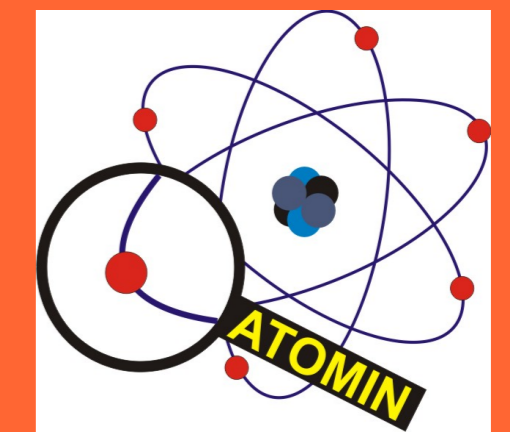


Molecular Spectroscopy  
and Quantum Information

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## Introduction

Entangled state is a specific correlated state of a system of two or more particles, in which the state of whole system is better described than the states of particular parts. In other words, the entangled state exists when the wave function of the composite system could not be represented as a tensor product of wave functions of individual components:

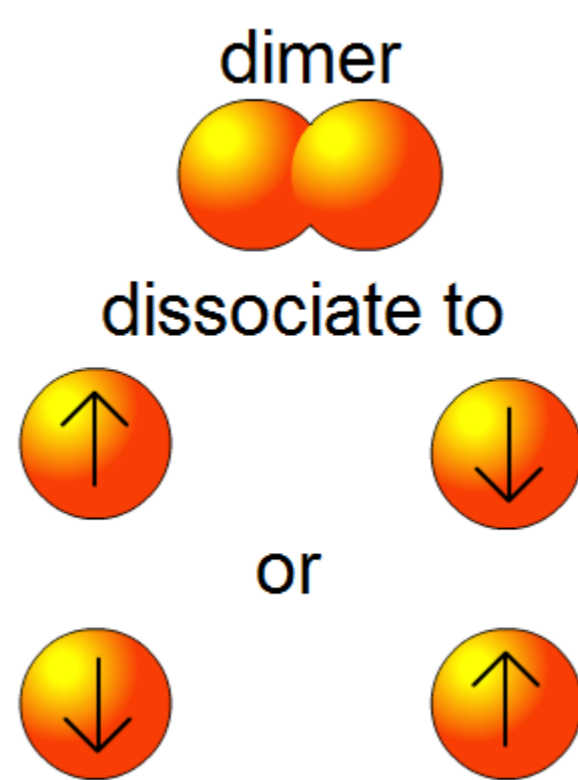
$$|\Psi_{AB}\rangle \neq |\Psi_A\rangle \otimes |\Psi_B\rangle \quad |\Psi\rangle = |\uparrow\rangle_A |\downarrow\rangle_B + |\downarrow\rangle_A |\uparrow\rangle_B$$

Consider a molecule in  $^1S_0$  state (it's orbital momentum, total electron momentum and angular total momentum are equal zero). The molecule is built with  $^{111}\text{Cd}$  atoms which has nuclear spin equal 1/2. If the molecule is dissociated during the process which conserve the momentum, the spins of resulted atoms have antiparallel orientation. Until the detection process the orientation of the spin of each atom is undefined. It means that the result of measurement process conducted on one of the two atoms, determines the spin orientation of both atoms (even if the atoms are spatially separated). The existence of process which instantly determines the results of measurements conducted on separated objects caused suspicions, that this process can violate the special relativity theory (STR) which constitutes that any interaction cannot propagate with a speed larger than the speed of light in vacuum.

In 1935 Einstein Podolsky and Rosen proposed a thought experiment, which – in intention of its authors – had indicated contradictions between Quantum Mechanics (QM) and special theory of relativity [1]. Roughly speaking they argued, that measurements conducted on entangled objects can be applied to anticipate the values of non commuting observables. So they concluded that either QM is not a complete theory (they postulated existence of so called hidden-variable theory, which should determine the results of measurement in the moment of creation of a pair of entangled object) or STR in some cases can be violated.

### Bell inequalities

In 1964 John Stewart Bell formulated and proved a theorem, that no hidden variable theory can reproduce all predictions of QM. He also formulated some inequalities, which have to be satisfied by any hidden variable theory but are violated by QM [2]. In our experiment we can test the violation of Bell-Cluser-Horne inequality by entangled cadmium atoms [3].



## General scheme of the experiment

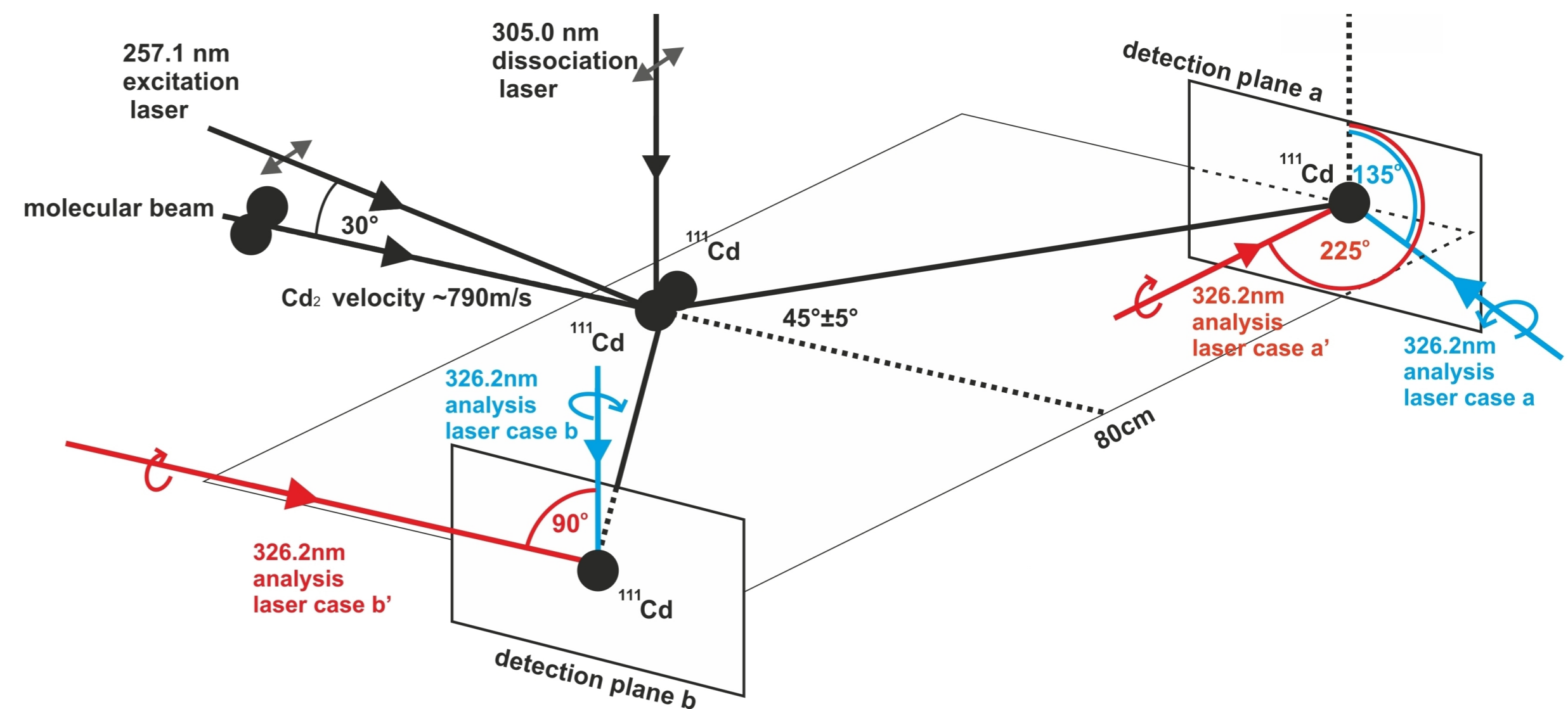


Fig. 2. The  $\text{Cd}_2$  molecule in supersonic beam is dissociated into two  $^{111}\text{Cd}$  atoms (black solid lines). In two parallel detection planes a and b, a spin selective detection of  $^{111}\text{Cd}$  atoms is taking place. The detection relies on two-photon excitation-ionization method (the ionization-laser beams are omitted for simplicity, see Fig. 5 for details). The angles between vertical direction perpendicular to the plane in which the atoms are propagating and analysis beams are selected in the way which ensures the maximum violation of Bell inequality.

## Experimental set-up

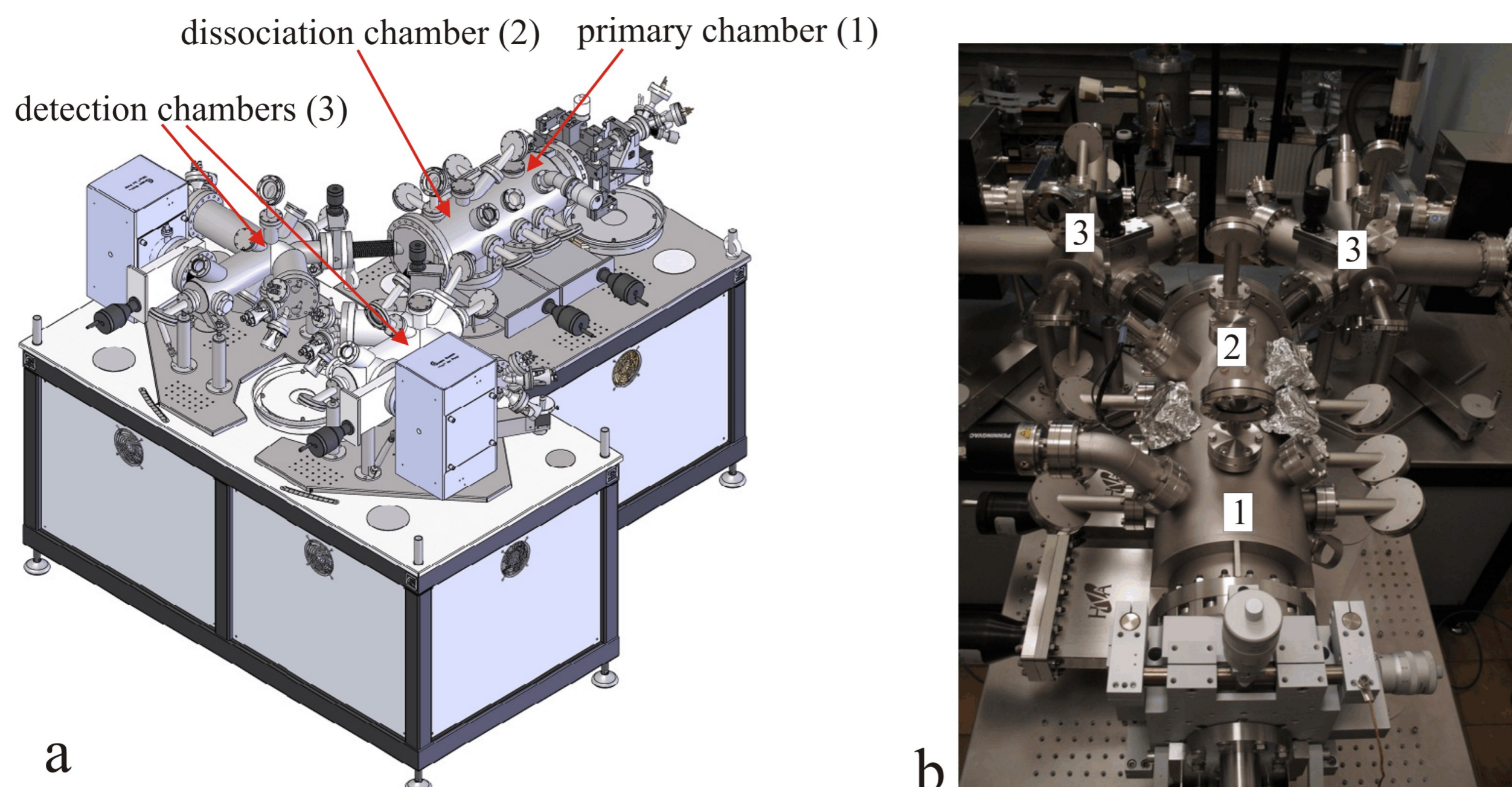


Fig. 1. (a) Visualization and (b) laboratory set-up of the apparatus. 1) *Primary* chamber in which the supersonic pulsed molecular beam source is located, 2) *dissociation* chamber, separated from the *primary* chamber by a skimmer (1.2 mm in diameter). Both *primary* and *dissociation* chambers are pumped down to  $10^{-6}$  mbar of ultimate pressure, 3) *detection* chambers in which nuclear spin selective detection of entangled atoms will be performed. Both *detection* chambers are equipped with ion pumps (ultimate pressure down to  $10^{-10}$  mbar).

## Molecular pulsed supersonic source

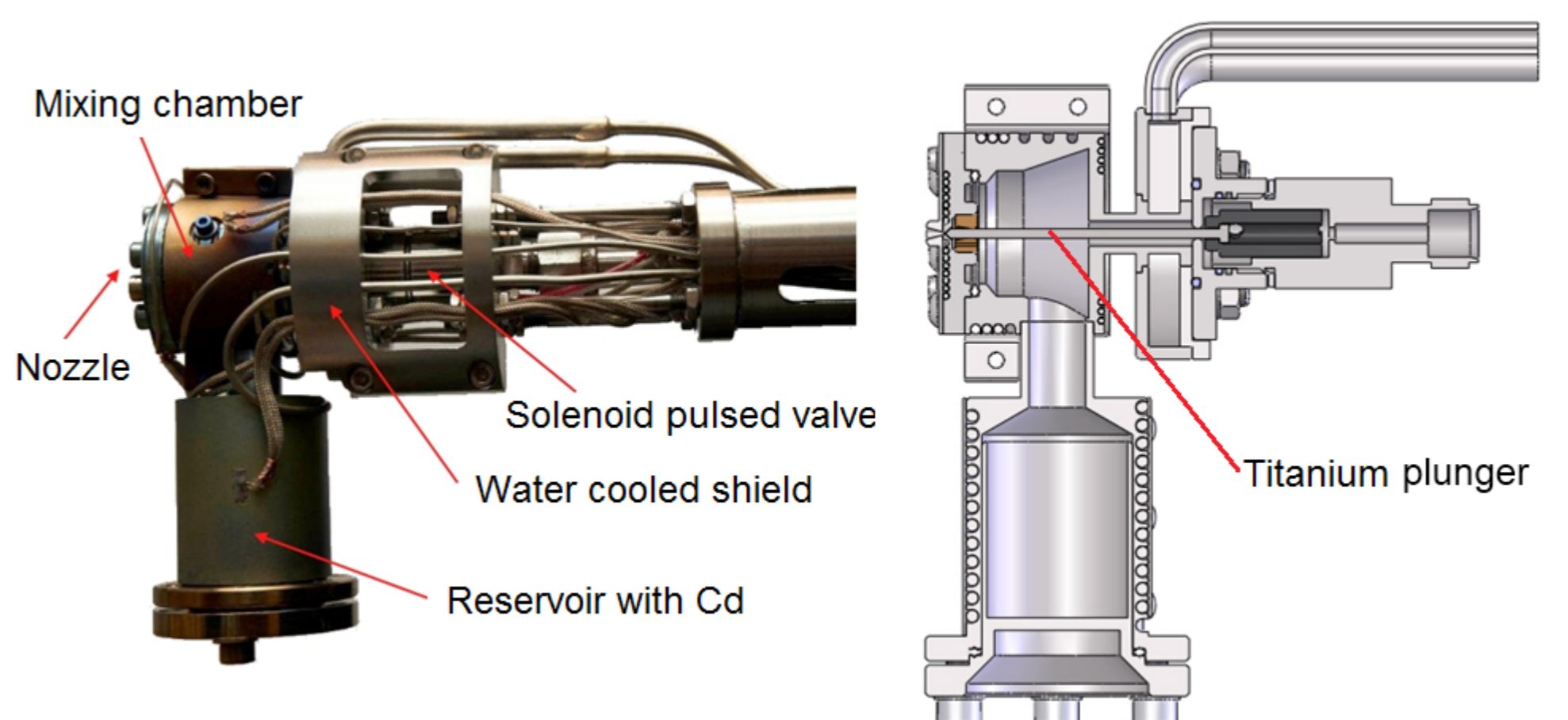


Fig. 3

In the experiment,  $\text{Cd}_2$  molecules are produced in a pulsed supersonic expansion beam. Cadmium metal is heated up to 980 K which is much higher than the cadmium melting point (594 K). Next, cadmium vapours enter the mixing chamber in which are mixed with carrier gas (noble gas, usually argon). The mixing chamber ends with a nozzle (with orifice of 0.15 mm in diameter) through which the mixture expands to the vacuum chamber forming a supersonic beam. The nozzle is periodically closed and opened with a plunger (made of titanium) with a help of electrically driven solenoid valve. Adiabatic expansion through a small orifice creates suitable conditions (internal cooling of vibrational and rotational degrees of freedom) for forming very weakly bound  $\text{Cd}_2$  van der Waals molecules.

## Creation of entangled cadmium atoms

In our experiment the ( $^{111}\text{Cd}$ - $^{111}\text{Cd}$ ) pairs of entangled atoms are produced by laser dissociation of  $^{111}\text{Cd}_2$  dimers produced in a pulsed supersonic beam (see Fig. 2). The laser dissociation of  $^{111}\text{Cd}_2$  takes place with a help of the stimulated Raman transition from the ground state  $X^1O_g^+(5^1S_0)$  via the  $A^1O_u^+(5^1P_1)$  excited and back to the repulsive part of the  $X^1O_g^+$  electronic state (see Fig. 4). Along with momentum conservation principle it creates a pair of entangled atoms each in  $(5s)^1S_0$  ground state. It is crucial, that the  $^{111}\text{Cd}$  isotope in its ground state possess only one non-zero angular momentum (nuclear spin  $I=1/2$ ) whereas the other atomic angular momenta ( $S$  – electronic,  $L$  – orbital and  $J$  – total electronic) are zero. Thus, along with the fact, that for  $^{111}\text{Cd}_2$  molecule in the  $X^1O_g^+(^1\Sigma_g^+)$  state all momenta are equal zero, it leads to the conclusion that the nuclear spins of the two  $^{111}\text{Cd}$  atoms (oriented in opposite directions) are entangled. In the process of the stimulated Raman transition it is important to excite the  $^{111}\text{Cd}_2$  molecule only to one strictly specified  $J'$  rotational level in the  $A^1O_u^+$  state. To achieve it, third harmonic of a pulsed tuneable ring alexandrite laser with 30-MHz spectral bandwidth will be used. It was estimated,

that the  $A^1O_u^+(\nu=40, J'=5) \leftarrow X^1O_g^+(\nu''=0, J''=6)$  transition, which corresponds to 257.1 nm wavelength lies in range of the third harmonic of the alexandrite laser. The dissociating transition (305.0 nm) can be stimulated by a second harmonic of tuneable Nd:YAG-laser-pumped-dye-laser with 2-GHz spectral bandwidth. It was calculated that the separation angle between the dissociated  $^{111}\text{Cd}$  atoms should be equal  $90 \pm 5^\circ$ .

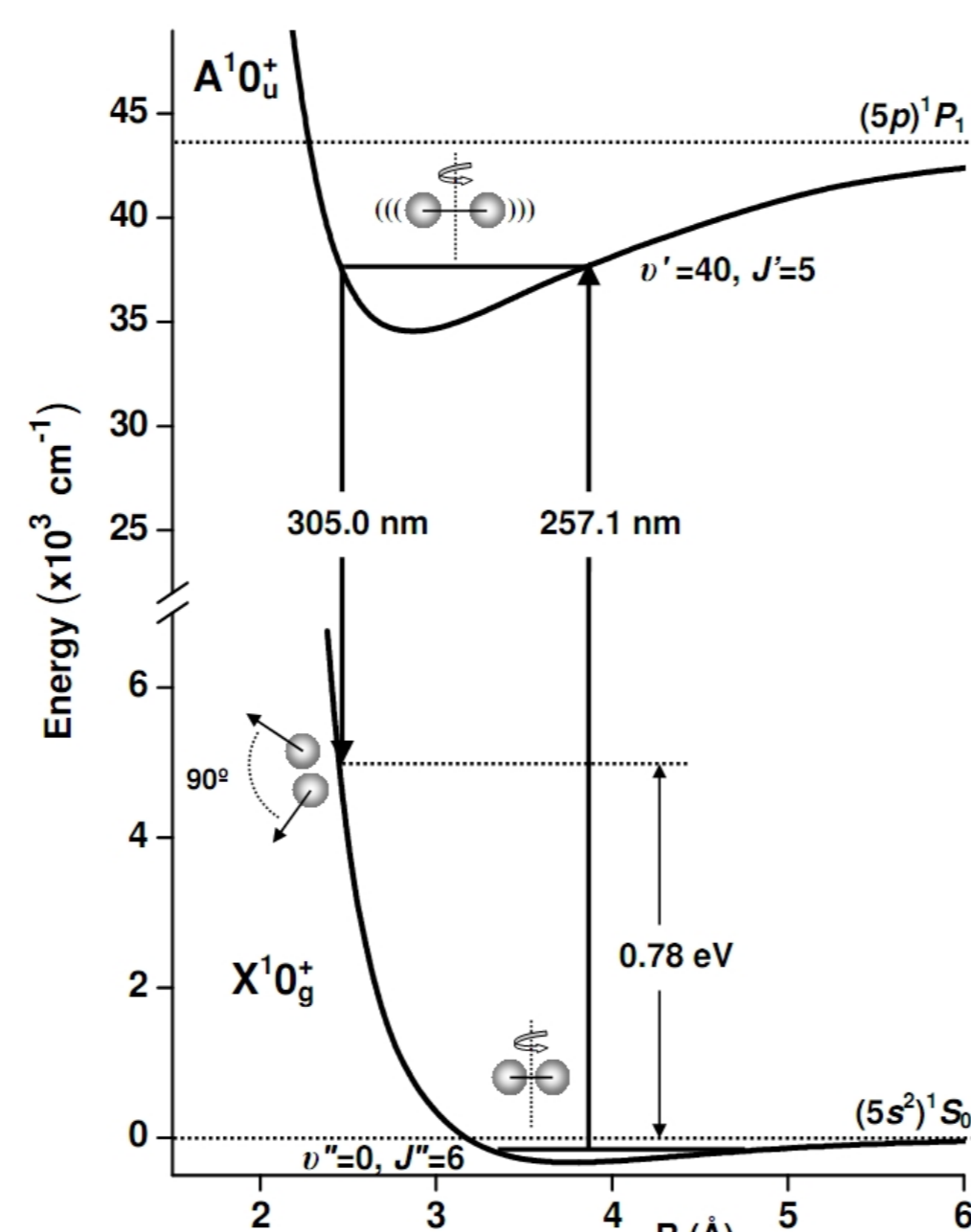


Fig. 5.

## Spin selective detection of atoms

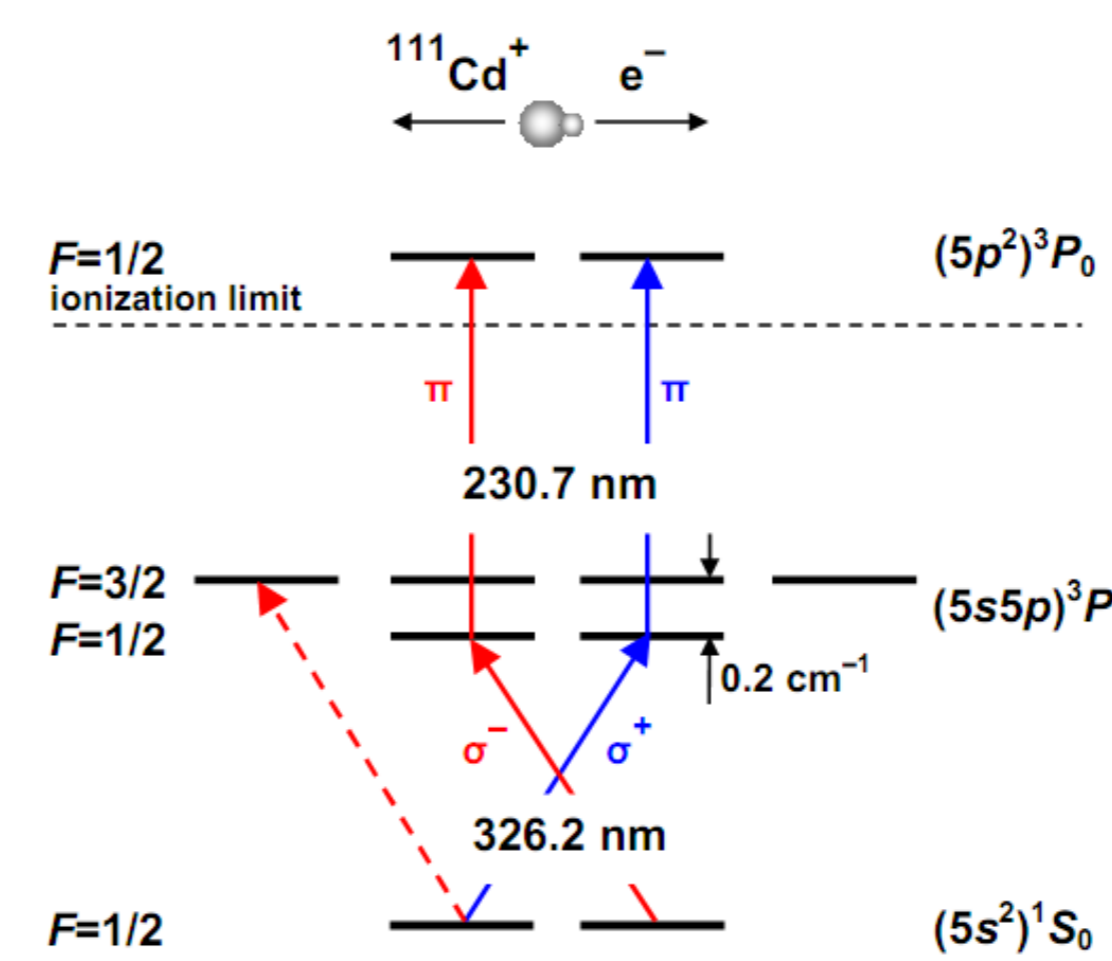


Fig. 4.

In order to selectively detect the orientation of nuclear spin we will use two-photon excitation-ionization method. Circularly polarized analysis-laser beam (326.2 nm, second harmonic of the dye laser) is spectrally sufficiently narrow (2 GHz), and can selectively excite only one  $F$  level in the hyperfine structure (HFS) of  $^3P_1$  state. The HFS splitting in this state of  $^{111}\text{Cd}$  atom is about 6 GHz ( $0.2 \text{ cm}^{-1}$ ). Along with the fact that the only non-zero angular momentum in the  $(5s)^1S_0$  state of  $^{111}\text{Cd}$  is its nuclear spin, one can anticipate that excitation of the  $^{111}\text{Cd}$  atom is possible only if orientation of the nuclear spin is properly correlated with circular polarization of the analysis-laser beam ( $\sigma^+$  and  $\sigma^-$  can only excite atoms with  $m_F = -1/2$  and  $m_F = +1/2$ , respectively). The second, ionization-laser beam (230.7 nm, second harmonic of the dye laser) is linearly polarized ( $\pi$ ) and ionizes the excited atom to the  $(5p)^3P_0$  state. After focusing by electrostatic lenses, products of the ionization process (ion and electron) can be detected by channeltrons.

## References

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## Acknowledgements

The project is financed by the National Science Centre according to the contract no. UMO-2011/01/B/ST2/00495.