Guiding slow polar molecules with a charged wire

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We demonstrate experimentally the guiding of cold and slow ND$_3$ molecules along a thin charged wire over a distance of $\sim 0.34$ m through an entire molecular beam apparatus. Trajectory simulations confirm that both linear and quadratic high-field-seeking Stark states can be efficiently guided from the beam source up to the detector. A density enhancement up to a factor 7 is reached for decelerated beams with velocities ranging down to $\sim 150$ m/s generated by the rotating nozzle technique.

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I. INTRODUCTION

Considerable experimental effort is directed towards creating dense samples of cold molecules for precision measurements [1], cold chemistry experiments [2–7], quantum information processing [8], degenerate quantum gases with dipolar interactions [9], etc. Established techniques for generating velocity controlled or trapped cold molecules include the deceleration using time-varying electric [10], magnetic [11, 12] and optical fields [13] and the velocity filtering of polar molecules out of an effusive source using static or time-varying electric fields [14, 15]. Alternative routes to producing cold molecules have been demonstrated utilizing the kinematics in elastically or reactively colliding molecular beams [16, 17].

A more general and conceptionally simple approach to producing slow beams of cold molecules is translating a supersonic jet to low longitudinal velocities by means of a rapidly counter-rotating nozzle. This technique was demonstrated by Gupta and Hershbach [18, 19] and recently improved in our group [20]. Using this technique we have demonstrated the production of dense beams of various atomic and molecular species with tunable velocity ranging from thousand of m/s down to $\lesssim 100$ m/s.

Since the molecules are not confined to any external potential this technique suffers from the drawback that beam density rapidly decay due to transverse beam expansion during beam propagation from the nozzle to the interaction region. This effect can be partly compensated by installing additional guiding elements such as electrostatic quadrupole guides [20]. However, such extended objects cannot easily be brought close to either the nozzle or the interaction region. Besides, electrostatic quadrupole or higher multipole guides produce confining potentials only for molecules in low-field-seeking rotational states.

As an alternative guide geometry we use a thin charged wire in this work, which is spanned through the whole molecular beam apparatus from the rotating nozzle up to the quadrupole mass spectrometer (QMS) that we use as a detector. This concept was proposed by Sekatskii [21, 22] and experimentally demonstrated by Loesch [23]. Recently, guiding of polar molecules in surface-based electrostatic potentials has been demonstrated [24, 25]. In our arrangement we capture the trapable molecules already in the supersonic expansion region and guide them all the way close to the detector. By comparison with classical trajectory simulations we find that ND$_3$ as well as CHF$_3$ molecules are guided in high-field-seeking states that feature both a linear and a quadratic Stark effect. An enhancement of the beam density on the beam axis due to the guiding effect of up to a factor 7 is measured for decelerated beams with velocities $v \lesssim 150$ m/s. The guiding concept is characterized in terms of optimum geometries and in terms of the applicability to slow molecules in the ground state.

II. EXPERIMENTAL SETUP

The experimental arrangement is identical to the one reported earlier [20] with the difference that the quadrupole guide placed between skimmer and QMS detector is replaced by a thin wire, as schematically shown in Fig. 1. We use a gold-plated beryllium-copper (BeCu) wire with a radius $R_w = 25 \mu$m. The total length of the wire from the jet expansion region up to the suspension in front of the detector amounts to 34 cm. The wire is attached at one end to a $x-y$-translation stage placed inside the source chamber such that the wire can be aligned transversally with respect to the beam axis to pass close by the nozzle (100 $\mu$m in diameter) and concentrically through the skimmer that has an aperture of 1 mm in diameter. Further downstream the wire passes through an intermediate chamber that serves as a differential pumping section and is suspended inside the detector chamber by a perpendicularly spanned second isolated copper (Cu) wire 15 mm in front of the crossed beam ionizer of the QMS. The BeCu wire is held under tension by a weight of 20 g such that the wire curvature at the point of suspension can be assumed to follow the radius of the Cu wire (50 $\mu$m). Owing to the resulting kink in the electric field a large fraction of the guided molecules are output coupled and enter the detection region of the ionizer of the QMS.
guiding efficiency was found to diminish considerably in
by setting the skimmer to high voltage. However, the
rotor arm. Sparking to the skimmer can be prevented
from the wire to either the skimmer or to the bored ti-
mum applicable voltage is limited to
age feedthrough inside the source chamber. The maxi-
mized directly in the guiding potential of the wire. Both
the filament and the channeltron were biased to constant
voltages with respect to the wire in order to ensure that
the detection efficiency is independent of the wire volt-
age. The measured signals followed the same trends as
the signals recorded using the QMS. However, a high
background signal level from ionized background gas and
fluctuating signal offsets caused the results to be less in-
dicative than those measured with the QMS.

The guide wire is electrically connected to a high volt-
age feedthrough inside the source chamber. The maxi-
mum applicable voltage is limited to \( U \approx 2.2 \text{kV} \) with re-
spect to the surrounding vacuum chambers by sparkover
from the wire to either the skimmer or to the bored ti-
nium ferrule that forms the nozzle at the tip of the
rotor arm. Sparking to the skimmer can be prevented
by setting the skimmer to high voltage. However, the
guiding efficiency was found to diminish considerably in
this case. Therefore all measurements presented here are
performed with the skimmer set to ground potential and
with a minimum distance \( \Delta x \) between the center of the
nozzle orifice and the wire center \( \Delta x \approx 350 \mu \text{m} \) to avoid
sparking. This, in turn, means that the nozzle is dis-
placed away from the beam axis by the same distance
since the wire is coaxially with the beam axis. As a re-
sult, the peak density of the transmitted beam without
guide voltage is reduced by about a factor 4 as compared
to the situation when no wire is installed and when the
nozzle position is optimized (\( \Delta x = 0 \)).

In the present study we use ND\(_3\) as test molecules to
demonstrate the potential of the charged wire setup
for guiding slow polar molecules. Since the energy dif-
ference between the vibronic ground state \( J = 0 \) and
the lowest rotationally excited state \( J = 1 \) is about
8.3 cm\(^{-1}\) mostly these two states are thermally populated
at the estimated low rotational temperatures in the jet
of \( T \lesssim 10 \text{K.} \) ND\(_3\) is particularly well suited for guid-
ing and deceleration experiments using electric fields due
to the strong linear Stark effect of both the high-field-
seeking state \( |J, KM\rangle = |1, 1\rangle \) and the low-field-seeking
state \( (1, 1, -1) \) correlating to \( J = 1 \) rotational level which
arises from the small inversion splitting in the absence of
electric fields [26]. The rovibronic ground state \( |0, 0\rangle \)
is high-field-seeking and features quadratic Stark effect.
When placing a ND\(_3\) molecule in the electric field of a
cylindrical capacitor at a distance \( r \) from the center,

\[
E(r) = \frac{U}{\ln(R_0/R_w)} \frac{1}{r},
\]

created by the charged wire of radius \( R_w \) inside a vac-
uum apparatus that is assumed to have cylindrical sym-
metry with inner radius \( R_0 \approx 20 \text{mm} \) we obtain a trans-
verse trapping potential \( V \) that scales as \( V(r) \propto r^{-1} \)
for the linear Stark state \( |1, 1\rangle \) and as \( V(r) \propto r^{-2} \)
for the ground state \( |0, 0\rangle \), see Fig. 2. The shaded area in
the center of the figure indicates the range excluded by
the wire. While the potential \( V \) is attractive for both
states in the shown range of distances \( V \) is much deeper

\[
\begin{align*}
\text{FIG. 1: Schematic representation of the experimental setup} \\
\text{used for guiding slow polar molecules along a thin charged} \\
\text{wire.}
\end{align*}
\]

\[
\begin{align*}
\text{FIG. 2: Transverse guide potential of ND}_3 \text{ molecules in ro-} \\
\text{tational states } |J, KM\rangle = |0, 0\rangle \text{ (quadratic Stark effect) and} \\
|1, 1\rangle \text{ (linear Stark effect). A wire diameter of 50\,\mu\text{m} \text{ and an} \\
\text{applied voltage } U = 1.5 \text{kV is assumed.}
\end{align*}
\]
and higher fields. Therefore a guiding effect may be expected only for a certain range of velocities in which the molecules are transiently bound to the wire and reach the detector before crashing into the wire or being expelled away from it. This situation is discussed in more detail at the end of the following section. Note that in the experiment performed by Loesch [23] using alkali-halide molecules even the rotational ground states were subjected to a $r^{-1}$-potential due to “brute force” orientation as a result of much larger dipole moments and higher fields.

III. CHARACTERIZATION OF WIRE-GUIDED BEAMS

The guiding efficiency characterized in this section is determined by comparing the detected beam density when switching on the wire voltage $U$ against the density of the unguided beam when the wire potential is set to ground ($U = 0$). Such a measurement using ND$_3$ (15%) seeded in krypton (85%) for variable beam velocities is depicted in Fig. 3 as open ($U = 0$) and as filled ($U = 2\, \text{kV}$) symbols. The drop of the absolute density of molecules (Fig. 3 (a)) with decreasing beam velocity is due to the transverse and longitudinal dispersion of the beam. This behavior is well reproduced by simple considerations based on the expansion of a bunch of molecules that has Gaussian velocity distributions in longitudinal and transverse directions (dotted line) [20]. Clearly, this drop can be mostly compensated by the wire guide when applying high voltage $U$ to the wire (filled symbols). Note that guiding is particularly efficient at low velocities in proportion to the unguided beam. The relative density increase due to guiding we call enhancement, which is illustrated in Fig. 3 (b). Thus, at beam velocities around 150 m/s we measure an increased beam density by up to a factor 7. A second measurement was done after the wire was replaced and newly aligned with respect to the nozzle, skimmer, and QMS detector. The two measurements are in good agreement at high beam velocities, whereas at low velocities there are slight deviations probably due to a slightly different distance $\Delta x$ between the nozzle and the wire.

The solid lines depict the result of classical trajectory simulations which account for the thermal population of rotational levels $J = 0$ and $J = 1$ at $T = 7\, \text{K}$ as well as for nuclear spin statistics [28]. Initial values for the spatial and velocity coordinates are determined by a Monte-Carlo method according to Gaussian velocity distributions and a longitudinal spatial slit opening function of the arrangement determined from fits to the experimental time of flight measurements of the unguided beam at various beam velocities [20]. One data point reflects the average of 5000 trajectories bound to the wire potential for each of the 10 rotational states correlating to $J = 0$ and $J = 1$. The two solid lines result from the same simulation and merely reflect the uncertainty in the effective cross section of the ionizer of the QMS. The upper and lower lines correspond to estimated circular cross sections with radius $R_D = 1.5\, \text{mm}$ and $R_D = 2\, \text{mm}$, respectively. Irrespective of this uncertainty, the simulation tends to overestimate the guiding effect. Possible detrimental effects in the experiment that are not accounted for in the simulation include modulations of the guide potential along the beam axis due to drastically changing outer radius $R_0$ of the assumed cylindrical capacitor configuration in particular when passing through the skimmer as well as the unknown efficiency of the output coupling process at the wire bend in front of the detector. According to the simulations, the enhancement of

FIG. 3: (a) Absolute peak densities of beams of decelerated ND$_3$ molecules detected behind the wire guide for wire voltage on (2 kV) and off (0 V). The dashed line represents a model of the free jet expansion based on Gaussian transverse velocity distributions. (b) Relative enhancement of the peak density due to guiding by the charged wire. The solid lines show the result of trajectory simulations (see text).
the guiding effect will rise steeply to exceed a factor of 10 as the speed of the molecules is further reduced below ~150 m/s. Unfortunately we did not reach this velocity range with the present setup due to the limited maximum rotor frequency (\(\lesssim 300 \text{ Hz}\)) [20].

The measured enhancement of the molecule density due to guiding as a function of the wire voltage \(U\) for different beam velocities \(v_0\) is depicted as symbols in Fig. 4(b). As \(U\) increases, the number of guided molecules grows monotonically, leading to a relative enhancement factor of up to 7 at \(v_0 = 150 \text{ m/s}\). At high voltages the enhancement slightly saturates. This is due to the dominating contribution of the linear Stark state \(|1,1\rangle\) which saturates at voltages \(U \gtrsim 1 \text{ kV}\), shown in Fig. 3(a). In this voltage range nearly all molecules in the guidable \(|1,1\rangle\)-state are actually captured by the confining wire potential.

The quadratic Stark state \(|0,0\rangle\) contributes much less in spite of its larger relative population as a consequence of the much weaker guide potential (see Fig. 2). The solid lines in Fig. 4(b) depict the results of trajectory simulations for \(v_0 = 150 \text{ m/s}\) when averaging over all Stark states correlating to \(J = 0\) and \(J = 1\). Again, \(R_D = 1.5 \text{ mm}\) and \(R_D = 2 \text{ mm}\) are assumed (upper and lower lines, respectively). Although the trend of a monotonically increasing guiding efficiency as a function of \(U\) is well reproduced, saturation sets in earlier in the simulation than in the experiment. This is presumably due to imperfections in the experimental setup as mentioned above.

The dependence of the enhancement factor on the distance \(\Delta x\) between the center of the charged wire and the nozzle orifice is shown in Fig. 5. In this measurement, the wire voltage is set to a moderate value \(U = 1.5 \text{ kV}\) to avoid sparking, the beam velocity is held constant at \(v_0 = 310 \text{ m/s}\), and the distance between the wire and nozzle is varied from 500 \(\mu\text{m}\) down to the minimum distance of about 350 \(\mu\text{m}\). This is achieved by shifting the whole baseplate that supports the rotating nozzle setup with respect to the position of the charged wire which is kept fixed. In this way, the geometry of the guiding field and of the detector is maintained unchanged during the measurement. Note that the nozzle to wire distance is obtained by viewing the nozzle position through a telescope along the wire axis. Therefore the value of \(\Delta x\) must be regarded as an estimate with an uncertainty of about 50 \(\mu\text{m}\).

![Figure 4](image1.png)

**FIG. 4:** (a) Simulated relative enhancement of the peak density of ND₃ molecules in the high-field-seeking states \(|J, KM\rangle = |0,0\rangle\) and \(|1,1\rangle\) due to guiding by the charged wire as a function of wire voltage for a beam velocity \(v_0 = 150 \text{ m/s}\). (b) Enhancement of the measured ND₃ peak density for various beam velocities (symbols). The calculations show the average of trajectory simulations for the low energy Stark states correlating to \(J = 0\) and \(J = 1\) and for two effective detector cross sections with radius \(R_D = 1.5 \text{ mm}\) and \(R_D = 2 \text{ mm}\) (upper and lower lines, respectively).

![Figure 5](image2.png)

**FIG. 5:** Measured (symbols) and simulated (lines) enhancement of the ND₃ peak density due to guiding by the charged wire as a function of the distance \(\Delta x\) between the center of the nozzle orifice and the center of the wire. The beam velocity and wire voltage are fixed to \(v_0 = 310 \text{ m/s}\) and \(U = 1.5 \text{ kV}\), respectively.
of molecules that pitch into the wire (dashed line). Possibly the position of the maximum shifts down to lower velocities as the wire radius is further reduced. Thus we conclude that while the charged wire may be useful for guiding beams of ground state molecules at moderate velocities in the range of hundreds of m/s, it is inapplicable for molecules decelerated well below $v_0 \sim 100 \text{ m/s}$.

IV. SUMMARY AND OUTLOOK

In conclusion, we have demonstrated that a simple thin charged wire placed along the axis of a beam of decelerated polar $ND_3$ molecules can be used for enhancing the molecule density even at the exit of the wire guide by up to a factor 7. $ND_3$ and $CHF_3$, that was also used, show similar guiding behavior for comparable experimental parameters. Classical trajectory simulations are found to be in reasonable quantitative agreement with the measurements and to reproduce well the systematic trends. While rotational states with linear Stark effect are guided along the wire in stable Kepler orbits the quadratic ground state is only transiently enhanced at $\sim 10 \text{ m/s}$ the guiding efficiency goes down again due to a sharp drop of the electric field. However, for practical reasons such as stability against tensile stress and electric sparkover we chose the BeCu wire with 50\,\mu m diameter.

The simulations presented so far show that $ND_3$ in both the linear $|1, 1\rangle$ and the quadratic Stark state $|0, 0\rangle$ can be guided along the charged wire in spite of the trajectories in a $r^{-2}$-potential being unstable. Therefore the question arises, under which conditions this instability becomes apparent as reduced guiding efficiency. In order to illustrate this effect we simulate the enhancement of the density of $ND_3$ molecules in the ground state $|0, 0\rangle$ for beam velocities reaching down to $v_0 \sim 20 \text{ m/s}$ (Fig. 7). The wire voltage $U = 1.5 \text{ kV}$, the nozzle position $\Delta x = 350 \mu m$ and the wire radius are held constant. As the velocity is decreased from $v_0 = 400 \text{ m/s}$ down to $v_0 = 100 \text{ m/s}$ the density enhancement first rises similarly to the state-averaged density shown in Fig. 6. However, at lower beam velocities $v_0 < 100 \text{ m/s}$ the guiding effect sharply breaks down due to an increasing fraction of molecules that pitch into the wire. Possible technical improvements of the present setup include a new nozzle design with a thinned end cap of the titanium ferrule in order to reduce the distance between the nozzle orifice and the wire surface down to $\sim 100 \mu m$. In this way both the guiding efficiency with respect to $U = 0$ is enhanced and the absolute beam intensity is increased due to better beam alignment. Furthermore, the wire voltage could be increased up to $U \gtrsim 3 \text{ kV}$ by insulating the tip of the rotor against the vacuum apparatus to suppress sparking. In total, higher peak densities by
about a factor $\gtrsim 5$ as compared to the reported guided beam densities should be attainable.

Several applications of the presented concept are conceivable. Since only polar molecules experience the electrostatic guiding force in contrast to the rare-gas atoms in the carrier gas of the seeded expansion such a guiding element can be used to separate the molecules out of the carrier gas beam, in particular if an additional bend section is incorporated. The implementation of a wire guide into novel intense sources of cold molecules that rely on buffer gas cooling in combination with expansion cooling may be promising [29, 30]. Such an approach may be particularly advantageous in applications where decelerated cold molecules are to be injected into micro-structured devices such as micro-cavities or atom chips.

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