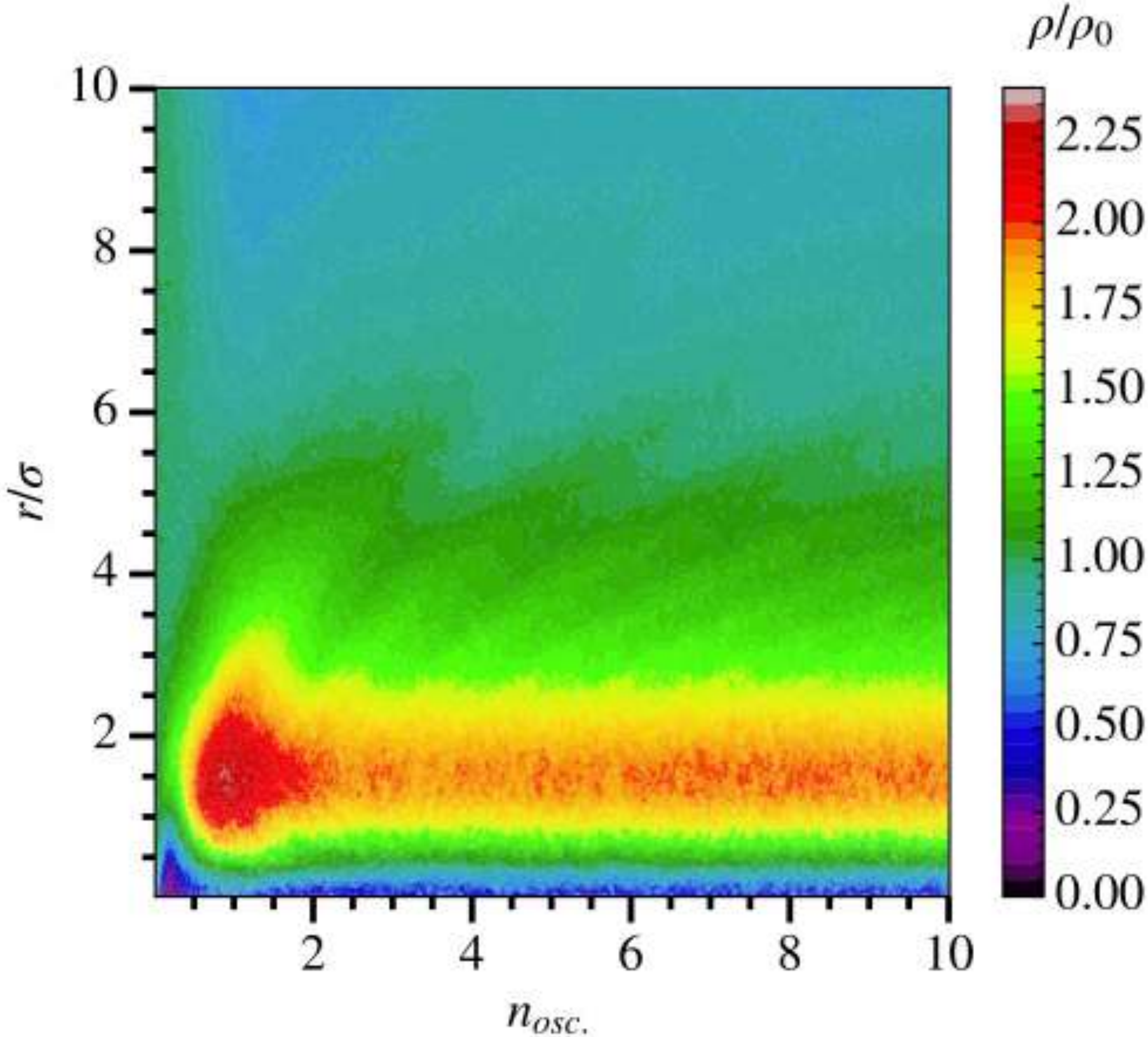
Cold molecules only in xy



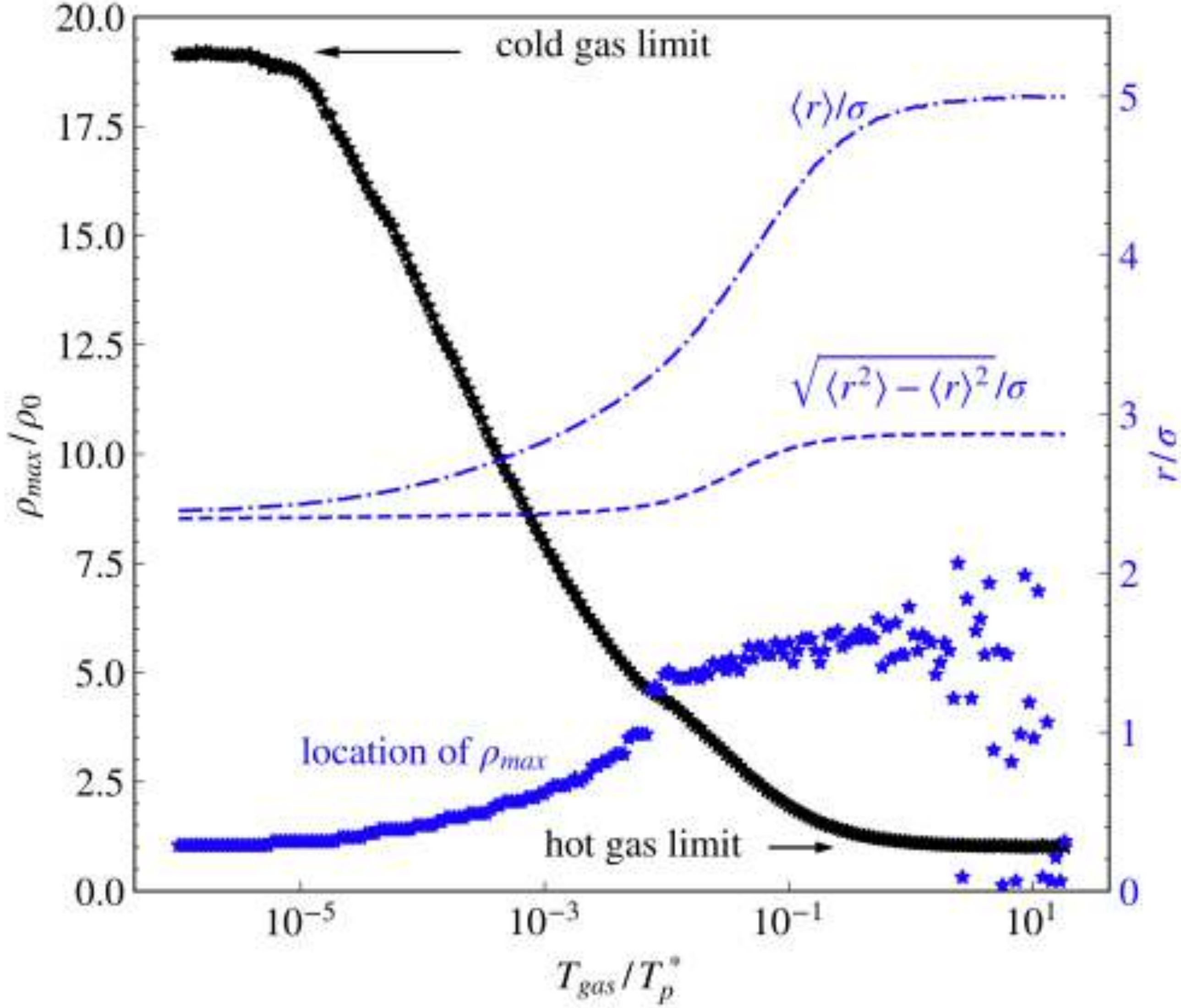
Radial density evolution



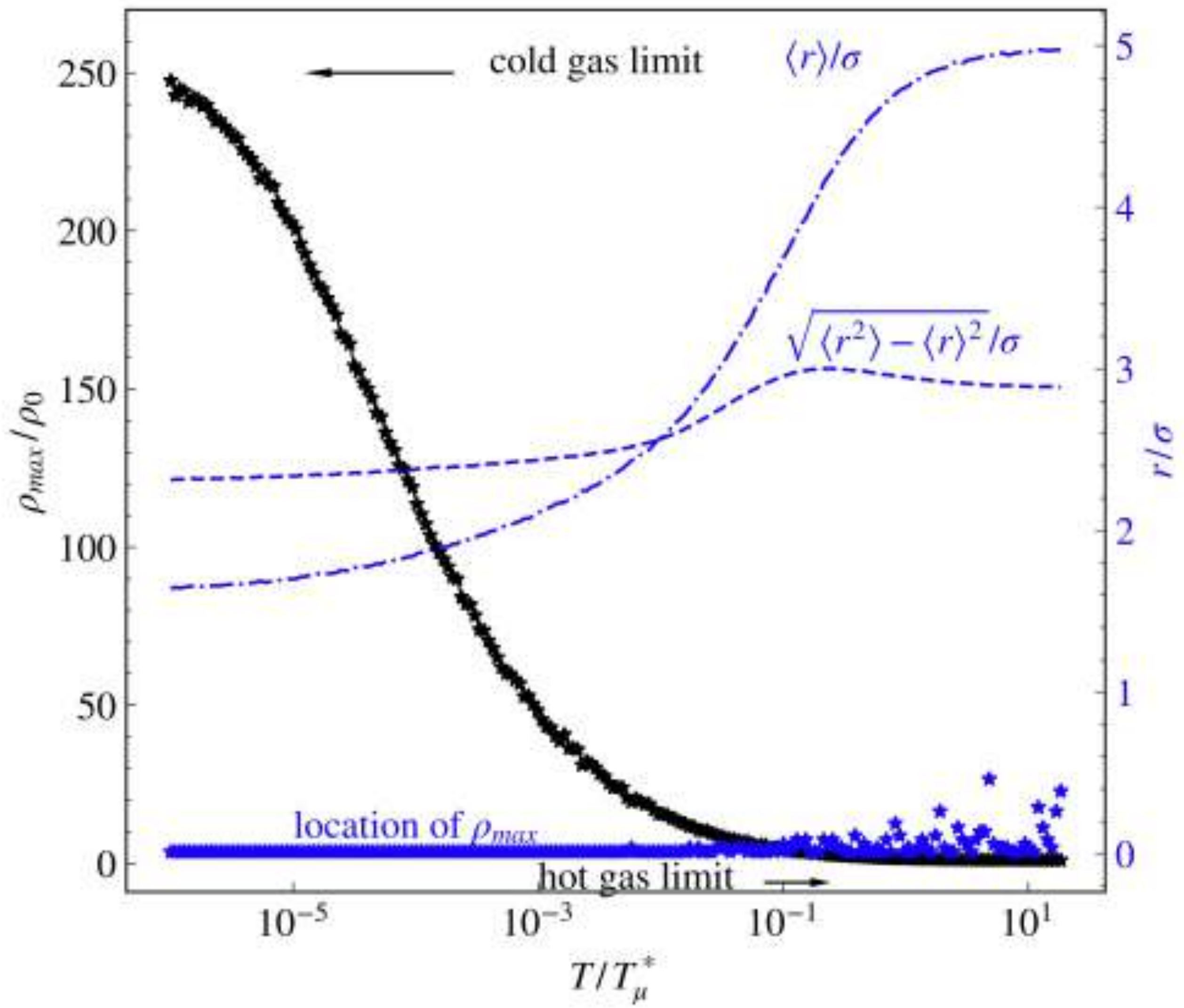
Molecules with $T/T^*_p = 0.1$



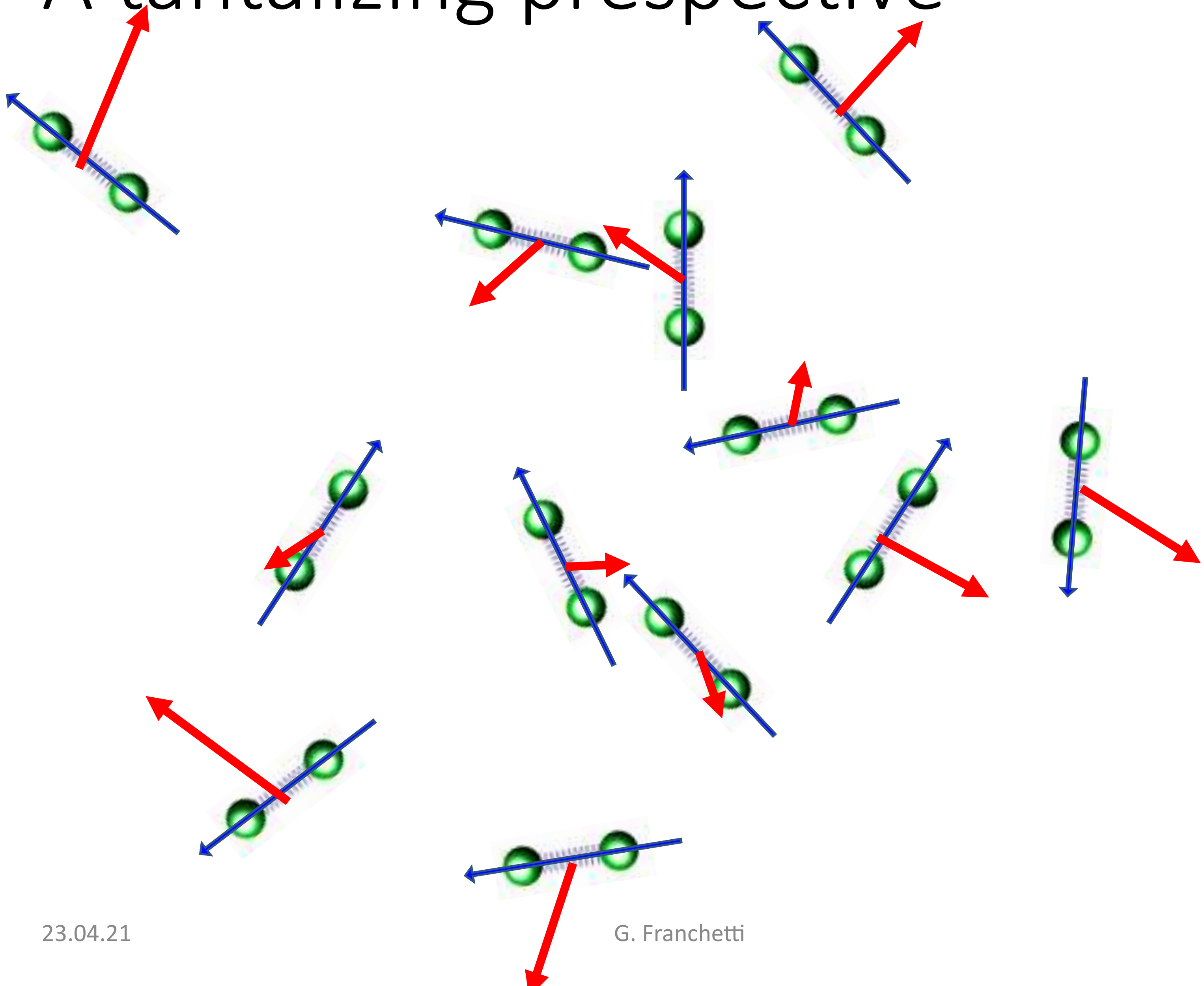
Density enhancement depends critically from T/T^*_p



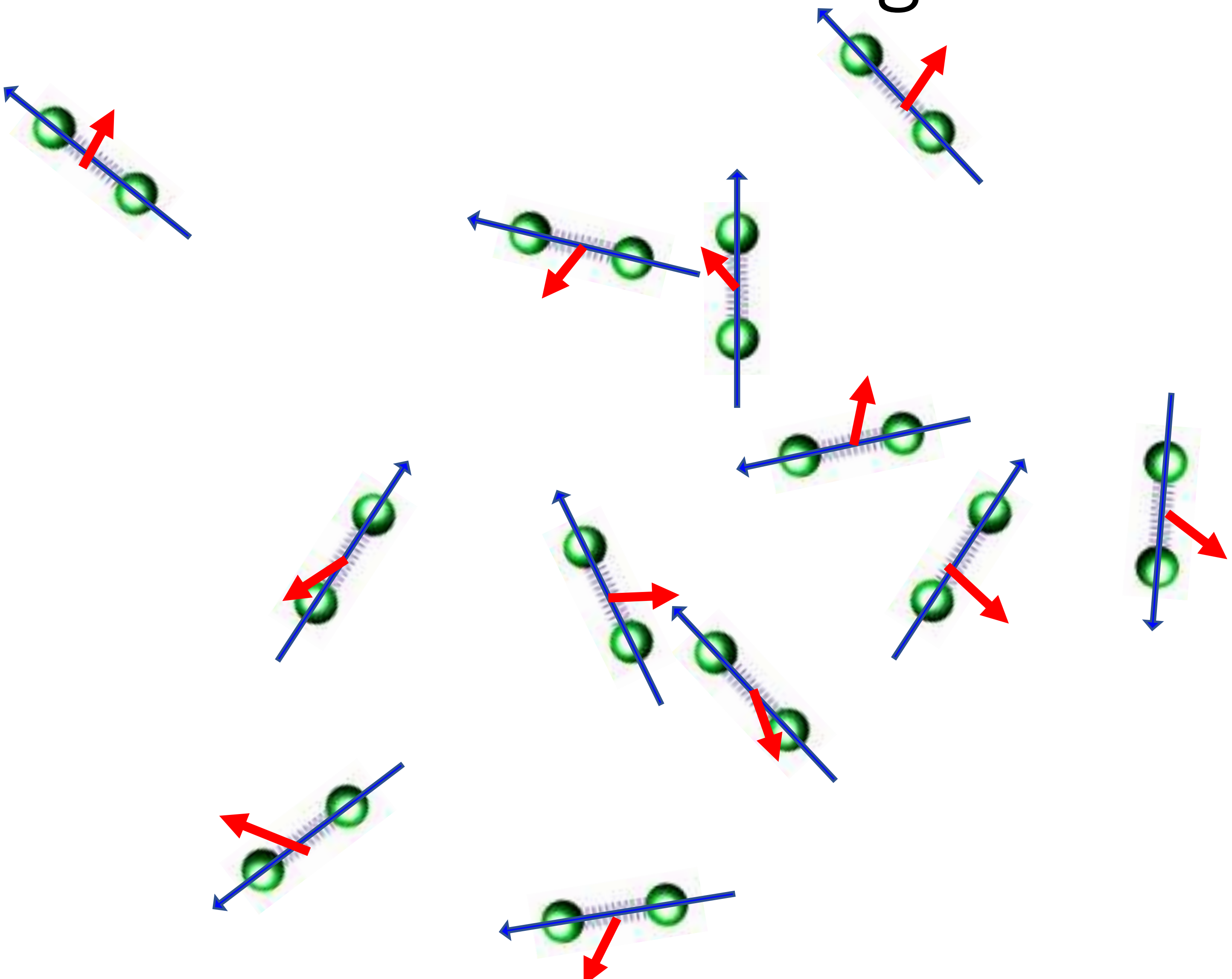
Density enhancement depends critically from T/T^*_μ



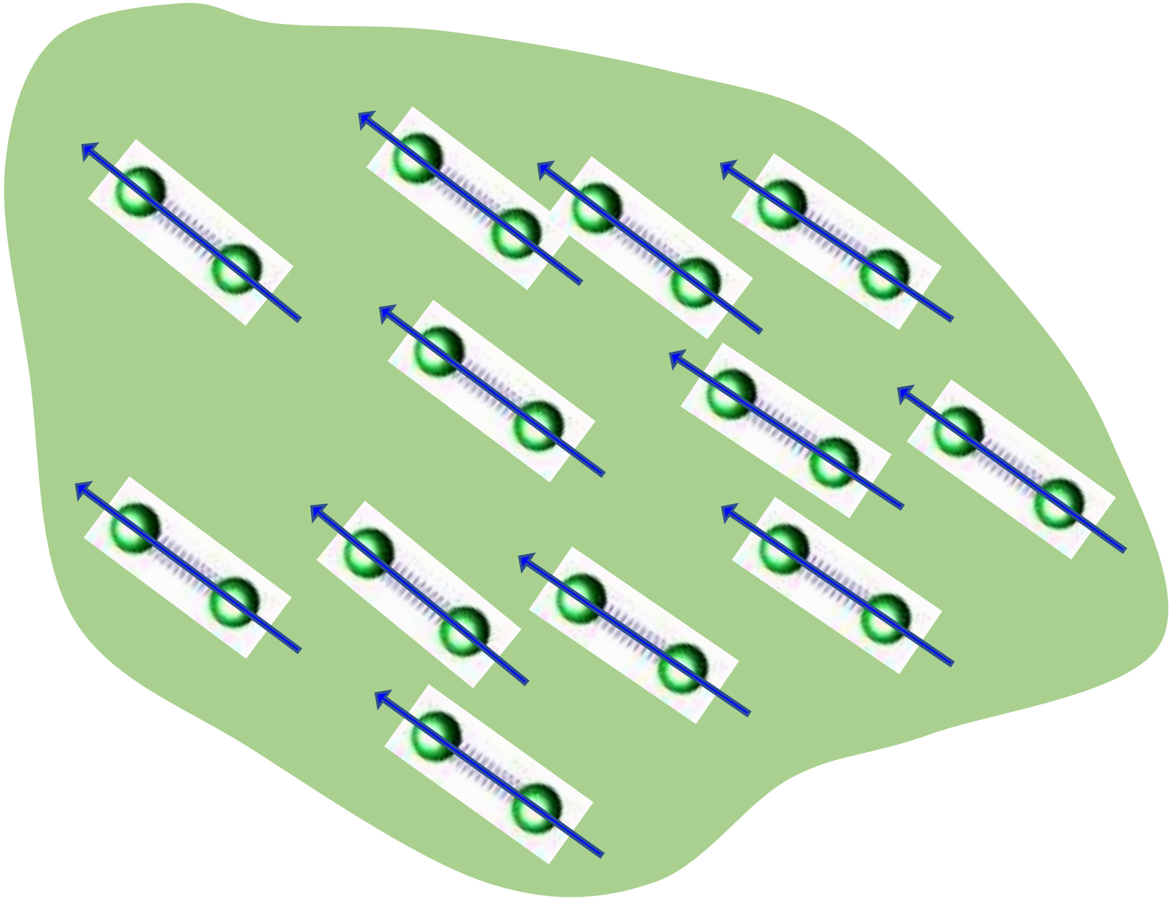
A tantalizing prespective



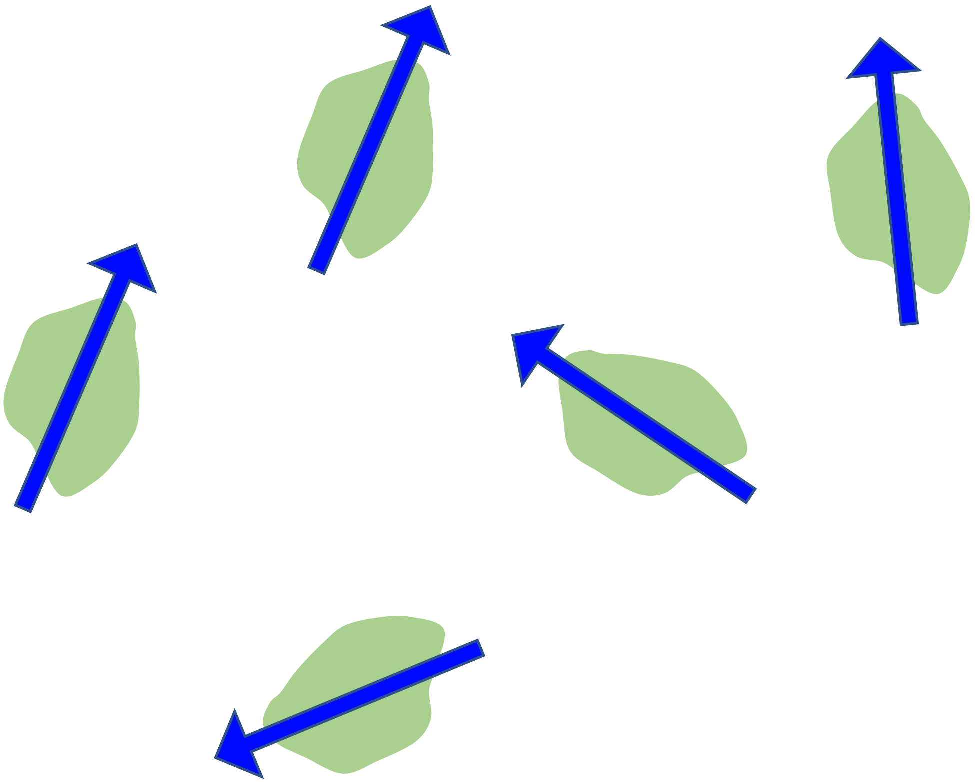
Molecules cold enough



Agglomeration or clustering



Gas of agglomerates or clusters



In thermal equilibrium, but have now lower temperature as the agglomerates have large mass

⇩

Very low T/T^* !!!

⇩

Large enhancement of vacuum density

Cluster-cluster aggregation with dipolar interactions

Particle-cluster aggregation with dipalar interactions
R. Pastor-Satorras and J. M. Ru
PRE, 51,6 1995

L978 *Letter to the Editor*

Figure 1. A typical cluster of 128 particles obtained without taking into account dipolar interactions nor the orientational dipole relaxation.

Paulo **M** Mors, Robert Botet and Rimi Jullien,
Phys. **A:** Math. Gen. **20(1987)L975-L980**

Dipole-Dipole Interactions of Charged- Magnetic Grains
Jonathan Perry, Lorin S. Matthews, and Truell W. Hyde, *Member, IEEE √*

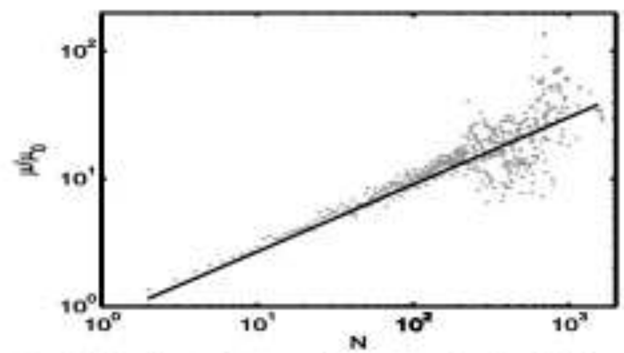


Figure 1. Normalized cluster magnetic moment as a function of N, the number of monomers in an aggregate. The fit line shows an exponential increase $\mu \propto N^{[illegible]}$.

No evident studies of aggregation at Accelerators cryogenic temperature

Summary

- Molecules with a magnetic dipole moment oscillate around the transverse center of the particle beam, whereas molecules with an electric dipole moment oscillate around a radial equilibrium position located at the edge of the beam.
- Description of the features of the dynamics as function of a trapping temperature T*
- Thermal motion of neutral molecules will be perturbed by the electromagnetic field of the beam, → trapping and density enhancement of such particles in the vicinity of the beam for T/T* small.
- Derived 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 time scale is problematic for simulations

Outlook → case for agglomeration formation studies

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

- Tools and methodologies developed for modeling aggregation phenomena may serve as a starting point for future studies of cluster formation and flake characteristics in accelerator beam vacuum systems.

Outlook → case for advanced beam dynamics studies

- Once a molecule or a flake comes close to the beam it may be ionized → dynamics is radically altered.
- Larger flake staying near the core of the beam would heat up, be charged, and then either evaporate or melt and explode, leaving behind a localized high-density mixture of ions, electrons, and molecules or atoms.
- A software package is under development at CERN, to study the interaction of such a complex mixture of species with the LHC proton beam → Lotta Mether
- Trapping and accumulation of individual neutral molecules or flakes of molecules in the vicinity of the beam enhances the effective gas density and can aggravate ion-induced beam instabilities
- The effect considered is particularly important in cryogenic vacuum systems, for high beam currents or for small beam sizes. Consequently, it will become more important for future generations of accelerators.