# **TRAPPING OF NEUTRAL MOLECULES BY THE ELECTROMAGNETIC BEAM FIELD**<sup>∗</sup>

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### *Abstract*

Trapping phenomena are common in physics and are of relevance for the accelerators. We discuss the phenomenon of neutral molecule trapping into the beam electromagnetic potential and highlight the potential influence on the vacuum density. The effect of molecule agglomerates is discussed for high energy accelerators.

### **INTRODUCTION**

At large accelerator laboratories, such as GSI [1], CERN [2], or BNL [3], the vacuum pressure in the beam pipe of storage rings ranges from 10<sup>-8</sup> to 10<sup>-10</sup> Pa. In cryogenic rings [4], the vacuum pressure  $p$  may reach a level of  $10^{-13}$  Pa or less, at a low temperature  $T$ . A low vacuum pressure ensures a low density of atoms and molecules, according to  $n = p/(k_bT)$ , with  $k_b$  the Boltzmann constant. The residual gas density  $n$  is a key quantity defining the "beam lifetime". In fact, the presence of neutral vacuum molecules in accelerator beam pipes lead to occasional collisions between beam particles and vacuum molecules, which may create several undesirable effects, ranging from the emission of beamstrahlung photons by beam electrons or positrons, over the stripping of electrons from partially stripped heavy-ion beam particles, to the fragmentation of the neutral molecule itself. The consequences of the beam-gas collisions may vary between a mild drop in the beam lifetime to a nearly catastrophic phenomenon, as in the case of a dynamical vacuum instability [5]. More generally, the presence of ionized gas molecules or liberated electrons inside the accelerator beam pipe can have undesired consequences, such as the creation of an electron cloud [6–10].

In this paper, we present a study of the dynamics of neutral molecules under the effect of the beam electromagnetic fields. We discuss a possible accumulation of neutral molecules in the vicinity of the beam [11], with potential negative impact on the beam lifetime.

## **DYNAMICS OF NEUTRAL MOLECULES AND APPROXIMATIONS**

At first sight, neutral particles are not affected by an electromagnetic field unlike particles carrying an electric charge. However, the situation can be different for neutral molecules which may exhibit a non-homogeneous charge distribution. To first order, this charge distribution  $\rho(\vec{r})$  is characterized

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hor(s), title of the work, publisher, and DOI by its electric dipole moment  $\vec{p} = \int \vec{r} \rho_M(\vec{r}) dv$ . A similar discussion applies to the intrinsic magnetic field of a molecule, which may be characterized by a magnetic dipole moment  $\vec{\mu}$ .

In general, the geometry of a molecule is not rigid, but exhibits an equilibrium configuration of its elementary particles subject to internal restoring forces, which, for example, give rise to natural vibration states of the molecule around an equilibrium mechanical geometry. The frequency of these internal oscillations is high and, therefore, we consider the geometry as rigid to a good approximation.

The effect of a homogeneous electric or magnetic field on a molecule with a dipole moment is to inflict a torque. If the field is not homogeneous a net force on the center of mass will also arise. These forces and torques are as follows [12]:

$$
\begin{cases} \vec{\tau} = \vec{p} \times \vec{E} + \vec{\mu} \times \vec{B} \\ \vec{F}_{\text{cm}} = (\vec{p} \cdot \nabla)\vec{E} + (\vec{\mu} \cdot \nabla)\vec{B} \end{cases}
$$
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Content from this work may be used under the terms of the CC BY 4.0 licence (© 2022). Any distribution of this work must maintain attribution to the author(s), title of the work, publisher, and DOI distribution of this work We observe that in both cases the torque in Eq. (1) disappears when the dipole moment has either the same or the opposite direction of the corresponding field. A stability analysis shows that the dipole moment dynamics is stable only if the dipole moment has the same direction as the field. Clearly, 2022). it is difficult that a molecule may simultaneously have  $\vec{p}$ and  $\vec{\mu}$  aligned with  $\vec{E}$  and  $\vec{B}$ . However, in our study we  $\odot$ consider only molecules equipped either with an electric dipole moment (EDM) or with a magnetic dipole moment licence (MDM). For example, in the case of an EDM molecule, the equation of angular motion of  $\vec{p}$  is  $\frac{1}{4}$ 

$$
\frac{d^2\theta}{dt^2}\hat{n} = \omega_E^2 \hat{p} \times \hat{E} , \qquad (2)
$$

the CC BY where  $\hat{p}$  and  $\hat{E}$  designate unit vectors in the direction of  $\vec{p}$  and  $\vec{E}$ , respectively, and  $\hat{n}$  is the unit vector orthogonal  $\sigma$ terms to  $\hat{p}$  and  $\hat{E}$ . The angle  $\theta$  is the angle between  $\vec{p}$  and  $\vec{E}$ . The quantity  $\omega_E = \sqrt{pE/I_i}$ , characterizes the oscillation frequency of  $\hat{p}$  around the equilibrium direction  $\hat{E}$ , and similarly, for MDM molecules we find  $\omega_B = \sqrt{\mu B/I_i}$ . We denote with  $I_i$  the moment of inertia of the molecule, which for a bi-atomic molecule is  $I_i = \frac{1}{2}mL^2$ , with L a characteristic length of the molecule and  $m$  an atom mass. The solution of Eq. (2) for small  $\theta$  is a harmonic oscillations of  $\theta$  around the equilibrium direction ( $\theta = 0$ ) with the characteristic angular frequency  $\omega_E$ . This frequency of oscillation is typically fast. For example, in a molecule of  $H<sub>2</sub>O$  the electric dipole moment is  $p = 1.87$  D, being D the unit of Debye,  $1D = 0.2082$  eÅ. An equivalent bi-atomic molecule, i.e. with equal dipole moment and the equal mo-Content mentum of inertia, will have size  $L = 0.65$  Å, hence we

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and DOI Content from this work may be used under the terms of the CC BY 4.0 licence (© 2022). Any distribution of this work must maintain attribution to the author(s), title of the work, publisher, and DOI find  $\omega_E/\sqrt{E} \simeq 4.44 \times 10^8 \text{ (rad/s)} (m/V^{1/2})$  . This formula publisher, shows that even a modest electric field of  $E = 1$  V/m will make  $\vec{p}$  oscillate with  $\omega_E = 4.4 \times 10^8$  rad/s, or a frequency of  $\simeq$  70 MHz.

It is convenient to define  $\vec{p} = p_0 \hat{p}$ , and  $\vec{E} = E_0 \vec{E}_n$ , where work,  $p_0$  is the strength of the EDM, and  $E_0$  is the maximum of the electric field in the region considered. Hence, with this definition  $|\vec{E}_n| \leq 1$ , and  $|\hat{p}| = 1$  and the dynamics of the to the author(s), title center of mass under the force given by the second formula of Eq. (1), reads

$$
\frac{d^2 \vec{r}_{\rm cm}}{dt^2} = \frac{p_0 E_0}{M} (\hat{p} \cdot \nabla) \vec{E}_n = \omega_E^2 \frac{I_i}{M} (\hat{p} \cdot \nabla) \vec{E}_n , \quad (3)
$$

where here  $M$  is the mass of the molecule. The ratio  $I_i/M$  yields the square of an effective molecule length, which is always less than the size of the molecule  $L$ , that is  $I_i/M \leq L^2$ . Therefore, we find that  $|d^2\vec{r}_{cm}/dt^2| \leq$  $\omega_E^2 L^2 \sum_{i=1,3} |\partial \vec{E}_n/\partial x_i|$  . The last term of this formula somehow measures the gradient of the normalized electric field. If this term is not too large, the dynamics is strongly controlled by  $L$  which is approximately of the order of one Angstrom or 10−<sup>10</sup> m. This effect becomes more visible if we re-scale the time in units of the period of oscillation of the EDM  $\tau_E = 2\pi/\omega_E$ , that is if we take the re-scaled time as  $\tau = t/\tau_E$ . Then Eq. (3) becomes

$$
\left| \frac{d^2 \vec{r}_{\text{cm}}}{d\tau^2} \right| \le (2\pi)^2 L^2 \sum_{i=1,3} \left| \frac{\partial}{\partial x_i} \vec{E}_n \right| . \tag{4}
$$

This formula says that during the time of one EDM oscillation  $\Delta \tau = 1$  the change of normalized velocity is negligible because  $L$  is very small, and this means that the motion of the molecule in this interval of time is "almost" uniform with velocity  $v_{\rm cm} = |d\vec{r}_{\rm cm}/dt|$ . The molecule motion will exhibit a local curvature radius  $r_c$  of the circle tangent to the trajectory. Therefore the quantity  $v_{\rm cm}/r_c$  is the instantaneous angular velocity of rotation of the center of mass. If this angular velocity is always much smaller than the natural instantaneous angular velocity  $\omega_E$ , i.e. if

$$
\frac{v_{\rm cm}}{\omega_E r_c} \ll 1 \ ,
$$

then an initially aligned EDM to  $\vec{E}$  will keep being aligned to  $E$  in the subsequent motion. This comparison of two frequencies is typical for requiring a condition of an adiabatic principle. The radius of curvature  $r_c$  depends also on the gradients of the electric field, and for smooth electric fields,  $r_c$  will never be too small. At  $T = 2$  K, a molecule of H<sub>2</sub>O has an rms thermal velocity of  $v_{cm} \approx 43$  m/s, and even assuming a curvature radius of  $r_c = 10^{-5}$  m, for  $\omega_e =$  $4.4 \times 10^8$  rad/s, this would yield  $v_{\rm cm}/(\omega_E r_c) \simeq 0.01$ .

If the initial orientation of the EDM has instead another direction than  $\vec{E}$ , then the EDM will oscillate around the electric field, and the average of the EDM positions will still be aligned to  $\vec{E}$ , but with a smaller effective strength (as coming from the averaging process).

We next explore the dynamics of neutral molecules under the assumption that the EDM/MDM is aligned with the elec-

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tric/magnetic field generated by the beam in an accelerator ("close alignment" condition).

### **FORCES FROM THE BEAM FIELD**

For an axi-symmetric coasting beam, the beam fields have a strength that is rotational symmetric, that is  $\vec{E} = E(r)\vec{r}/r$ , and  $\vec{B} = B(r) \vec{r}/r \times \hat{z}$ , with  $E(r)$ ,  $B(r)$  the modulus of the electric and magnetic field at radius  $r$ , and  $\hat{z}$  the unity vector pointing to the direction of motion of the beam. The field  $E(r)$ ,  $B(r)$  are completely defined by the particle distribution in the coasting beam. As the fields created by the coasting beam are only on the transverse plane, and we consider the molecules with EDM or MDM aligned with the beam field, then the dipole moment must be  $\vec{p} = p \vec{r}/r$  for the EDM molecules and  $\vec{\mu} = \mu \vec{r}/r \times \hat{z}$  for the MDM molecules. Here  $p$  is the EDM strength and  $\mu$  the MDM strength in absence of external fields. Inserting these "always aligned" dipole moments in Eq. (1) we find the following force

$$
\vec{F}_{\text{cm}} = \left[ -\mu \frac{B(r)}{r} + p \frac{dE(r)}{dr} \right] \frac{\vec{r}}{r} . \tag{5}
$$

This is the total force valid for the special case of a molecule having both  $\vec{p}, \vec{\mu}$  aligned with the respective field, but for our study we consider only molecules having either EDM or MDM. Note, in Eq. (5), the appearance of the derivative of  $E(r)$ , which is rather counter-intuitive, and is the result of requiring the dipole moment alignment.

By considering a beam with a Gaussian particle distribution, the strength of the electric and magnetic field is dependent only on the radial distance of a particle from the beam center according to

$$
B(r), E(r) \propto \frac{I}{\sigma} \times \frac{\sigma}{r} \left[ 1 - \exp\left( -\frac{1}{2} \frac{r^2}{\sigma^2} \right) \right] \,, \qquad (6)
$$

with *I* the beam current, and  $\sigma$  the rms beam size. Consequently, the force on the center of mass of the molecule is not the usual one created by space charge but assumes a peculiar pattern sketched in Fig. 1 (see in [11] for more details).



Figure 1: Forces exerted on the center of mass of a molecule, as a function of normalised transverse position. Note the substantial difference between EDM (black markers), and MDM (red markers), but also the difference with respect to usual space-charge forces expected from the beam fields.

For the EDM case, the force disappears at  $r_e/\sigma \approx \pi/2$ : note that  $r_e$  depends only on the beam size and not on the

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beam current. Note also that in Fig. 1 the force becomes discontinuous through the origin. This is a consequence of the finite value of  $E'(r)$ ,  $B(r)/r$  in the origin, contrarily to the strength of  $E(r)$ ,  $B(r)$  which goes to zero at  $r = 0$ , hence removing the discontinuity. This behaviour of  $F_{\rm cm}$  is valid if the molecule is aligned with the field. However, an instantaneous flip of the orientation of the dipole moment because of the flip of the force is not possible. Therefore, Eq. (5) will not hold for molecules going through the beam center, as these will lose the "close alignment" condition, and their dynamics will become more complex, since the force  $F_{\rm cm}$  will acquire a *coupling* with the orientation of the dipole moments. However, this anomaly applies only to those particles that cross the beam center, and these are a minor fraction of all molecules possibly found in the beam pipe.

### **TRAPPING BY THE BEAM FIELD**

The first hint of molecule trapping is from Fig. 1 where we see for a Gaussian distribution the existence of the equilibrium radius  $r_e/\sigma \simeq \pi/2$ . Molecules in the vicinity of this radius are focused to oscillate around  $r_e$ . An indicator of the focusing strength is the natural frequency of oscillation. By expanding the force around  $r_e$  the equation for small oscillations becomes linear, and a harmonic motion will take place. The angular frequency of this oscillation is

$$
\omega \simeq \sqrt{\frac{e}{10} \frac{p}{2\pi\epsilon_0 Mc \sigma^3} I},\qquad (7)
$$

where here  $e = 2.718...$  is the Euler number, not to be confused with the electron charge. The effect of this focusing force can be visualized by tracking the motion of the molecules. We take a set of cold molecules, i.e. with initial  $dx/dt = 0$ , equally distributed on the horizontal plane while keeping  $y = 0$ .

The result of tracking few particles is shown in Fig. 2 (top) where the oscillation pattern around  $r_e$  is clearly visible. Figure 2 (middle) presents the same simulation with more molecules, leading to a complex structure produced by the special choice of initial conditions. However, if we repeat the same simulation for cold molecules randomly populating the transverse section of the beam pipe the resulting trajectories do not produce a clear structure, as we can see in the bottom picture of Fig. 2. To complicate the matter further, rarely molecules will have  $dx/dt = 0$ , as the initial conditions of the neutral molecules are determined by the thermodynamics of a gas in equilibrium. At equilibrium the molecules follow a Maxwell-Boltzmann velocity distribution, which is characterized by the transverse rms velocity

$$
v_{rms} = \sqrt{\frac{k_b T}{M}} \,,\tag{8}
$$

where  $k_b$  is the Boltzmann constant, and T is the molecule's temperature. Therefore, it is not straightforward even to assess whether a molecule is trapped or not.

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Figure 2: Trajectories of test molecules started at rest along the horizontal axis and aligned with the beam field. The top picture presents the trajectories of a few particles, clearly revealing that these particles oscillate around  $r_e$  (the red lines). On the abscissa, the time is scaled in units of the oscillation period near  $r_e$ , i.e. in the unit of  $\Delta t = 2\pi/\omega$ . The middle picture shows a similar simulation, but now with 49 molecules. The bottom picture instead displays the trajectories of particles randomly placed in the  $x - y$  plane.

To assess whether a molecule is trapped by the electromagnetic beam field, we have to invoke a more general principle. The equation of motion of molecule center of mass, in a "closely aligned  $\vec{p}$ " condition, reads

$$
M\frac{d\vec{v}}{dt} = p\frac{dE(r)}{dt}\frac{\vec{r}}{r},
$$

here for simplicity we have dropped the label  $cm$  from  $r$  and v. By multiplying both sides by  $\vec{v}$  we easily get

$$
\frac{1}{2}v^2 - \frac{p}{M}E(r) = D,
$$

where  $v^2 = v_x^2 + v_y^2$  and D is a constant determined by the initial condition. Note the very peculiar situation that  $E(r)$ becomes the potential in the energy conservation equation. From this formula, it is clear that a particle is trapped only if  $D < 0$ . Next, we observe that the electric field generated by an arbitrary axisymmetric beam distribution has the general form

$$
E(r) = \frac{1}{2\pi\epsilon_0 c} \frac{I}{\sigma} f\left(\frac{r}{\sigma}\right) ,
$$

with  $f(u)$  a function that depends on the type of transverse distribution: for the Gaussian distribution, it is the term after

the "×" in Eq. (6). Therefore,

$$
\frac{1}{2}v^2 - \frac{p}{M}\frac{1}{2\pi\epsilon_0 c}\frac{I}{\sigma}f\left(\frac{r}{\sigma}\right) = D.
$$
 (9)

As previously mentioned, the initial condition of a molecule is strongly influenced by Eq. (8), as the initial  $v_{x0}$ ,  $v_{y0}$  of a molecule located at  $r_0$  are determined by a Maxwell-Boltzmann distribution characterized by the rms velocity given in Eq. (8). Therefore  $v_{x0} = \xi_x v_{rms}, v_{y0} = \xi_y v_{rms}$ with  $\xi_x, \xi_y$  two independent random numbers generated from a Maxwell-Boltzmann distribution with unitary velocity spread. Hence the constant  $D$  of Eq. (9) is found as

$$
\frac{1}{2}\frac{k_bT}{M}(\xi_x^2+\xi_y^2)-\frac{p}{M}\frac{1}{2\pi\epsilon_0c}\frac{I}{\sigma}f\left(\frac{r_0}{\sigma}\right)=D.
$$

This formula shows that it is convenient to define the temperature

$$
T_p^* = \frac{1}{\pi \epsilon_0 k_b c} \frac{I}{\sigma} p \tag{10}
$$

a quantity resulting from a combination of beam properties such as beam current I, beam size  $\sigma$ , and the dipole moment strengths  $p$ . Therefore, we find that the trapping of a particle, i.e.  $D < 0$ , requires

$$
\xi_x^2 + \xi_y^2 - \frac{T_p^*}{T} f\left(\frac{r_0}{\sigma}\right) < 0 \,. \tag{11}
$$

This expression allows an interpretation of the meaning of  $T_p^*$ . If the temperature of the molecules T is lower than  $T_p^*$ there is a higher chance that a particle (i.e. the  $\xi_x, \xi_y, r_0$ ) satisfies Eq. (11), and hence is trapped into the beam potential. Now we extend the meaning of *"trapping"* referring it to a particle that does not collide with the beam pipe while being under the influence of the beam fields. Even in this case the ratio  $T/T_p^*$  is the key quantity determining the number of trapped particles: the smaller it is the more molecules get trapped.

# **DYNAMIC EFFECTS ON VACUUM DENSITY**

In the previous section, we showed that  $T/T_p^*$  determines how many particles are trapped in the beam potential. Figure 2 (middle) suggests that the trapped molecules may evolve with trajectories that lead to special high-density structures in the transverse space. At the same time, Fig. 2 (bottom) shows that, for a random spatial position of cold molecules, the molecule density pattern is not so clearly visible. Hence, a more thorough investigation is necessary to unravel the general properties of the system.

We continue the study by tracking a gas of molecules initially being in thermal equilibrium, i.e., having temperature  $T$ , and the EDM strength  $p$  is chosen so as to create a specific trapping temperature  $T_p^*$ . The complete randomness of the initial molecule distribution in a circular pipe and their random velocity, together with the axial symmetry of the beam suggests that the local molecule density evolves axisymmetrically as well. A large number of macro-molecules are tracked and at a constant intervals of time, the average

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 $\rho/\rho_0$ 10 4.5 4.0 8 3.5 3.0 6 2.5 *<sup>r</sup>*/ 2.0 4 1.5 2 1.0 0.5 0.0 2 4 6 8 10 *nosc*.  $20.0$ cold gas limit  $17.5$  $15.0$  $12.5$  $\sqrt{\langle r^2 \rangle - \langle r \rangle^2}/c$  $10.0$  $7.5$  $5.0$ location of  $2.5$ hot gas limit  $0.0$  $10^{-}$  $10<sup>°</sup>$  $10^{-}$  $T_{gas}/T_{n}$ 

Figure 3: Top: Radial density evolution for EDM molecules for  $T/T_p^* = 0.02$ . Bottom: Beam density enhancement as function of  $T/T_p^*$  (form Ref. [11]).

radial molecule density is computed from the distribution for all radii in the vacuum chamber. The result for the case  $T/T_p^* = 0.02$  is shown in Fig. 3 (top), where the full simulation is presented. It is visible that the molecule density varies and pinch within one oscillation  $n_{osc}$  of molecules around  $r_e$ . Afterward, the peak density lowers a little and remains stable at  $\rho/\rho_0 \simeq 3.6$ . Note that the region of  $r/\sigma < 0.5$  is evacuated as those molecules are strongly repelled towards  $r_e$ . In conclusion, Fig. 3 (top) shows that the effect of the beam field for a specific  $T/T_p^*$  is of enhancing the initial molecule density  $\rho_0$  of a certain factor  $\rho_{\text{max}}/\rho_0$  at a certain specific radius, and also that the radial molecule density has a certain spread that we may quantify via statistical analysis (average and standard deviation). A more global survey of the dynamical effect of the beam field on the density of the molecules is obtained by repeating the simulation as for Fig. 3 (top), but for a different  $T/T_p^*$ . The result of this scan is shown in Fig. 3 (bottom). The black curve shows the dependence of the  $\rho_{\text{max}}/\rho_0$  from  $T/T_p^*$ , and exhibits a very interesting pattern: for  $T/T_p^*$  larger than one, we find  $\rho_{\text{max}}/\rho_0 = 1$ , so that no effect on the molecules is detected, this is a sort of "hot gas limit" because the thermal motion of the molecules is too strong and wins over the forces exerted by the beam. The contrary is the case if  $T/T_p^*$  is less than one. The density enhancement becomes stronger for smaller

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 $T/T_p^*$ , and reaches a limit of  $\rho_{\text{max}}/\rho_0 \sim 19$  for  $T/T_p^* \to 0$ ("cold gas limit"). These results further confirm that  $T_p^*$  has the role of trapping temperature.

# **ARE AGGREGATES OR FLAKES MORE SENSITIVE TO THE BEAM FIELD?**

The trapping temperature of Eq. (10), can be understood as a general trapping temperature  $T^* = 1/(\pi \epsilon_0 k_b c)(\tilde{p}I/S)$ , with  $S$  denoting the characteristic length scale of trapping, and  $\tilde{p} = p$  or  $\mu/c$  (see the next section). The remarkable property of the trapping temperature is that it does not depend on the mass of the molecules, but only on their dipole moment  $\tilde{p}$ .

Suppose that the neutral molecules in the beam pipe carry the dipole moment  $\tilde{p}$  and that the beam has the parameters  $(I, \sigma)$ , so that there is a certain trapping temperature  $T^*$ . As previously discussed, the fraction of trapped molecules depends on  $T/T^*$ . Now also suppose that a process of agglomeration or clustering will take place, involving groups of  $N$  molecules. The resulting flakes will have a dipole moment  $\tilde{p}_f \sim N\tilde{p}$ , so that the trapping temperature of these flakes will be  $T_f^* \sim NT^*$ . We observe that the flakes are in the vacuum pipe and in thermal equilibrium with the environment (i.e., with the other molecules and beam pipe); hence they will also have the temperature  $T$ . It follows that the amount of trapped flakes is now governed by  $T/T_f^* \sim (T/T^*)/N$ . Therefore, if the temperature of the accelerator is approximately equal to the trapping temperature of the vacuum molecules, then for the flakes  $T/T_f \sim 1/N$ , and clustering of, for example,  $N \sim 100$  molecules will bring the flake component of the vacuum closer to the cold gas limit shown in Fig. 3 (bottom). As a consequence an enhancement of  $\rho_{\text{max}}/\rho_0$  will occur.

We also observe the following interesting features of the EDM molecules. The time scale of the pinch process is given by the frequency of the oscillation of molecules around  $r_e$ , i.e.  $\Delta t = 2\pi/\omega$ , but we easily see that Eq. (7) can also be written as  $\omega^2 = (e/20)(k_b T_p^*)/(M\sigma^2)$ . Therefore, the angular frequency  $\omega$  will not be altered by the clustering process as long as  $p_f = pN$ . The physical reason for the higher sensitivity of flakes to the beam field is that the force on the flakes is  $\sim N$  times larger, but for a mass also N times larger. Hence, the acceleration of the flakes will be the same as for the other, regular molecules, while the thermal same as for the other, regular molecules, while the thermal<br>velocity of the flakes will be  $\sqrt{N}$  smaller, rendering the initial conditions of the flakes more susceptible to the trapping process.

# **DYNAMICS AND TRAPPING OF MDM MOLECULES**

For MDM molecules the analysis is similar, the magnetic field  $B(r)$  from the axisymmetric beam is

$$
B(r) = \frac{\mu_0 I}{2\pi\sigma} f\left(\frac{r}{\sigma}\right) ,\qquad (12)
$$

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and the equation of motion of the center of mass is

where

$$
M\frac{d\vec{v}}{dt} = -\mu \frac{B(r)}{r} \frac{\vec{r}}{r} \ . \tag{13}
$$

The energy conservation, defining  $N_2(u) = \int_0^u f(u')/u' du'$ , reads

$$
\frac{v^2}{2} + \frac{k_b T^*_{\mu}}{2M} N_2 \left(\frac{r}{\sigma}\right) = E,
$$

$$
T_{\mu}^{*} = \frac{1}{\pi \epsilon_0 k_b c} \frac{I}{\sigma} \frac{\mu}{c} \ . \tag{14}
$$

This expression shows that particle trapping in the beam pipe is again governed by  $T/T^*_{\mu}$ . The equation of motion Eq. (13) is more transparent in the following form

$$
\frac{d\vec{v}}{dt} = -\frac{1}{2} \frac{k_b T^*_{\mu}}{M \sigma} \left[ \frac{\sigma}{r} f\left(\frac{r}{\sigma}\right) \right] \frac{\vec{r}}{r},\qquad(15)
$$

and shows that the larger  $T^*_{\mu}$  the faster the dynamics of neutral molecules because of the beam field. As mentioned earlier the instantaneous flip of a dipole moment is not possible, hence this equation will not be valid for the MDM molecules that cross the beam center. Note that the function in the square brackets of Eq. (15) vanishes only at  $r \to \infty$ , therefore, differently from the case of EDM molecules, we cannot define any natural frequency  $\omega$  as in Eq. (7), where it was characterizing the period of the EDM pinch process. A scan over  $T/T^*_{\mu}$  also shows that for MDM molecules there is a cold limit (see Ref. [11]), which reaches maximum density values an order of magnitude higher than that for EDM; compare Fig. 3 (bottom). Lastly, we remark that the discussion on the sensitivity of EDM flakes equally applies to MDM flakes, with the same conclusions.

### **OUTLOOK**

We have analyzed the motion of neutral molecules equipped with EDM, or MDM, and investigated the effect of the beam field on such molecules. According to our study, the trapping of molecules is controlled by a temperature  $T^*$  which directly can be compared with the vacuum temperature  $T$ . The general indication is that a local density enhancement is likely if  $T/T^* < 1$ . The potential presence of aggregates amplifies the effect of the beam. We have shown that, in consequence, flakes are more prone to being trapped. The dependence of the forces on the field gradient indicates that the application of solenoid magnets, whose fringe fields exhibit a high gradient, will disrupt the dynamics that the beam imparts on the neutral molecules. Hence, local installation of weak solenoid magnets could mitigate the formation of high density structures [13, 14]. More detailed analyses are needed to quantify the effect of breaking the "close alignment" condition, and the dynamical change of beam density in the case of bunched beams.

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