VISTA Seminar

Seminar 68

May 1, 2024

10:00 am – 11:30 am EDT / 3:00 – 4:30 pm BST London / 4:00 pm – 5:30 pm CEST Paris / 10 pm – 11:30 pm CST Beijing

TOC:

NMR Spin Relaxation Calculations

Jochen Autschbach

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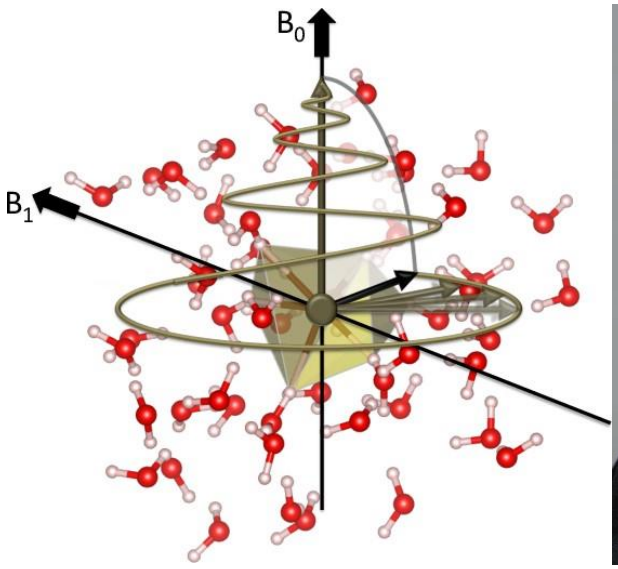

During the past 12 years, some of the effort in my research group has been directed toward calculations of NMR spin relaxation rates driven by quadrupolar, dipolar, and spin-rotation interactions. I will give a brief overview of the relaxation rate formalism and its implementation via molecular dynamics simulations with forces obtained from force fields or from density functional calculations. Examples will cover quadrupolar relaxation of group-1 and -17 ions including the curious case of Na(-), dipolar relaxation of protons in liquid water and acetonitrile, and dipolar vs. spin rotation relaxation in methane and water covering a wide range of pressures and temperatures.

Vibrational strong coupling in liquid water from cavity molecular dynamics

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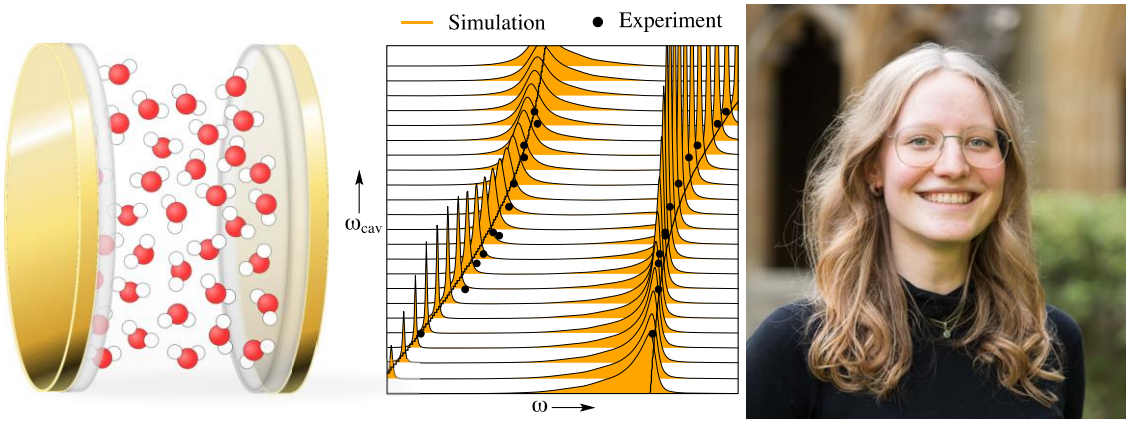

We assess the cavity molecular dynamics method for the calculation of vibrational polariton spectra using liquid water as a specific example. We begin by disputing a recent suggestion that nuclear quantum effects may lead to a broadening of polariton bands, finding instead that they merely result in anharmonic red shifts in the polariton frequencies. We go on to show that our simulated cavity spectra can be reproduced to graphical accuracy with a harmonic model that uses just the cavity-free spectrum and the geometry of the cavity as input. We end by showing that this harmonic model can be combined with the experimental cavity-free spectrum to give results in good agreement with optical cavity measurements.
Since the input to our harmonic model is equivalent to the input to the transfer matrix method of applied optics, we conclude that cavity molecular dynamics cannot provide any more insight into the effect of vibrational strong coupling on the absorption spectrum than this transfer matrix method, which is already widely used by experimentalists to corroborate their cavity results.

References:

A. Z. Lieberherr, S. T. E. Furniss, J. E. Lawrence and D. E. Manolopoulos. *J. Chem. Phys.* **158**, 234106 (2023)

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 68
Time: May 1, 2024 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/96573295278?pwd=aVJHV3pScTVqdGIvUWVuY08vbjVpUT09

Meeting ID: 965 7329 5278
Passcode: 448687