QSS24 - Jessie Zhang, Ryan MacDonnell, Gonzalo Carvacho - Questions & Answers

Jessie Zhang, Ryan MacDonnel, Gonzola Carvacho

Table of Contents

1. Jessie Zhang

What do you mean by "rich internal structure" of a molecule?

JESSIE: Atoms in general have internal structure consisting of hyperfine, fine and electronic states. On top of these degrees of freedom, molecules also have additional internal structure, including vibrational and rotational degrees of freedom. These can be used, for example, as qubit states, to generate interactions, or even in some more sophisticated proposals as “synthetic dimensions” of the system.

Would you mind to repeat how long take the sequence of the preparation of this molecules?

JESSIE: The overall duty cycle is roughly 2Hz (depending on the exact sequence being run). The atoms are loaded directly from a MOT which takes 2-300ms or so to load. Cooling the atoms to their motional ground states and preparing the states takes 10s of ms, and the molecule formation process itself takes around 100ms, mostly limited by the time to ramp the large magnetic fields.

What are the most sensitive parts of the preparation sequence for the molecules, and what limits the final yield of molecules in the ro-vibrational states in current experiments? Is it more sensitive to preparation and cooling of the atoms, or the process of transferring the atoms in to the molecular ground state?

JESSIE: Essentially it is the preparation and cooling of the atoms. The conversion efficiencies from atoms to weakly-bound molecule and weakly-bound molecule to rovibrational ground state are ~45% and ~85% respectively. The first step of forming the weakly-bound molecule by magnetoassociation effectively picks out only those atoms pairs that are in the relative motional ground state. So it is sensitive to the fidelity that we can prepare them in that state. Once they are prepared in the right state though, the conversion efficiency is near unity. I should mention all of these are technically limited at the moment and should not have any fundamental limit in our system.

How does the efficiency of the molecule association in the tweezer compare to the efficiencies that have been achieved in bulk gases? What is better / worse in the two cases?

JESSIE: One big advantage of optical tweezers is that we can prepare exactly one of each atom species with really high fidelity. In bulk gases, the first step of magnetoassociation gets hit by three body collisions with other atoms. In optical lattices, it is quite difficult to load exactly a single atom of each species into each site. Our conversion efficiency from atom to weakly-bound molecule of ~45% is actually one of the highest in heteronuclear bi-alkalis so far (starting from atoms).

Do you use fluorescence for detection? **JESSIE**: Unfortunately the molecules we form do not have any cycling transitions for direct detection with fluorescence. So the detection is actually done entirely on the atoms. Because both steps of the molecule formation process are reversible, we can dissociate the molecules back into atoms with very high fidelity.

2. Ryan MacDonnell

For the types of Chemistry problems that you're looking at, with which level of quantiative accuracy do you need to do the simulation to calculate something useful that is not possible for current classical simulations? How does this compare with the typical level of accuracy in existing analogue quantum simulators?

RYAN: As mentioned earlier in the talk, it's difficult to estimate at what point we can achieve a quantum advantage. A state-of-the-art classical computing method like ML-MCTDH achieves numerical convergence of the wavefunction for systems of 10-1000 modes, but it is highly dependent on the molecule of interest. We expect that our advantage will come from including system-bath interactions, which complicates classical simulation considerably, but we are still investigating the sensitivity of our approach to experimental errors. One of the principal uses of vibronic coupling models is for the prediction of quantitatively accurate absorption spectra, and we have early results to suggest that our approach can predict accurate spectra beyond the ability of other techniques such as boson sampling.

You have presented a model for simulating pyrazine? What is the specific interest of this particular molecule?

RYAN: Pyrazine is to vibronic coupling Hamiltonians as the hydrogen molecule is to electronic structure. The molecule is small and fairly rigid, and its lowest two electronic states are very well represented by with a linear vibronic coupling model. Whereas pyrazine has 24 vibrational modes, there are only 6 modes that are active in a linear vibronic coupling model due to symmetry, and using just the dominant two modes gives a great qualitative picture of dynamics through a conical intersection.

About the mapping: You explained the mapping of the molecule to a single ion, but it involved entangling operations. How many ions do you need in the chain, or can it be done with only 2?

RYAN: Sorry, I may have explained this aspect poorly during the talk. For the two-state, two-mode model system I presented, you only need a single ion. The light-matter interactions are in the same form as conventional multi-qubit entangling gates, but in our case the desired entanglement is between the qubit internal states and the bosonic modes rather than between multiple qubits. In fact, for larger calculations it is simpler to use a single qudit ion coupled to many modes (e.g. with inactive or "shelved" ions) to avoid the complications of entangling multi-qubit states with the bosonic modes.

3. Gonzalo Carvacho

How does establishing violations of your inequalities in these networks relate to our usual understanding of bipartite entanglement (e.g., standard Bell's inequalities)? Can we bound bipartite entanglement across different bipartitions from these measurements?

GONZALO: The violation of Bell inequalities allows us to certificate nonclassical behaviour and hence stablishing this phenomenon within a network proves that in complex systems is possible to find new and truly complex behaviour such as Bilocality violations. These measurements are optimized for the violation of n-locality, I guess is possible to bound entanglement for some set of measurements but what can be done surely is to bound the bilocality for different bipartitions.

Based on the outcomes of these measurements, if we obtain a violation by a certain amount, what

can we say about the potential usefulness of the resulting states (e.g., for quantum communication or computation?).

GONZALO: Yes! The correct violation allows us to exploit the setup for protocols of quantum communication, generation of random numbers and so on. According of the protocol/application there would be a minimum amount of violation to ensure the quality for instance of a raw key, or the level of randomness generated. There are also some protocols for improving the outcomes avoiding experimental bias.

Could you also check these inequalities in butterfly networks?

GONZALO: Yes! It is possible to find/adapt the inequalities for different causal structures as they allow a correct Markov description.

The obtained violation seems independent on n (number of sources). This is rather unusual in terms of scaling with local errors. What is limiting the strength of the violation?

GONZALO: What is independent on n (number of sources) is not the violation obtained, but the upper bound of the inequality which is dependent only on the number of measurements that is performed at each node. What limits the strength of the violation is the noise involved in the experiment, the quality of the generated states, our capacity to perform the correct measurement optimized for the violation and other experimental issues.