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Electronic Supplementary Information for PCCP article:

Magnetic deflection of neutral sodium-doped ammonia clusters

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S1 Mechanical deflector design

The dimensions of the deflector and its position in the deflection chamber are shown in Fig. 1b to d. All metal body parts of the deflector are machined from magnetic steel (1080 carbon steel). As mentioned in section 2.1, the deflector consists of three electromagnets, each 7 cm in length, leading to an assembled deflector length of 21 cm. Each electromagnet consists of a metal body on which a coil, made from 15 turns of insulated copper wire is mounted. The cross section of the metal body with its coil is shown in Fig. 1d. The metal bridge, placed in the centre of each coil is 5.6 cm long and 2 mm wide, and acts as a pole shoe. The flight channel reaches a maximum height of 3.75 mm. The asymmetric geometry of the flight channel creates an inhomogeneous magnetic field with a strong gradient in the *z*-direction. The coils are set in epoxy to mechanically protect them and to increase heat conduction to the metal bodies. These bodies are mounted onto a single, liquid-cooled aluminium plate. A cooling liquid consisting of 30% glycol 70% water mixture is circulated by a closed-cycle chiller at -10 °C through the aluminium plate. The deflector is mounted on two *x,z*-translation stages (one at each end) to allow fine alignment of the flight channel relative to the molecular beam. The detection skimmer is positioned 21.5 cm after the deflector exit to select the non-deflected species.

S2 Electronic deflector design

Each electromagnet is driven by a 3-stage Pulse Forming Network (PFN) circuit designed to generate a high current square pulse of 1000 A with a pulse of 270 µs. High power thyristors are used to switch the PFN circuits, which resemble Cauer topology low-pass filters using three capacitors and two inductors each. The PFNs are individually triggered by a delay generator (Stanford Research Systems DG535), using one channel for the master offset (t_d) and three others for the relative delays (t_1, t_2, t_3). Auxiliary signals (energy recovery and recharging sequences) are generated by a complex programmable logic device.

To verify the actual performance when driving an electromagnet (of about 32 µH impedance and 75 mΩ resistance), both current pulses and resulting magnetic field pulses were measured for various charging voltages. The form of a typical magnetic field response measured in our setup (about 300 µs width) is included in Fig. 2. Charging voltage is provided from an external buffer capacitor bank, which is charged by a modified programmable power supply (TDK-lambda genesis 1000-10). With the current deflector design we are able to collect data at a repetition rate of 5 Hz when pulsing the electromagnetic coils with up to 300 A peak pulses

(~150 V charging voltage). Working at higher currents is only feasible if the magnetic field pulse repetition rate is reduced. Operating the deflector with 700 A peak pulses (~350 V charging voltage) is achievable, if the repetition rate is reduced to 1 Hz. The limit in repetition rate and peak pulse currents arises from thermal loads generated in the in-vacuum coils that cannot be efficiently dissipated by our cooling method. Attempts to operate with higher thermal loads are prevented by the onset of outgassing, accompanied by a total loss of signal at about 10^{-4} mbar l/s, which we attribute to obstruction of the flight channel. As this mechanism of signal extinction would compete with signal loss due to deflection, we choose repetition rates that keep the pressure rise in the deflector chamber below 3×10^{-8} mbar. A typical base pressure in the chamber housing the deflector is about 1×10^{-7} mbar.

The pulsed deflector design introduces several time dependent effects (time dependent field strengths, eddy currents, field fluctuations along the propagation axis). Our MD model, which includes time dependent magnetic fields (see section 2.3), reproduces the observed deflection of effusive Na-atoms quantitatively over the range of magnetic field strengths studied (see section S3, and also Fig. 7 for $NaNH_3$). A magnetic deflector being operated in a pulsed manner becomes very favourable when coupled to a photoelectron spectrometer with velocity map imaging (VMI) detection. The VMI detection of photoelectrons is very sensitive to external magnetic fields. With a pulsed magnetic field, it is easier to reduce such interfering magnetic fields and measure an undistorted photoelectron image. In addition, a pulsed deflector reduces the thermal load produced in the electromagnetic coils, which facilitates miniaturization and in-vacuum placement of the complete electromagnetic setup.

S3 Deflection of effusive Na atoms

To test the performance of the deflector, we attempted to deflect sodium atoms in an effusive beam, produced by heating the sodium oven to 265 °C. Photoionization was performed with a 212 nm laser pulse and sodium ions were detected via TOF mass spectrometry. Fig. S1 shows the relative sodium TOF signal plotted as a function of t_d (circles) at I_d = 400 A (Fig. S1a) and I_d = 800 A (Fig. S1b) peak current. For comparison, the results of the MD-simulations (see section 2.3) are shown as diamonds. The experimental relative intensities and the MD-simulations show good general agreement within 2σ of the former. The standard deviation σ was determined from the four latest timings (Fig. S1a), when θ_{rel} = 1 and the field is switched

on after the detected clusters have already passed the deflector. For these initial measurements and MD-simulations, the individual coils were switched on simultaneously, $t_1 = t_2 = t_3$. For I_d = 400 A, the relative signal decreases to a minimum of approximately θ_{rel} = 0.5. By increasing the current to 800 A (Fig. S1b), a stronger depletion of θ_{rel} = 0.3 can be observed. This trend is reproduced by the MD-simulations. For our MD approach, we choose to describe the effusive sodium velocity distribution as a 1D-Maxwell-Boltzmann distribution at 265 °C convoluted with a transmission function. This transmission function emulates residual gas in the deflector channel, which preferentially transmits the higher velocities contained in the initial velocity distribution leaving the sodium oven. The transmission is mathematically described by $T(v) = 1 - \exp(-bv^2)$ where b is a fit parameter which is proportional to an effective channel pressure. The remaining signal deviations of experimental data and MD simulation may be due to inaccuracies in the modelling of the effusive sodium velocity distribution.

For light Na atoms (23 amu) deflected at these high currents, one might expect a largely reduced signal $\theta_{rel} \approx 0$. This can neither be seen in the experiment nor in the MD-simulation. The reason for this limited deflection is the broad velocity distribution (FWHM = 870 ms^{-1}) of the effusive sodium atoms (see Fig. 3b) in conjunction with the pulsed operation of the deflector. Considering the path from the deflector to the ionization volume, the flight time differences among the particles being ionized are larger than the operation time of the deflector. Therefore, only a timing-dependent fraction of the ionized particles had been exposed to the magnetic field. The amount of deflected particles can be increased by either lengthening the magnetic field pulse in time or by narrowing the velocity distribution. These two different approaches are discussed in section 3.

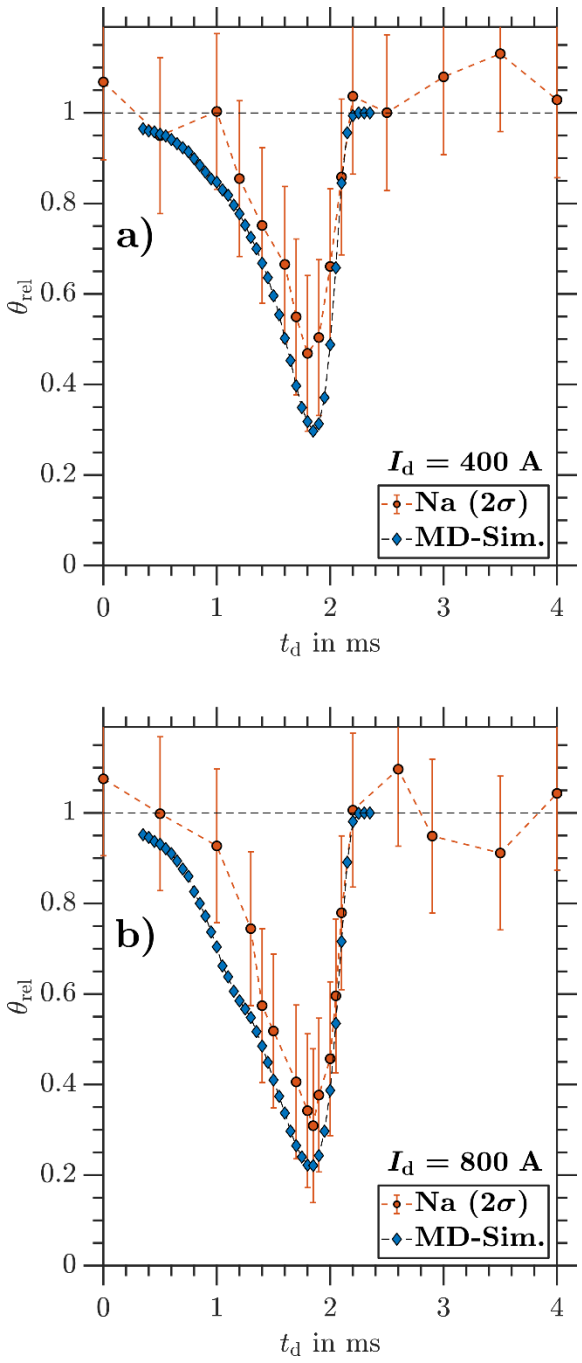

Fig. S1: Circles: relative integrated TOF signal (750 shots per data point) of Na atoms as a function of t_d. The error bars indicate an uncertainty of two standard deviations: Diamonds: MD-simulations. Examples are shown for two different electromagnet currents **a)** I_d = 400 A and **b)** I_d = 800 A.