Science & Technology Facilities Council
ISIS Neutron and Muon Source

Introduction to Ionic Motion (and muon and electron motion)

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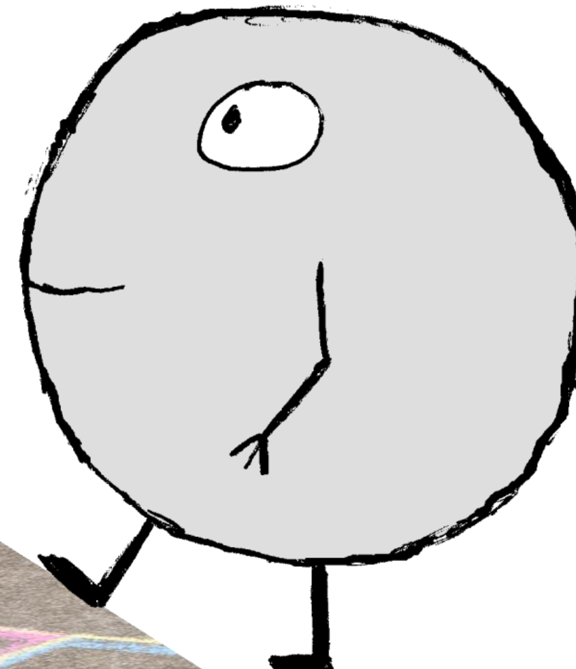


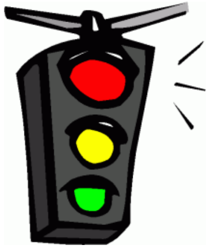
Why study ionic motion?

- Batteries!
- Hydrogen fuel cells and storage
- Solar cell materials
- Electron transport in polymers

- Because it's interesting…

Why study it with muons?

- Ionic motion changes on different length scales – muons probe the atomic scale
- Timescale of ~μs is about right for ions moving at the atomic level
- Probes individual materials, not just devices
- Works in paramagnetic materials
- Muons can impersonate (light) protons
- Muonium is a lighter version of hydrogen



What ions can you study?

Nucleus	Moment	Abundance (%)	Chance of success
^{1}H	+4.84	99.9885	Have to separate μ^+ and H^+ motion
^{7}Li	+4.20	92.41	Excellent and well-studied
^{19}F	+2.63	100	Not promising due to F-μ bonds
^{23}Na	+2.86	100	Excellent and some existing work
^{25}Mg	-0.86	10.13	Works but with a small signal
^{27}Al	+3.64	100	Promising
^{43}Ca	-1.49	0.135	Terrible unless enriched
^{51}V	+5.15	99.76	Promising
^{67}Zn	+0.875	4.1	Not promising
^{127}I	+2.81	100	Excellent

Also consider:

- Do nuclei move faster than muons?
- Is the environment magnetic too?
- Does NMR work?
- If not, why not?

What else can you study?

Muon motion

- Hydrogen by analogy
  - Impurity behaviour in pure metals
  - Fuel cell/hydrogen storage component materials
- Muon is probing its own behaviour
- Need to consider how it is different from real hydrogen

Electron motion

- Conducting polymers
  - Polyacetylene
  - DNA
- Muon is an active probe that displaces an electron
- Electron needs to go away and come back on the right timescale

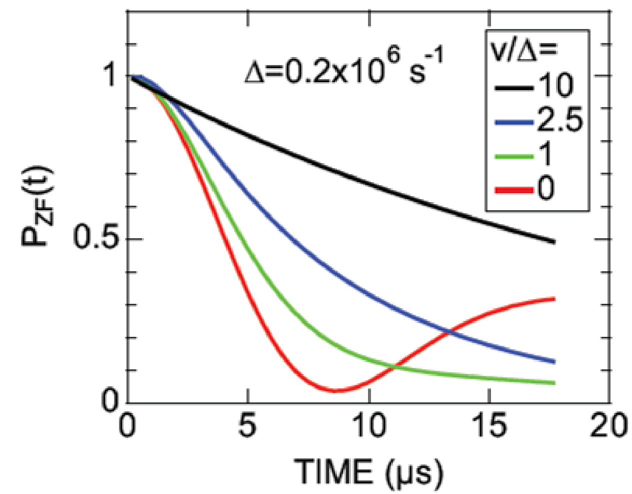
HOW DOES IT WORK?

Physical situation

- Spin-polarized muon stops in sample
- Fields from nearby nuclei cause incoherent spin precession
  - Fields from electrons can cause spin relaxation
- Ion with nuclear magnetic moment moves near muon and flips the muon spin
  - Muon motion studies do this in reverse
- Muon decays and positron detected
- Signal depends on how often the muon spin was flipped

The Kubo-Toyabe function

- Incoherent muon precession in a Gaussian field distribution
  - Static Gaussian Kubo-Toyabe
- Add Markovian dynamics
  - Dynamic Gaussian Kubo-Toyabe
- Nuclei in the sample and where the muon stops determines Δ
- Ion hopping rate determines ν
- Can infer D_{Li} almost directly at the microscopic level
  - Need to know the possible diffusion pathways



$$D_{\mathrm{Li}} = \sum_{i=1}^{n} \frac{1}{N_i} Z_{\nu,i} s_i^2 \, \upsilon_i$$

R.S. Hayano *et al.*, Phys. Rev. B 20, 850 (1979)

The Abragam function

- Similar idea to Kubo-Toyabe function but for use in transverse fields:

$$G_z(t) = \cos(2\pi\omega t + \phi) \times \exp(-\sigma^2\tau^2 t^2 \times [\exp(t/\tau) - 1 + t/\tau])$$

- Expressed in terms of correlation time $\tau=1/\nu$
- Useful for:
  - Sensitive on different timescale to Kubo-Toyabe
  - Systems containing muonium (can remove its signal)
  - When zero field compensation isn't available
- Keren applied this model to LF-μSR

A. Abragam, *Principles of Nuclear Magnetism* (1961)
A. Keren, Phys. Rev. B 50, 10039 (1994)

The Risch-Kehr function

- Muonium attaches to polymer chain displacing electron
- Electron randomly walks along chain
- Muon spin flips each time electron passes it

$$G_z(t) = \exp[\Gamma(B)t]\mathrm{erfc}\sqrt{[\Gamma(B)t]}$$
$$\Gamma(B) = \lambda/(1 + D_{\parallel}\omega_0^{-2}\sqrt{2\omega_e\lambda})^2$$

- Useful to measure as a function of both temperature and magnetic field to build up full picture

R. Risch and K.W. Kehr, Phys. Rev. B 46, 5246 (1992)

Why might it not work?

- Sample too magnetic so electronic fields too large
  - Magnetic order present (unusual at relevant T)
  - Strongly paramagnetic (rare problem)
- Ion moves too fast or slow
  - Can normally change temperature to find useful range
- Wide band gap insulator means muonium formed
  - Use suitable weak transverse field and Abragam function
- Ion doesn’t have a nuclear moment
  - Nothing to see here (without isotopic enrichment)
- Muon moves faster than ion
  - Nothing to see here (unless muon motion is of interest)
  - Has proved rare so far

Conclusions

- Studying ionic motion is a very popular use of muons
- Experiments and data analysis are fairly easy
- Gives atomic scale information
- Useful to combine with results from bulk techniques to understand ionic motion (and how to improve it)
- Most ions of technological interest are easy to probe
- Muon and electron motion can be interesting too