

Assistant Professor Matjaž Gomilšek

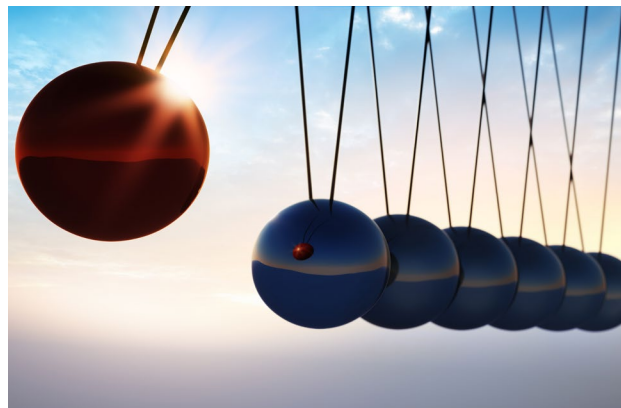
Ghost in the Material: Using Muons to Study the Effects of Quantum Jitters

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PHYSICAL SCIENCES & MATHEMATICS

Nothing can ever be perfectly still, no matter how cold you make it. Take solid nitrogen, for example, which freezes at a bone-chilling -210°C . You might expect its molecules to be frozen rigidly in place but, even at such extreme temperatures, they have a life of their own. At the microscopic level, quantum effects become important and random fluctuations ensure that molecules of solid nitrogen will jitter unceasingly. In the limit of absolute zero temperature, these tiny movements can have a considerable influence on the properties and behaviour of whole materials. New work published by a collaboration of scientists from Slovenia and the UK has sought to develop a better understanding of the effects of this quantum motion.



Nothing Can Ever Be Perfectly Still

When you cool a material down, it loses energy. That's what temperature is – the average kinetic energy of particles as they bash each other around in a substance. Decreasing temperature, therefore, reduces the kinetic energy and leads to the slowing down of all the constituent particles. So, what happens if you keep cooling something down – that is, all the way to absolute zero? You might think that eventually all the energy is lost and that the particles end up frozen and unmoving, but that's not the case. At the microscopic level, quantum mechanics rules the roost and its laws dictate that particles can never stop moving entirely. However close you get to absolute zero, random quantum fluctuations will always jostle particles around, meaning that even when they're supposed to be frozen in one place by the cold, they will continue to fidget – we call this zero-point motion (ZPM).

The size of a particle's ZPM depends on what kind of particle is involved. Heavier atomic nuclei aren't too affected by quantum fluctuations because of their hefty mass. But lighter particles, like hydrogen nuclei that consist of just a single proton, will feel them far more and end up with large ZPM. It's like the difference between basketballs and ping-pong balls. A force big enough to easily knock a ping-pong ball around will barely move a basketball. As more and more research has been devoted to the study of the quantum properties of materials, physicists are now aware that nuclear ZPM can play a critical role in explaining the onset of phenomena such as superconductivity. An improved

understanding of ZPM has also contributed to the development of more efficient hydrogen storage techniques – essential for the usability of hydrogen fuel, that can be stored in ever denser, more compact ways.

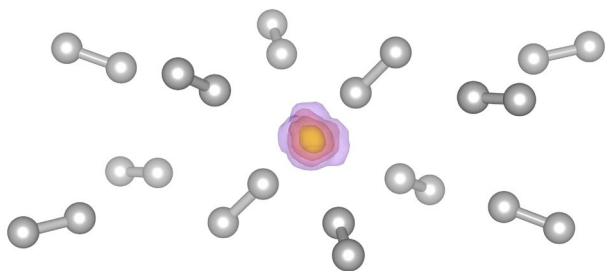
Studying Atomic Properties Using Muons

While physicists have developed a range of tools for incorporating the effects of ZPM on material properties, many of these are not suitable for use in situations where ZPM becomes very large. This is an issue that Asst Prof Matjaž Gomilšek from Ljubljana, Slovenia and a team of researchers based in Durham and Harwell Campus in the UK, have tried to address. One of their concerns was with a method called muon spectroscopy (μSR), commonly used to study the properties of materials at the atomic scale. In these experiments, lightweight particles – known as muons – are fired into a material to probe its inner structure and its magnetic properties.

To most of us, muons are an unfamiliar kind of particle, but they can be routinely produced using modern particle accelerators. They belong to the same class of particles as the electron, and have many similar properties, except they're a lot heavier and less stable. In μSR , muons entering the material can become lodged in between the constituent molecules and disrupt the electric and magnetic fields in the area. The muons only last for a couple of microseconds, but during that time they behave like little probes of their surrounding environment. Think space probe Voyager, but on the quantum scale! When their lifetime expires, the muons decay into other particles; when these leave the material, we can detect them to obtain information about the environment where the muon was situated.

The Difficulties of Modelling Particles as Light as Muons

A key problem identified by Asst Prof Gomilšek and his collaborators was that results of μSR experiments are heavily affected by the muons' ZPM. Muons are heavier than electrons, but still much lighter than objects like atomic nuclei – a single proton is around 9 times heavier than a muon. Because of this, muons are extremely susceptible to quantum fluctuations and experience a larger ZPM than any atomic nucleus.



This is what led Asst Prof Gomilšek and his collaborators to challenging some of the traditional approaches of modelling the behaviour of muons and light nuclei within materials. They considered the specific case of muons injected into solid nitrogen.

First of all, the locations of “stopping sites” – where the muons wedge themselves in between nitrogen molecules – are usually predicted using a technique known as density functional theory (DFT). But, to work out their positions, DFT assumes that both the nitrogen nuclei and the muon are classical particles – like solid marbles. This may not be a bad approximation when dealing with heavier nuclei, but it’s certainly not appropriate for dealing with the very lightweight, very quantum muons.

To account for quantum effects, Asst Prof Gomilšek noted that at least one of two simplifying assumptions are typically made to go beyond standard DFT: adiabaticity or harmonicity. In adiabatic approximations, muons are treated as either being totally independent of the surrounding nitrogen molecules, or as being extremely strongly bound to them. In either of these regimes, the behaviour becomes easier to model. On the other hand, harmonic approximations assume that interactions between the muon and the nitrogen nuclei take the simplest possible form – that of an ideal spring. What Asst Prof Gomilšek and his collaborators discovered is that neither of these approximation schemes are appropriate for muons embedded in solid nitrogen. They demonstrated that the muons are neither weakly nor very strongly bound to their surroundings, and that their interactions with neighbouring nitrogen molecules cannot be considered spring-like. The muons and nitrogen nuclei seemed to move together in a much more complex pattern.

High Precision Measurements of Muons in Solid Nitrogen

When a muon becomes lodged in solid nitrogen, its charge disturbs the electric and magnetic fields in its vicinity, and a central, positively charged complex is formed. This causes nearby nitrogen molecules to become electrically polarised – they become positively charged at one end and negatively charged at the other. Since opposite charges attract, the nitrogen molecules then reorient themselves to ensure that their negatively charged zones point towards the muon complex. The resulting arrangement is called a “polaron”.

This complex behaviour means that the ZPM of muons in solid nitrogen doesn’t fit into the neat categories of adiabaticity or harmonicity. The muons and nitrogen nuclei become partially quantum entangled, so that they’re neither weakly nor strongly bound to each other. Instead, they move together in an imperfectly correlated fashion. Because the usual methods for modelling ZPM aren’t equipped to deal with an intermediate case such as this, Asst Prof Gomilšek turned to a technique known as Path-Integral Molecular Dynamics (PIMD). This method is more computationally demanding, but had been effectively used before to deal with the ZPM of light nuclei, such as hydrogen.

The researchers developed simplified, less computationally demanding models that still manage to capture the salient features of the partially quantum entangled regime. These general models can be used either in place of the more expensive PIMD method, or, as the team also demonstrated, in conjunction with PIMD to further improve its results. The team also defined new observables (called entanglement witnesses) that can be used to easily detect the presence of partial quantum entanglement in muon–nuclear systems based on straightforward DFT calculations, even without running a full PIMD simulation.

To test their new framework, Asst Prof Gomilšek and his collaborators extracted a property of solid nitrogen called the Nuclear Quadrupolar Coupling Constant (NQCC). This quantity can be determined experimentally and is a measure of how symmetrically electrons are distributed around the nitrogen nuclei. Previous values of the NQCC came with significant uncertainty, but in their new, more advanced analysis based on quantum effects of muons and nuclei, the researchers managed to pin down the constant to (-5.36 ± 0.02)

MHz—substantially improving accuracy over the earlier accepted (-5.39 ± 0.05) MHz, and providing the most precise value to date.

A Unified Scheme for Dealing with ZPM

The high-precision determination of the NQCC for solid nitrogen is an impressive validation of the work of Asst Prof Gomilšek and his collaborators. By applying PIMD and related methods to muons, they’ve now established a unified framework that can be applied generally to account for the ZPM of muons and light nuclei. It’s well known that ZPM plays a crucial role in interesting and varied quantum phenomena – with superconductivity being one of the most famous examples. Looking towards the future, the team hopes that their methods can now be used to explore the quantum effects of light particles with unprecedented accuracy in a wide range of materials.



Article written by Matthew Davies, PhD





MEET THE RESEARCHER

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Matjaž Gomilšek is an assistant professor at the Faculty of Mathematics and Physics within the University of Ljubljana in Slovenia and a scientific associate at the Jožef Stefan Institute in Ljubljana, Slovenia. He earned his PhD in 2018 from the same university, focusing on experimental characterization of highly-entangled quantum states called quantum spin liquids. Some of his main areas of academic interest now include quantum muon and nuclear effects, topological magnetism (skyrmions), and frustrated magnetism (quantum spin liquids). He has written more than 30 academic papers, two of which appeared in Nature Physics where he now serves as a reviewer for Nature Communications, and one review paper on frustrated magnetism. Asst Prof Gomilšek is the principal investigator or leader of several funded research projects studying the quantum properties of light particles in materials, especially through the use of muon spectroscopy. He is also the head of the Laboratory for Numerical Physics at the Jožef Stefan Institute in Ljubljana.



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FURTHER READING

M Gomilšek, F Pratt, S Cottrell, *et al.*, *Many-body quantum muon effects and quadrupolar coupling in solids*, *Communications Physics*, 2023, 6 (142). DOI: [10.1038/s42005-023-01260-7](https://doi.org/10.1038/s42005-023-01260-7)

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