

# THE USE OF ELECTRIC MULTIPOLE LENSES FOR BENDING AND FOCUSING POLAR MOLECULES, WITH APPLICATION TO THE DESIGN OF A ROTATIONAL-STATE SEPARATOR\*

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## Abstract

The dipole interaction (Stark effect) of a polar molecule allows one to use an inhomogeneous electric field to bend and focus a neutral beam in a transport line. The dependence of the optics on the Stark potential energy is discussed and we describe the type of multipole-field lenses that are needed. The special features that differ from charged particle optics are discussed. The RMS envelope equations are used to design a rotational-state separator to be built at LBNL. Its performance is simulated using the non-linear trajectory equations (with off-energy molecules included) and we find good state selection.

## STARK POTENTIAL ENERGY

The Hamiltonian for a non-relativistic neutral beam in an electric lens-field is  $H = \frac{1}{2} m_0 v^2 + W_S(E)$ , where  $W_S$  is the Stark potential energy which depends only on the magnitude  $E$  of the electric field and not its direction. If the derivative of the potential with respect to the field is negative  $dW_S/dE < 0$ , then the neutral particle is strong-field-seeking. This includes neutral atoms and polar molecules in the ground state, as well as all rotational states in the limit of large fields. Excited rotational states for which  $dW_S/dE > 0$ , are weak-field-seeking.

Two simple forms of the Stark interaction energy are:

(I) A constant dipole moment ( $\mu_d$ ):  $W_S = -\mu_d E$  (1)

(II) A constant polarizability ( $\alpha_p$ ):  $W_S = -\frac{1}{2} \alpha_p E^2$  (2)

Neutral atoms are strong-field-seeking, with induced dipole moments and a quadratic field dependence.

The Stark energy for polar molecules is not as simple – for methyl fluoride, an analytic approximation for the ground state gives [1]

$$W_S = -W_C(E/E_C)^2/[1 + (E/E_C)] \quad (3)$$

where  $W_C = 4.3$  K and  $E_C = 11$  MV/m. This molecule is strong-field-seeking, and the Stark energy starts from a quadratic (type-II) dependence at low fields, to a linear one (type-I) at high fields.

We do not have this variability in the interaction energy for charged particles, for which the interaction energy is the same  $W_S = q_0 \Phi$ , and the charge state  $q_0$  is constant.

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## ELECTROSTATIC LENS FIELD

A charged particle we can deflect with a dipole field and focus with a quadrupole field.

For a neutral beam, we need a quadrupole field to bend it and a sextupole field to focus it, in combination with a dipole field to provide a non-zero field on axis [2]. There is an exception for weak-field-seeking molecules, where a pure sextupole field will focus the beam linearly in both transverse planes. A disadvantage is that the field is zero at the beam center and molecules can drop out of their excited rotational state.

Choosing skew multipoles for greater horizontal clearance, the lens potential, to order ( $r^3$ ), is:

$$-\Phi = E_{y0}(z)[y + (\sigma_2/r_0)xy + (a_3/r_0^2)(x^2y - 1/3y^3) - 1/6(\sigma_2/r_0\rho_0)y^3] - 1/6E''_{y0}(z)y^3 \quad (4)$$

where  $E_{y0}$  is the vertical dipole field on midplane and  $E'_{y0} = dE_{y0}/dz$ , etc. The quadrupole field polarity is given by  $\sigma_2 = \pm 1$ , and the sextupole field strength is  $a_3$ . The curvature of the electrodes is specified by  $r_0$  the lens-field scaling length. This length  $r_0$  also determines the range of the non-linear fields which arise from the coupling between the multipole fields [1]. For example, in a simulation of a long 60°-FODO transport line [1], the dynamic aperture was found to be about 40% of the scaling length  $r_0$ . The curvature  $\rho_0$  of the optic axis in a sector bend-lens with local coordinates,  $x = r - \rho_0$ ,  $y = -Z$  and  $z = \rho_0\theta$ , contributes the  $\rho_0$ -term to the potential. The lens end fields contribute the  $E''_{y0}$ -term to the potential, and affect only the vertical motion.

The total electric field in the lens to order ( $r^2$ ) is

$$E^2 = E_{y0}^2 \{1 + 2(\sigma_2/r_0)x + [(\sigma_2^2 + 2a_3)/r_0^2]x^2 + [(\sigma_2^2 - 2a_3 - \sigma_2 r_0/\rho_0)/r_0^2]y^2\} + [E'_{y0}{}^2 - E_{y0}E''_{y0}]y^2 \quad (5)$$

and contains all the terms needed for linear optics. For calculating non-linear trajectories, the field to order ( $r^4$ ) was used.

## LINEAR OPTICS

From the Stark potential energy and the total lens field, we can now obtain the equations of motion for neutral particle linear optics.

### Trajectory Equations

These, with dispersion included, have the usual form

$$x'' + K_x x + \delta_o/\rho_o = 0 \quad y'' + K_y y = 0 \quad (6)$$

where the lens focusing strengths are

$$K_x = a_x K_O \quad K_y = a_y K_O - U_O k_{ye} \quad (7)$$

and  $k_{ye}$  is the contribution from the end field. Table 1 gives the bend and focusing parameters for the two types of Stark potential considered here.

Table 1: Lens parameters for field  $E_O$  ( $\sigma^2 = 1$ ).

Type	(I) Linear	(II) Quadratic
$W_O$	$-\mu_d E_O$	$-\frac{1}{2} \alpha_p E_O^2$
$1/\rho_o$	$\sigma_2 U_O / 2r_o$	$\sigma_2 U_O / r_o$
$K_O$	$U_O / r_o^2 = 2 / (\sigma_2 r_o \rho_o)$	$U_O / r_o^2 = 1 / (\sigma_2 r_o \rho_o)$
$a_x$	$+a_3 + \sigma_2(r_o / 2\rho_o)$	$+2a_3 + \sigma_2^2 + \sigma_2(r_o / \rho_o)$
$a_y$	$-a_3 + \sigma_2^2 / 2 + \sigma_2(r_o / 2\rho_o)$	$-2a_3 + \sigma_2^2 - \sigma_2(r_o / \rho_o)$
$k_{ye}$	$[E'_{yo}{}^2 - E_{yo} E''_{yo}] / 2E_O E_{yo}$	$[E'_{yo}{}^2 - E_{yo} E''_{yo}] / E_O^2$

The bend radius and the focusing strengths are proportional to the energy ratio  $U_O = W_O / T_E$ , where  $W_O$  is the Stark energy and  $T_E = \frac{1}{2} m_o v_E^2$  is the kinetic energy. If the lens field is static then the Hamiltonian is conserved and the kinetic energy inside is  $T_E = T_O - W_s(E_O)$ . Strong-field-seeking molecules gain energy upon entering a field while weak-field-seeking ones lose it (this is reversed on leaving). This effect with pulsed fields is used to decelerate [3] and bunch neutral beams. The inverse energy ratio  $|U_O^{-1}|$  can also be taken as a measure of the rigidity of a neutral beam, and the dispersion term in Eq.(6) is given in terms the deviation  $\delta_o = \delta U_O / U_O$ .

In the bend lenses the total dimensionless multipole field strengths ( $a_x, a_y$ ), plotted in Fig.1, are controlled by the sextupole component  $a_3$  – equivalent to the field-index in a gradient bend magnet. If  $a_x > 0$ , a strong-field-seeking molecule ( $U_O < 0$ ) is defocused in the x-plane, while a weak-field-seeking will be focused.

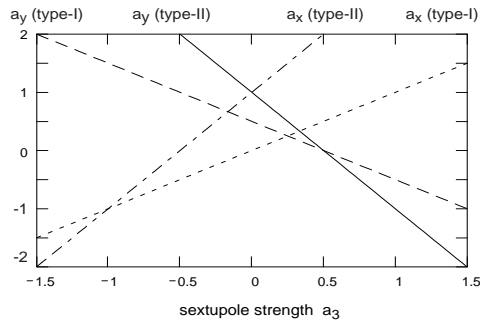


Figure 1: Total multipole strengths  $a_x$  and  $a_y$ .

We see that for  $a_3 = \frac{1}{4}$  (type-I), or 0 (type-II), a bend lens has equal defocusing for strong-field-seeking molecules, but equal focusing for weak-field-seeking ones. This can be used to make the size of a synchrotron ring much smaller for a weak-field-seeking molecule [4].

The vertical focusing by the end field is significant, since the field goes to zero over a short distance. A complication is that the end fields are affected by the location and potential of neighboring electrodes. For example, by using a short lens spacing and equal fields, we can make the end-field focusing negligible between the two lenses.

As a model for the lens end field next to a drift space, we can use the field of two parallel plates with half-gap  $r_p$ . The axial field  $E_{yo}$  with its derivatives, and the resulting vertical focusing field  $k_{ye}$  (type-I), are plotted in Fig.2.

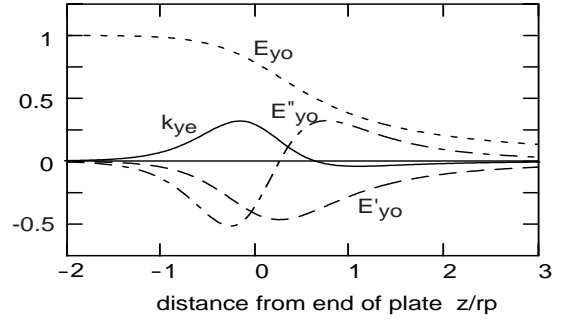


Figure 2: Parallel plate end fields (normalized to 1).

The first term  $E'_{yo}{}^2$  is the dominant one and is always positive, so both ends act the same, with focusing for weak-field-seeking and defocusing for strong-field-seeking molecules. In general  $k_{ye}$  can have a number of focusing regions of different sign, such as the negative tail in Fig.2.

Since the lens field scales with the half-gap  $r_p$ , we can approximate the end-field focusing by a constant strength  $k_{ye} \approx a_{ye} / r_p^2$  over an effective length  $L_{ye} \approx \lambda_{ye} r_p$ . The parameters  $a_{ye}$  and  $\lambda_{ye}$  will depend on the electrode shape, and for the separator electrodes with curved ends (radius  $\frac{1}{2} r_p$ ) we estimate  $a_{ye} = 0.175$  and  $\lambda_{ye} = 1$ .

### RMS Envelope Equations

A beam can be characterized by the second moments of the distribution function

$$\begin{aligned} \sigma_x^2 &= \epsilon_x \beta_x & -\sigma_{xx'} &= \epsilon_x \alpha_x & \sigma_x'^2 &= \epsilon_x \gamma_x \\ \sigma_y^2 &= \epsilon_y \beta_y & -\sigma_{yy'} &= \epsilon_y \alpha_y & \sigma_y'^2 &= \epsilon_y \gamma_y \end{aligned} \quad (8)$$

which we can express in terms of the associated envelope functions ( $\beta, \alpha, \gamma$ ), and the invariant RMS emittances

$$\epsilon_x = (\sigma_x^2 \sigma_x'^2 - \sigma_{xx'}^2)^{1/2} \quad \epsilon_y = (\sigma_y^2 \sigma_y'^2 - \sigma_{yy'}^2)^{1/2} \quad (9)$$

with the envelope functions related by

$$\gamma_x \beta_x - \alpha_x^2 = 1 \quad \gamma_y \beta_y - \alpha_y^2 = 1 \quad (10)$$

This gives us the RMS envelope equations, F. J. Sacherer [5], in a form independent of the emittance,

$$\begin{aligned} \beta_x' + 2\alpha_x &= 0 & \beta_y' + 2\alpha_y &= 0 \\ \alpha_x' + \gamma_x - K_x(z)\beta_x &= 0 & \alpha_y' + \gamma_y - K_y(z)\beta_y &= 0 \end{aligned}$$

$$\gamma_x' - 2K_x(z)\alpha_x = 0 \quad \gamma_y' - 2K_y(z)\alpha_y = 0 \quad (11)$$

which apply to all phase-space particle distributions.

### BERKELEY MOLECULAR SEPARATOR

The Berkeley molecular separator (BMS) consists of a jet source followed by a triplet of focusing lenses Q1F-Q2D-Q3F, that transport the beam to a focusing doublet Q4D-Q5F and a horizontal-bend lens BH1. The design optics with the acceptance beam sizes ( $\sigma_x$ ,  $\sigma_y$ ) and the horizontal dispersion  $\eta_x$ , is shown in Fig.3.

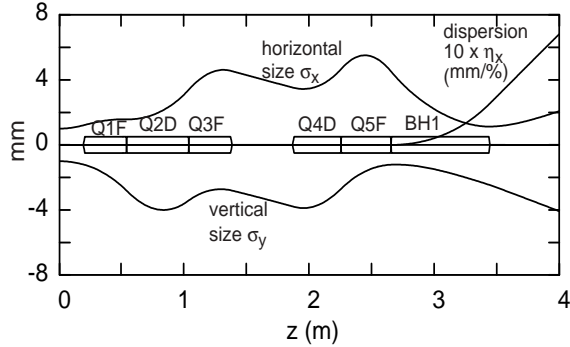


Figure 3: Berkeley Molecular Separator (BMS).

Table 2, lists the BMS separator elements, together with their focusing parameters. The lens fields given are for the ground state of the 196.5 K (310 m/s) methyl fluoride beam that will be used to test the separator.

Table 2: BMS separator parameters

	$L_{\text{eff}}$ cm	$E_0$ MV/m	$K_0$ $\text{m}^{-2}$	$a_3$	$r_0$ mm	$r_p$ mm
Drift	19.80					
End	0.40		17.9			
Q1F	34.05	2.51	7.26	-1	15	4
Q2D	49.80	2.51	7.24	+1	15	4
Q3F	34.05	2.51	7.26	-1	15	4
End	0.40		17.9			
Drift	49.60					
End	0.40		17.5			
Q4D	38.25	2.48	7.10	+1	15	4
Q5F	40.00	2.74	8.45	-1	15	3.5
BH1	78.74	3.00	7.96	0.5	16.74	3
End	0.30		43.1			

The horizontal bend-lens BH1 deflects the beam  $3^\circ$ , with a bend radius of 15 m and a sextupole field  $a_3 = 0.5$ , so vertically it's a drift space (Fig.1). There are cleanup collimators just upstream of the triplet and doublet lenses and a final one 16 cm downstream of BH1.

The lens apertures and non-linear forces, limit us to beam acceptances of about 3.5 mm-mr in both planes. The initial jet-source aperture radius is 1 mm, so the angular acceptance is  $\pm 3.5$  mr. The kinetic energy acceptance, from the simulations, is about 2 % RMS.

At the last collimators ( $z = 3.6$  m), the horizontal mono-energetic beam size is 1.3 mm and the dispersion is 0.373

mm/%. This should allow us to separate rotational states that differ in rigidity by 10 to 20%. The lens fields for  $\text{CH}_3\text{F}$  are low enough that we can scan over rotational states three times as rigid.

The BMS separator performance was simulated using the nonlinear trajectory equations with beam energy spread included. Fig.4 shows the transverse particle distribution just after the last collimators ( $z = 3.6$  m), for three rotational states with rigidity  $\delta_0 = 0, \pm 10\%$ , and an initial 2 % RMS energy spread. Here, Fig.4(a) is the distribution for no collimators, and Fig.4(b) with them – resulting in a well separated beam.

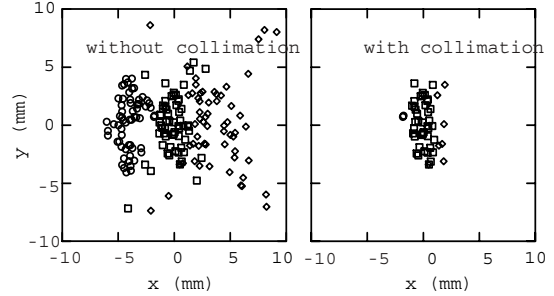


Figure 4: Separation of rotation states with  $\delta_0 = -10\%$  (circles), 0 (squares),  $+10\%$  (diamonds).

### CONCLUSIONS

Neutral beam optics is significantly affected by the sign and the electric field dependence of the Stark potential. Electric multipole lenses can be used to bend and focus beams of neutral atoms or polar molecules, but they have inherent non-linear fields that limit the acceptances. Optics for strong-field-seeking molecules is made more difficult by the defocusing in the end fields and from the quadrupole component in the bend field.

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### REFERENCES

- [1] J. G. Kalnins, G. Lambertson, and H. Gould, "Improved Alternating Gradient Transport and Focusing of Neutral Molecules", Rev. Sci. Instr. 73, 2557 (2002); LBNL-49088
- [2] G. Lambertson, "Beam Dynamics in a Storage Ring for Neutral (Polar) Molecules", in this proceedings, Portland, May 2003.
- [3] J. A. Maddi, T. P. Dinneen, and H. Gould, Phys. Rev. A 60, 3882 (1999).
- [4] H. Nishimura, G. Lambertson, J. G. Kalnins, and H. Gould, "Lattices for Milli-eV Neutral Molecules", in this proceedings, Portland, May 2003.
- [5] F. J. Sacherer, IEEE Trans. Nucl. Sci., NS-18, 1105 (1971)