Electrostatic Collimation and Guiding of ThO (Draft)

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Collimation by an ideal potential

Consider a potential $U(r)$ in a cylindrical geometry. In order to act as a focusing lens, the potential should vary as $U(r) \propto -r^2$, so that the force $F(r) \propto -\vec{r}$. Let $U(r) = -\frac{1}{2}kr^2$ and $F(r) = -k\vec{r}$. Assume that the potential only exists in a finite region $d < z < d + \ell$ and $0 \leq r < R$.

Consider a point source of atoms at $r = z = 0$. The atoms have velocity vector $v_0(\hat{z}\cos(\theta)+\hat{r}\sin(\theta))$ before entering the potential. Because the longitudinal motion is not affected, let's only consider the transverse motion $v_r = v_0\sin(\theta)$ and $r(t)$. When the atom enters the potential, it has position $r(0) = d\tan(\theta)$ and $v_r(0) = v_0\sin(\theta)$. The equation of motion for the particle is

$$m\dot{v_r}(t) = -kr \qquad r(0) = d\tan(\theta) \qquad v_r(0) = v_0\sin(\theta)$$

The solution to this equation is

$$\begin{aligned} r(t) &= \frac{v_0}{\omega}\sin(\theta)\sin(\omega t) + d\tan(\theta)\cos(\omega t) \\ &\approx \frac{v_0}{\omega}\theta\sin(\omega t) + d\theta\cos(\omega t) \end{aligned}$$

where $\omega = \sqrt{k/m}$ and we have assumed small angles θ. We would like to collimate the particles so that $v_r(\Delta t) = 0$, where Δt is the transit time through the potential, $\Delta t = \ell/v_z = \ell/v_0\cos(\theta) \approx \ell/v_0$. Therefore we require

$$\begin{aligned} 0 &= v(\Delta t) \\ &= v_0\theta\cos(\omega\Delta t) - d\omega\theta\sin(\omega\Delta t) \\ \tan(\omega\Delta t) &= \frac{v_0}{d\omega} \\ \Delta t &= \frac{1}{\omega}\arctan\left(\frac{v_0}{d\omega}\right) \\ \ell &= \frac{v_0}{\omega}\arctan\left(\frac{v_0}{d\omega}\right) \\ \ell &\approx \frac{\pi}{2}\frac{v_0}{\omega} \end{aligned}$$

where the last approximation assumes that $v_0 \gg d\omega$. In other words, we need $v_0/\omega \approx \ell \gg d$, i.e. the distance to the guide entrance should be much shorter than the guide, which is easily the case in the situations we will consider.

Collimation by a multipole guide

Now we consider a specific system: a dipolar molecule moving through the electric field created by an $n-$pole. The interaction potential of a molecule in an electric field $\vec{\mathcal{E}} = \mathcal{E}(r)\hat{r}$ is $V = \vec{\mu}\cdot\vec{\mathcal{E}} = \mu|\mathcal{E}| = \mu\mathcal{E}$. The force is then $F(r) = -\nabla(\mu\mathcal{E})$. We consider two cases: the linear and non-linear stark regimes.

Linear stark regime. This would be the case if we wanted to guide the ThO H state, which is polarized in extremely small fields. Thus we may assume that μ is a constant, so a stark energy of $W(r) = -\mu\mathcal{E}(r) \propto r^2$ requires $\mathcal{E} \propto r^2$. The electric field from an $n-$pole varies as $r^{(n-2)/2}$, so in this

case we would like a hexapole ($n = 6$). However, we do not want to guide the H state − the H state will be prepared in the interaction region! We want to guide the X state, which means the non-linear stark regime.

Non-linear stark regime. Here the stark energy is $W = -\alpha\mathcal{E}^2$, where α is the polarizability. To have $W \propto r^2$ we want $\mathcal{E} \propto r$ and therefore a quadrupole guide.

Stark Shifts of the ThO X state

We shall use the value $\mu_X = 2.8$ D reported by Alexei Buchachenko, and $B_X = 0.33$ cm^{-1} reported by Alexei and the standard ThO literature. We will be working in the quadratic stark regime, so the parameter of interest is the polarizability α, where the stark shift is given by $W(\mathcal{E}) = -\alpha\mathcal{E}^2$. Because we work with units of cm^{-1} for W and kV/cm for $\mathcal{E}$, α has units of cm^{-1}/(kV/cm)^2. The conversion to other common units are are follows:

$$\frac{\text{cm}^{-1}}{(\text{kV/cm})^2} = 1.986 \times 10^{-33}\frac{J}{(\text{V/m})^2} = 17.85 \times 10^6 (4\pi\epsilon_0)\mathring{A}^3$$

Perturbative Calculation

We can find the polarizabilities of the rotational states by using the following formula[1]:

$$\alpha = -\frac{\mu^2}{2hcB}\left(\frac{J(J+1) - 3M^2}{J(J+1)(2J-1)(2J+3)}\right) = -(62000 \times 4\pi\epsilon_0\mathring{A}^3)\left(\frac{J(J+1) - 3M^2}{J(J+1)(2J-1)(2J+3)}\right)$$

where in the second equation we plugged in the values for the X state. We want states with a large, negative polarizability; this will ensure that the state has a higher energy in higher fields, and is therefore a low-field seeker and will therefore be pulled into the center of the guide. Therefore, we can see that $M = 0$ is the best choice; increasing $|M|$ from $M = 0$ reduces the magnitude of α if $\alpha < 0$, and makes α larger if $\alpha > 0$. Therefore, we can simplify the above expression with $M = 0$:

$$\boxed{\alpha = -\frac{\mu^2/2hcB}{(2J-1)(2J+3)} = -\frac{62000 \times 4\pi\epsilon_0\mathring{A}^3}{(2J-1)(2J+3)}}$$

Now we must determine over what electric field ranges the quadratic stark regime is valid. To use perturbation theory we want the stark shift $|W| = |\alpha|\mathcal{E}^2$ to be much smaller than the rotational spacing $2hcBJ$ between the J and $J-1$ levels, i.e.

$$\mathcal{E} \ll \mathcal{E}_* \equiv \sqrt{\frac{2hcBJ}{|\alpha|}} = \frac{2hcB}{\mu}\sqrt{J(2J-1)(2J+3)} = (14 \text{ kV/cm})\sqrt{J(2J-1)(2J+3)}$$

(For $J = 0$, use $J = 1$ since the nearest level is the $J = 1$ level). Notice that as we increase J we get a smaller magnitude of the polarizability, but we have quadratic stark shifts for larger ranges of $\mathcal{E}$. Thus as the maximum field we can create gets larger, we can have stronger and stronger guiding by choosing a state with higher and higher J. We shall see that technical limitations impose $J \leq 2$ for us.

J ($M = 0$)	$\alpha[4\pi\epsilon_0\mathring{A}^3]$	$\mathcal{E}_*$[kV/cm]
0	20,000	40
1	-12,000	40
2	-3,000	56

Polarizabilities in units of $4\pi\epsilon_0\mathring{A}^3$ are reported with two significant figures here and after. Since $J = 2$ starts to leave the quadratic stark regime around electric fields we could reasonably produce, it isn't worth calculating higher levels. Therefore, depending on how high an electric field we can create, the $J = 1$ or $J = 2$ ($M = 0$) levels are the best for guiding.

[1] Herzberg, (V,96). We also used $W = -\alpha\mathcal{E}^2$ and $I_0 = h/8\pi^2 cB$

Hamiltonian Diagonalization Calculation

We must diagonalize the matrix containing the rotational energies and the coupling between the rotational states[2]. Say that we have an electric field in the $z-$direction, which will be the quantization axis for J. Of course it is not true that we have an electric field in the $z-$direction, but each molecule travels along a trajectory at a constant angle with respect to the axis of the guide, so each molecule sees an electric field in a fixed direction. Thus

$$\langle J'M'\Omega'|H|JM\Omega\rangle = \delta_{J,J'}BJ^2 + \mu\mathcal{E}\sqrt{\frac{2J+1}{2J'+1}}\langle J'M'|1,0;J,M\rangle\langle J'\Omega'|1,\Omega'-\Omega;J,\Omega\rangle$$

Here B is the rotational constant, μ is the electric dipole moment, and $\mathcal{E}$ is the electric field. In our situation we have $\Omega = \Omega' = 0$ (since we are considering the X state), so

$$\langle J'M'|H|JM\rangle = \delta_{J,J'}BJ^2 + \mu\mathcal{E}\sqrt{\frac{2J+1}{2J'+1}}\langle J'M'|1,0;J,M\rangle\langle J'0|1,0;J,0\rangle$$

By diagonalizing this Hamiltonian we can check the perturbative calculation, get a better idea about over which ranges the perturbation is valid, and get the actual potential energy curves if we wanted to simulate a real trajectory. We calculate the Stark shifts $W(\mathcal{E})$ in the states $J = 0$ up to $J = 2$, which we shall see are the states of interest in the ranges of electric fields that we can access in the lab. We will cut off the matrix at $J = 6$ since that level is much higher in energy than $J = 0, 1, 2$; the energy of 2.8 D in 50 kV/cm is ≈ 2.4 cm^{-1}, while the rotational energy of the $J = 6$ state is ≈ 12 cm^{-1} above the $J = 2$ state. The real test is to check whether the values reported below change if we include the $J = 7$ state as well, which they do not.

The stark shifts are plotted in figure 1. To calculate the polarizability α, we fit a parabola to the Stark energy $W = \alpha\mathcal{E}^2$, as shown in figure 2

Guiding the ThO X state

Say that the electric field varies linearly from $r = 0$ to $r = R$, where it reaches a maximum value $\mathcal{E}_0$, so $\mathcal{E}(r) = (\mathcal{E}_0/R)r$. The potential energy experienced by the molecules is then

$$U(r) = \frac{1}{2}kr^2\alpha\mathcal{E}^2 = \alpha\mathcal{E}_0^2r^2/R^2 \quad \Rightarrow \quad k = 2\alpha\mathcal{E}^2/R^2$$

The spring constant ω is then given by $\omega = \sqrt{k/m} = \sqrt{2\alpha\mathcal{E}_0^2/mR^2}$, where m =248 amu. Plugging in numerical values gives

$$\omega = \frac{\mathcal{E}_0}{R}\sqrt{\alpha} \times (1.6 \text{ Hz})$$

where α is in units of $4\pi\epsilon_0\mathring{A}^3$, $\mathcal{E}$ is in kV/cm, and R is in mm. If we assume a beam forward velocity of v_0 =150 m/s, and use $\ell_{\text{guide}} = \frac{\pi}{2}\frac{v_0}{\omega}$, we have

$$\boxed{\ell_{\text{guide}} = \frac{R}{\mathcal{E}_0\sqrt{\alpha}} \times 145 \text{ m}}$$

We can consider $R/\mathcal{E}_0\sqrt{\alpha}$ as a figure of merit for guiding; notice that switching to $J = 2$ from $J = 1$ would require doubling the electric field to have the same figure of merit.

Some reasonable estimates are $\mathcal{E}_0 = 10$ kV/cm and $R = 1$ mm. We could probably go up to 50 kV/cm peak field, but remember that for an electrostatic lens we want $\mathcal{E}$ to be uniform over a radius R, thus $\mathcal{E}_0$ can be considered the maximum field value where the field is still approximately uniform.

For the smaller field of 10 kV/cm we want $J = 1$ with $|\alpha| = 12,000$, so $\omega = 360$ Hz in this case. To completely collimate the molecules, we would need a guide of length $\ell_{\text{guide}} \approx 13$ cm.

[2]See Brown and Carington, p.823

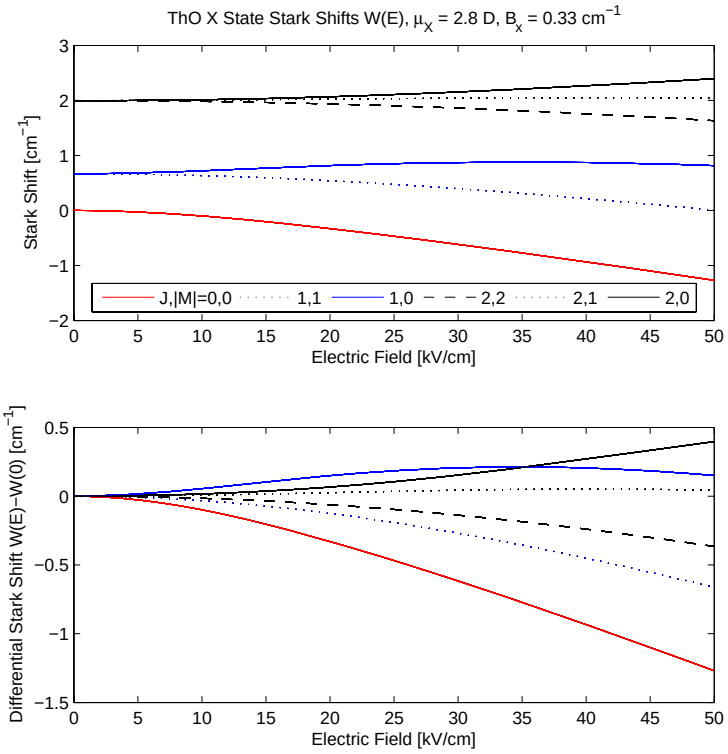

Figure 1: Calculation of stark shifts.

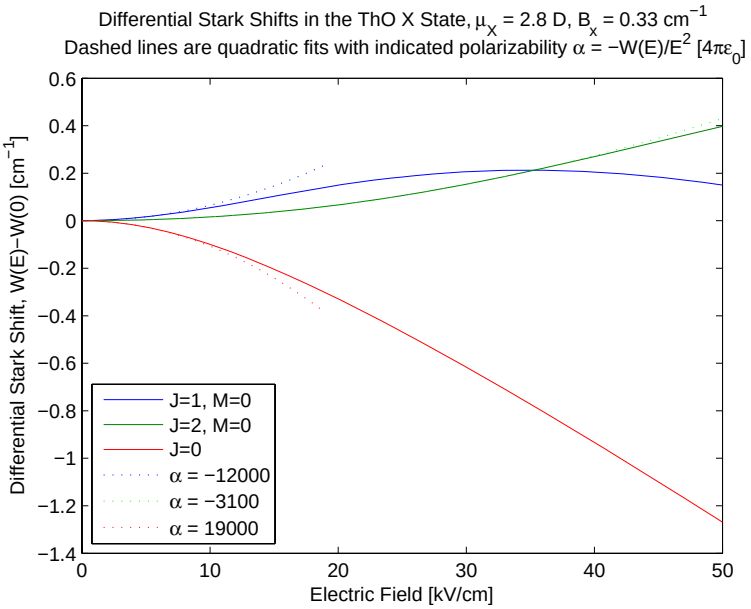

Figure 2: Calculation of polarizability.