MOLECULAR QUANTUM SCIENCE & TECHNOLOGY

Conference 2024

Poster Abstracts

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Poster session: Thursday February 1, 2024 @ 17:30 - 21:00 in the ATI 1st floor hallway

Please set up your poster at the numbered station indicated in the program. You may set up your poster on Wednesday and leave it up for the duration of the conference. It must be taken down by Friday @ 13:00.

Snacks & refreshments will be provided. We thank AQT for sponsoring the poster session.

AQT

Contents

1 Molecular docking with neutral atoms

Noé Bosc-Haddad
CentraleSupélec

New computational strategies are emerging that can speed up the drug discovery process, such as Virtual screening (VS). VS optimizes drug discovery by highlighting molecules that fit the target. VS structure-based methods rely on molecular docking to predict the activity of the candidate molecules at the binding site of the proteins, helping select those with desirable behavior and rejecting those with undesirable behavior. For large chemical libraries, it is desirable to search and score configurations using as few computational resources as possible but still with high precision. In this work, a mapping of the Molecular docking problem to a graph problem is performed. The graph can be mapped onto a maximum-weight independent set (MWIS) problem on a unit-disk graph (UDG) in a Physical Neutral Atom Quantum Processor, where each vertex represents an atom trapped by optical tweezers. The Variational Quantum Adiabatic Algorithm (VQAA) approach is used to solve the problem. Results using VQAA in small instances of the molecular docking problem are presented, demonstrating the potential for future NISQ applications.

2 Sensing with single organic molecules at room temperature

Anežka Dostálová
Palacký University Olomouc

Sensors based on single fluorescent molecules and their clusters hold a promise of significant advancement of quantum sensing. The implementations of such sensors are predominantly limited to cryogenic temperatures, thereby significantly reducing their applicability. We present the utilization of organic molecules as sensors operated at room temperature. We monitor statistical properties of light emitted by single molecules and their clusters and study changes in the dynamics under various ambient conditions. Our approach is based on a fluorescence microscope scheme with confocal, wide-field and total internal reflection regimes possible. A sample containing terrylene molecules embedded in a crystal host is prepared by spin-coating. Advanced techniques are utilized for emission characterization, such as multiplexed photon-number-resolving detection, photon statistics reconstruction, and novel machine learning modalities. We experimentally demonstrated the single-photon nature of light emitted by terrylene molecules. Photon statistics and correlation properties of the detected signals were examined to resolve the number of individual emitters. We are working towards enhancement of sensing abilities and the counting of single emitters aided by deep learning, ensuring less sensitivity to noise. The room temperature operation and novel statistical readout methods open the path to a broad range of new applications, including minimally-invasive and in-vivo sensing.

3 Dissipative protection of molecular rotational states against blackbody radiation and spontaneous decay

Brandon Furey
Universität Innsbruck

Novel quantum information encoding schemes are possible in the rotational degrees of freedom in molecules which are not available in atoms.[1] However, these codes are vulnerable to rotational transitions induced by the environment; namely, blackbody radiation and spontaneous decays. Encoding in a single rotational manifold may enable protection against such decoherence.[2] Theoretically, we are developing a dissipative quantum error correction (QEC) scheme which can be continuously applied to stabilize a rotational superposition. Experimentally, we aim to demonstrate state preparation, coherent control, and the creation of superpositions of rotational states in CaH^+ or $CaOH^+$ molecular ions using Raman setups with two CW laser beams and another with an optical frequency comb.[3] This could pave the way for exploring QEC codes based on trapped molecular ions.

[1] V. Albert, et al. Phys. Rev. X 10, 031050 (2020)

[2] S. Jain, et al. arXiv:2311.12324 [quant-ph] (2023)

[3] C. Chou, et al. Science 367, 1458 (2020)

4 Laser cooling Barium monofluoride molecules

Tatsam Garg
University of Stuttgart

Ultracold molecules have recently drawn widespread interest as promising platforms for precision measurements to probe fundamental physics and for studies of quantum chemistry. While their rich internal structure complicates the realisation of direct laser cooling, there has been significant progress towards this goal over the last two decades. We will report on the experimental realisation of laser cooling for the bosonic isotopologues of barium monofluoride (BaF), a polar diatomic molecule. Due to its high mass, resolved hyperfine structure in the excited state, and narrow linewidths, this molecular species is notoriously difficult to cool. We will present our progress leading up to the first observation of Sisyphus-type forces in one-dimensional transversal cooling of ^{138}BaF. In this, we present a characterization of the molecular beam, observations and characterization of long lasting optical cycling with on the order of 500-1000 scattering events, and high-fidelity imaging and optical cycling in the rare isotopologue ^{136}BaF. Our work has enabled the laser cooling of the abundant species, and paved the way to readily extend the technique to its rare bosonic isotopologues.

5 Towards ultracold Calcium monofluoride molecules

Phillip Groß
5. Physikalisches Institut, Universität Stuttgart

The production of ultracold molecular quantum gases promises to add long-range dipolar interactions to the quantum simulation toolbox. Here we first show theoretically that such dipolar interactions can lead to the formation of new phases of matter in bulk molecular Bose-Einstein condensates, such as droplet states and supersolids. Second, we present a setup to realize these phases of matter in an experiment. In this setup we work with calcium monofluoride molecules, which are characterized by large electric dipole moments and well-established laser cooling strategies. In a first step to create a gas of these molecules with high phase space density, we present the design and characterization of a cryogenic buffer gas beam source, as well as measurements of the collisional cross-sections of barium monofluoride and calcium monofluoride with helium in the buffer gas cell.

6 Microwave coupling of spins in cryogenic solids: from atoms to molecules

Andrew Kanagin
TU Wien

Noble gas crystals form a weakly interacting, inert, matrix which aims to preserve the favorable vacuum properties of the impurity of choice. As a proof of concept we have demonstrated strong coupling of an ensemble of alkali atoms (Na) embedded in solid neon to a superconducting resonator. The hybrid quantum system collectively couples to the hyperfine transition of the 10^{12} spins which are directly deposited on top of the superconducting resonator. The impurity linewidths are competitive compared to other spin impurity systems, suggesting that the cryocrystal is a suitable host matrix for other impurities.

Moving beyond atomic impurities, we aim to couple embedded polar molecular impurities to superconducting resonators. Molecular impurities, which can be coupled electrically rather than magnetically, results in roughly a thousand times stronger coupling per impurity ($u_d \gg u_B$). The molecular impurity of choice we plan to initially explore is deuterated ammonia (ND_3). Ammonia is known to have a tunneling transition, or inversion transition, at low microwave frequencies which hopefully will allow one to couple the capacitive component of the superconducting resonator directly to the electric dipole moment of the molecule. These transitions are known to still exist while in the cryocrystal.

7 Superradiance in a Hybrid System of NV Centers Coupled to a Microwave Resonator

Wenzel Kersten
TU Wien

We present our experimental system which strongly couples an ensemble of nitrogen-vacancy spins to a novel superconducting microwave resonator [Kersten2023], exhibiting superradiant behavior [Angerer2018]. Using this setup, we implement a protocol to create an uniformly inverted spin ensemble. To this end, we rapidly detune the ensemble after a microwave inversion pulse to keep the spin inversion stored for up to 20 ms—four orders of magnitude longer than the characteristic superradiant timescale of our system. The inverted ensemble constitutes a highly unstable and sensitive system, responsive to weak microwave pulses on the order of 10^{-11} photons per spin. By varying the stored inversion, we explore a threshold behavior for the spontaneous appearance of superradiant pulses. Surprisingly, the initial superradiant decay is followed by a sequence of pulsed revivals, evolving into a quasi-continuous masing emission. These revivals occur significantly later than the typical timescales of both cavity and spins. After the initial superradiant decay, resonant spins are de-excited and a spectral hole is created. We introduce a new mechanism for this pulsed behavior: repumping of the spectral hole, facilitated by spin-spin interactions with off-resonant spins, propels the ensemble back above the inversion threshold, enabling the emergence of self-pulsed superradiant masing emission.

8 Modeling laser cooling of barium monofluoride molecules

Felix Kogel

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Cold molecular gases are the starting point for studies of cold chemistry, quantum simulation and precision measurements of fundamental physics. Here, we report on our effort towards the first realization of Sisyphus-type laser cooling of BaF molecules. We perform high-resolution absorption spectroscopy to derive an improved set of molecular constants for the bosonic isotopologues 138BaF and 136BaF and use these constants to model laser cooling using simulations based on the optical Bloch equations. We find effective Doppler, sub-Doppler, and coherent cooling strategies for the bosonic, as well as for the fermionic BaF isotopologues. This provides important guidance for the corresponding experiments ongoing in our group, and paves the way for tests of fundamental symmetries using these molecules.

9 Towards frequency comb Raman spectroscopy for quantum logic

Elyas Mattivi
University of Innsbruck

One of the most attractive quantum computing platforms is that of atomic ions. We aim to investigate an alternative approach that substitutes atomic ions with molecular ions, which allows for the utilization of rotational degrees of freedom for quantum information encoding. However, due to the complex internal structure of molecules, advanced methods are required to manipulate and readout their quantum states. In order to prepare, control, and characterize molecules at the quantum level, we are developing a setup for two-beam frequency comb Raman spectroscopy. The two-beam frequency comb Raman setup allows precise control over driving rotational transitions in molecular ions. We will drive two-beam frequency comb Raman carrier transitions between the electronic D-levels in Ca^+. The same system will be used for driving rotational state transitions in CaH^+ and $CaOH^+$. The possibility of directly driving sideband transitions with the frequency comb will also be explored. Driving rotational transitions in molecules, especially sideband transitions, requires higher intensities, necessitating the use of an amplifier. Dispersion in the optical path also decreases Raman efficiency. My project focuses on the amplification and dispersion compensation of the comb light used in this Raman setup.

10 Towards state preparation, readout, and control of polyatomic molecular ions using quantum logic spectroscopy

Mariano Monsalve
University of Innsbruck

Molecular ions offer more degrees of freedom than atomic ions. These larger Hilbert spaces are rich and interesting landscapes to explore, possibly enabling quantum information applications such as quantum error correcting (QEC) schemes not available in atomic ions. This requires efficient and precise control of the molecular ion states. Co-trapping a molecular ion with an atomic ion facilitates state preparation and readout via quantum logic spectroscopy. Our group aims to use calcium-based molecules, e.g., CaH^+ or $CaOH^+$, co-trapped with a $^{40}Ca^+$ ion for exploring these applications in QEC and precision spectroscopy. Coherent control within a rotational manifold of a molecular ion can be achieved by driving two-beam Raman transitions, as direct transitions between the sublevels in the same manifold are forbidden by selection rules.

11 Highly-resolved Stark effect measurements of Rydberg states in thermal nitric oxide

Fabian Munkes

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We demonstrate Stark effect measurements at room temperature of high-lying Rydberg states in nitric oxide. These states are generated using a three-photon continuous-wave excitation scheme. The readout is based on the detection of charged particles created by collisional ionization of Rydberg molecules. A theoretical discussion of the obtained experimental results is given.

12 Apparatus for deterministic ionization and loading of molecules

René Nardi
Universität Innsbruck, Institut für Experimentalphysik

We study the complex rovibrational structure of trapped molecular ions and their potential applications in molecular quantum information processing. Our experiments are currently limited to investigating $CaOH^+$, which are created from chemical reactions of trapped Ca^+ and free H_2O. In order to load other molecular species, we are building a test setup where a molecular gas is injected in a vacuum chamber, photoionized, and then guided into an ion trap. This test setup features a time-of-flight mass spectrometer to determine the ions created by photoionization of N_2^+ and acetylene. Mass filters and ion optics can then be added to steer and focus the molecule of interest through a differential pumping region towards a linear Paul trap in a UHV chamber. Molecular ions can be injected into the trapping region through an aperture in the end-cap electrode for axial confinement in our linear ion trap.

13 Molecules research at DQC – Dipole-phonon quantum logic and sympathetic cooling of molecular ions

Swapnil Patel
Duke Quantum Center, Duke University

We will present the two main areas of molecular ion research currently being pursued at the Duke Quantum Center. The first involves using quantum logic to prepare and measure quantum information encoded in the internal state of a molecular ion through the dipole-phonon interaction (DPI). We report on progress toward observing the DPI in a CaO^+-Ca^+ ion chain. We have demonstrated sympathetic sideband cooling to the shared ground state of motion and preservation of the ground motional state through the adiabatic ramping of the secular frequency. We outline our experimental plan and the preliminary results of searching for DPI. The second experiment aims to demonstrate a technique for sympathetic cooling of molecular ions. This involves cooling the translational motion of molecular ions (CaH^+) by co-trapping them with Doppler- cooled atomic ions (Ca^+) and cooling the internal motion using quenching collisions with ultracold neutral atoms (K) trapped in a 3D MOT. We have also investigated and observed charged exchange between Ca^+ and K, and CaH^+ and K. As a prerequisite for demonstrating internal cooling, we are currently working toward rotational spectroscopy of CaH^+ using REMPD. This helps us probe the internal state population, which can be used as a tool to show internal state cooling.

14 Microwave resonator design for strong coupling to polar molecules

Elena Redchenko
TU Wien

Although the molecules strongly coupled to microwave resonators have been suggested for quantum computing almost two decades ago, due to the challenging trapping scheme, strong coupling between a microwave resonator and a single molecule has never been realized. Recent developments in cryogenic matrix isolation technologies allow us to overcome these challenges and tarp molecules $\sim$ 100 nm away from the circuit surface. Now, the only obstacle left to overcome is a correct microwave resonator design. Here, I will demonstrate the resonator design that combines high-kinetic inductance material with vacuum-gap design and guarantees a strong coupling at a single emitter level.

15 Towards high precision quantum logic spectroscopy of single molecular ions

Till Rehmert
QUEST, PTB Braunschweig

High precision spectroscopy of trapped molecular ions constitutes a promising tool for the study of fundamental physics. Possible applications include the search for a variation of fundamental constants and measurement of the electric dipole moment of the electron. Compared to atoms, molecules offer a rich level structure, permanent dipole moment and large internal electric fields which make them exceptionally well- suited for those applications. However, the additional rotational and vibrational degrees of freedom result in a dense level structure and absence of closed cycling transitions. Therefore, standard techniques for cooling, optical pumping and state detection cannot be applied. This challenge can be overcome by quantum logic spectroscopy, where a well controllable atomic ion is co-trapped to the molecular ion, both coupled strongly via the Coulomb interaction. Using a calcium ion, we implemented a quantum logic scheme to detect population transfer on a co-trapped spectroscopy ion, induced by a far detuned Raman laser setup. Here, we present the latest progress of the experiment, including the successful compensation of Raman laser induced light shifts as well as spectroscopy on complex, mono-atomic systems. All aiming at high precision quantum logic spectroscopy of single molecular ions.

16 Many-body perturbation theory for 1D atomic chains

Matej Veis
Comenius University - Bratislava, Slovakia

Contributions to the correlation energy at second order Møller–Plesset perturbation theory (MP2) are examined for a finite chain of hydrogen atoms. We demonstrate that restricting oneself to a subset of MP2 terms, such as pair-states, either doesn't involve a scaling reduction or vanishes at the thermodynamic limit. Similarities between the terms do appear, and allow for them to be classified by three effective parameters, i.e. momentum transfer, depth and asymmetry of the corresponding diagram. Formulating the perturbative series with respect to these parameters not only gives an insight regarding the magnitude of terms, but also allows for their separation into similar groups. Integrating over such groups leads to a size extensive scheme, with bounds on error, that does involve a scaling reduction. As a proof of concept the method was benchmarked against full MP2 and CCSD with STO-6G and cc-pVDZ.

17 State-dependent force spectroscopy for trapped ions

Stefan Walser
Insitut für Experimentalphysik, Universität Innsbruck

Optical trapping and laser cooling are techniques that founded a revolution of quantum experiments in which atoms and molecules are manipulated using optical forces induced by laser light. A particularly useful technique are optical tweezers which are routinely used in many scientific disciplines. Certain trapped ions are an excellent basis for high precision spectroscopic experiments due to the available electronic structure for state preparation and read-out at the single atom level. Within this project we aim to combine state-dependent optical tweezers to manipulate the motional modes of a linear ion crystal with quantum logic spectroscopy. We plan to co-trap a well controllable $^{40}Ca^{+}$ logic ion with a molecular ion of interest which is inaccessible to the standard spectroscopic techniques in ion traps. By applying a state-dependent force on the molecular ion using an optical tweezer, the overall trapping potential is modified. This consequently changes the frequency of the ion's common motional mode. That frequency shift can be measured via the logic ion. Thereby we realize a quantum non- demolition measurement of the molecule's internal vibrational and rotational states. We hope that this project will facilitate the nondestructive state detection of molecules with the outlook of providing a basis for a compact spectrometer for atomic and molecular systems.

18 Photodissociation spectrum of a single trapped $CaOH^+$

Zhenlin Wu
University of Innsbruck

Electromagnetically trapped molecular ions can be sympathetically cooled and crystallized in atomic ion crystals, which are ideal for molecular spectroscopy on the single molecule scale. Their application in quantum information processing and the exploration of fundamental physics has also been proposed and demonstrated. Investigating the internal structure of trapped molecular ions mainly relies on dissociation-based state detection methods and quantum logic spectroscopy via co-trapped atomic qubit ions. In our experiment, we aim to study triatomic $CaOH^+$ molecular ions generated in trapped Ca^+ ion experiments in the presence of water vapor. As the first step towards quantum logic spectroscopy of a single trapped polyatomic ion, we investigate the single-photon and two-photon photodissociation process of $CaOH^+$ which excites the molecule to its unbound first electronic excited state. We report the photodissociation cross section spectrum of $CaOH^+$ obtained from measurement of a single $CaOH^+$ located in an ion chain. This result paves the way for dissociation-based spectroscopy of the rovibrational structure of $CaOH^+$. In addition, the reported spectrum can be useful in large-scale trapped Ca^+ quantum experiments where photodissociation can be used for recycling Ca^+ ions when they form undesired $CaOH^+$ ions via background gas collisions.

19 Preparation of dual-species two-ion crystals for spectroscopy of molecular ions

Maximilian Jasin Zawierucha
Physikalisch-Technische Bundesanstalt

High precision spectroscopy of trapped molecular ions constitutes a promising tool for the study of fundamental physics. Possible applications include the search for a variation of fundamental constants and measurement of the electric dipole moment of the electron. Quantum logic spectroscopy is a versatile approach for the investigation of such complex systems. In order to use this technique, a two- ion crystal needs to be prepared, consisting of a molecular ion and a well-controllable atomic ion. We present our setup for high precision spectroscopy of molecular ions and our methods for efficient and deterministic preparation of a two-ion crystal, consisting of a $^{40}Ca^{+}$ and a $^{24}MgH^{+}$ ion, among other two-species combinations which will be subject of future investigations by quantum logic.