Dr. Michal Leskes

**Mapping the Homogeneity of Paramagnetic Dopants via Nuclear Spin Relaxation**

When placing matter in a magnetic field, the degeneracy of the nuclear spin states is lifted due to the Zeeman interaction. For a spin ½ two distinct energy levels become possible, differentiating whether the spin is aligned parallel or antiparallel with respect to the magnetic field. The probability of populating the different levels is given by Boltzmann statistics. This energy-and population difference is the basis of medical MRI and the widely used spectroscopic technique NMR. The time constant that describes how long a system needs from being placed in the magnetic field until reaching Boltzmann equilibrium is called relaxation time. Unlike in other spectroscopies, this relaxation process is not spontaneous, but requires a coupling of the nuclear spins to the lattice. Introducing paramagnetic center (unpaired electron spins) creates a relaxation “shortcut” for the surrounding nuclei, strongly increasing their relaxation time.

This property is exploited in MRI, where paramagnetic species are introduced to create image contrasts via differential relaxation; and in NMR they are introduced to reduce experiment times significantly.

The degree of relaxation caused by a paramagnetic species on a nuclear spin depends on their distance, decreasing with an r-6 dependence. In a sample with many nuclear spins but only few paramagnetic centers, there will be a large distribution of relaxation times, reflecting the distribution of distances (Figure1). As the spatial distribution of dopants can strongly affect the materials properties, having a simple analytical tool for determining dopants distributions would be of great value for materials scientists and is the goal of this project. We are interested in understanding how the distribution of the paramagnetic centers will affect the shape of the observed summation curves, which is what we actually can measure with NMR. The analysis will be done with numerical simulations mapping the relaxation of individual spins from their spatial coordinates. Students will create multidimensional grids and explore the effect of introducing paramagnetic centers in different spatial arrangements on the distance, and consequently relaxation distribution.

Prerequisites: No prerequisites required. Simulations will be performed using MATLAB or other programming tools depending on the student experience.

References:

[A. Labouriau,](https://doi.org/10.1103/PhysRevB.54.9952) *[Phys. Rev. B](https://doi.org/10.1103/PhysRevB.54.9952)* **[1996](https://doi.org/10.1103/PhysRevB.54.9952)**[,](https://doi.org/10.1103/PhysRevB.54.9952) *[54](https://doi.org/10.1103/PhysRevB.54.9952)*[, 9952](https://doi.org/10.1103/PhysRevB.54.9952)

Omer Yaffe

**One-dimensional simulation of a particle inside an anharmonic potential well:**

Our group investigates the structural dynamics of anharmonic crystals, that is, crystals where the harmonic approximation, which assumes Hook-law ion-ion interactions, breaks down.

To better understand the time and temperature dependent motion of a particle trapped inside an anharmonic potential well, we would like to create a classical simulation of the motion inside an arbitrary one-dimensional potential.

The main goal of the project is to create a flexible simulation, capable of producing the location time series x(t) for a particle moving under the influence of a prescribed potential function V(x). With a reliable simulation tool at hand, we may try and answer a host of interesting questions regarding the relationship between potential shape and resulting motion.

Prof. Yaakov (Koby) Levy

Proteins often have disordered regions that are essential for their function. These disordered tails may have different properties. Unique cases of interest are those where the disordered tails have non-zero net charge. For example, disordered tails which are positively charged are quite common in DNA-binding proteins and contribute to the interactions to DNA, both thermodynamically and kinetically. Disordered tails of other proteins may be negatively charged and some proteins may have both positively and negatively charged disordered tails. Charged disordered tails can contribute to other biological functions. In this project, we aim at achieving a comprehensive survey of charged tails in the genome of several organisms using various computational approaches. Quantification of the occurrence of charged tails and their properties for different functions may shed light on their functional role.

Jacob Klein

**Molecular dynamics simulation of lipid membrane system under an electric field**

Molecular dynamics (MD) simulation is a computational tool which provides theoretical predictions of structures at sub-micron scale and dynamics at sub-microsecond scale, often useful for providing molecular level insights of macroscopic experimental observations. The idea of MD is based on simulating the interactions between large numbers of molecules forming a physical system – in this case lipid bilayers, which form the membrane of living cells – and seeing how such an assembly of molecules (composed of individual atoms) develops in time under the forces between them. A particularly attractive aspect of this is that the developing molecular assemblies can be visualized on the screen (see e.g. below). In this project, we will apply the MD simulation technique to understand the effect of an electric field on a lipid bilayer. Electric fields are known to alter the structure of a lipid membrane by initiating pores in the membrane through dipole alignment. Understanding the details of this effect is particularly useful for us to explain the change in surface forces measured between two lipid bilayers when an electric field is applied. Students will learn to generate membrane structures using the CHARMM-GUI tool, perform energy minimisation, equilibration, and production simulations using the software package GROMACS. Students will analyse the results using GROMACS and/or MATLAB and be introduced to visualisation using the software VMD. After being familiarised with the process, we will investigate the effects of lipid chain length and unsaturation and the effects of cholesterol content.

Prerequisite: basic Linux command line, vim, access to high performance computing unit

References:

[1] Böckmann, R. A., De Groot, B. L., Kakorin, S., Neumann, E., & Grubmüller, H. (2008). Kinetics, statistics, and energetics of lipid membrane electroporation studied by molecular dynamics simulations. Biophysical Journal, 95(4), 1837–1850. <https://doi.org/10.1529/biophysj.108.129437>

[2] Kotnik, T., Rems, L., Tarek, M., & Miklavčič, D. (2019). Membrane Electroporation and Electropermeabilization: Mechanisms and Models. Annual Review of Biophysics, 48(1), 63–91. <https://doi.org/10.1146/annurev-biophys-052118-115451>

[3] Jo, S., Kim, T., & Im, W. (2007). Automated builder and database of protein/membrane complexes for molecular dynamics simulations. PLoS ONE, 2(9). https://doi.org/10.1371/journal.pone.0000880

Yohai Kaspi

The recent Juno and Cassini missions to Jupiter and Saturn have provided a wealth of new evidence about their atmospheres and interiors through gravity, infrared, microwave and magnetic measurements. This allowed understanding the depth of the atmospheric flows on both planets, how the atmosphere interacts with their fluid interior and how the magnetic fields control their flows. One remaining puzzle is the existence of a 3D structure to Jupiter’s magnetic field while the Saturn magnetic field is very axisymmetric. In this project, the student will use new data to develop better understanding of the differences between the magnetic fields of both planets and how the atmospheric dynamics might relate to this phenomenon, using a combination of observational, theoretical and numerical tools.

Itay Halevy

**Modeling cave drip deposits with applications in paleoclimate reconstructions**

The oxygen isotopic composition of calcium carbonate cave deposits (speleothems) has been widely studied as a proxy for reconstruction of climatic and hydrological conditions over the past millennia. Such reconstructions rely on an assumption of isotopic equilibrium between the calcium carbonate and the fluid from which it precipitated. However, disequilibrium isotopic compositions are often observed. Extracting meaningful paleoclimatic and paleohydrological information from speleothem oxygen isotopes requires an understanding of the processes that govern the speleothem’s isotopic composition. We have recently shown with a dynamic model of dissolved inorganic carbon (DIC) chemistry and mineral precipitation that the geometry of the precipitating solution (i.e., its thickness, its flow velocity, etc.) affects the isotopic composition of the carbonate mineral precipitates. In the current project, we would like to quantitatively model the time-dependent geometry of the solution: a drop of water falls, hits the inclined speleothem surface, spatters and begins to flow down the surface. Together, the fall height, drip rate and slope of the speleothem surface determine the flow velocity, thickness and width. The flow geometry, in turn, controls the rate of CO2 degassing and carbonate mineral precipitation, thereby affecting the net isotopic effect expressed during the formation of cave deposits. The project will entail the development of a Matlab program that includes the physics governing the geometry of a dripping cave solution, which will later be coupled to our existing dynamic model of DIC chemistry and isotopes.

Gershon Kurizki

**Quantum thermodynamics**

Nir Gov

**High-wire act: modelling cellular motility on grids**

Cells migrate in our bodies during the development of the embryo, during wound healing and immune system response, and also during cancer metastasis. Often cells move along quasi-one-dimensional paths, such as fibers and thin capillaries. We wish to extend a theoretical model that we have recently developed for migration along simple 1D lines [1], to describe motion on networks, mazes and grids of 1D stripes and fibers. The theoretical results will be compared to experimental data obtained in different labs.

[1] "One-dimensional cell motility patterns", Jonathan E. Ron, Pascale Monzo, Nils C. Gauthier, Raphael Voituriez, and Nir S. Gov. Phys. Rev. Research 2, 033237 (2020).

Itamar Procaccia

**Turbulence, fractals and glass formation**

Nir London

**Discovering new compounds for chemical biology**

Eli Pollak

**Time dependent quantum mechanics**

Rei Chemke

**The scale dependent response of atmospheric waves to human activity**

Atmospheric waves play a central role in shaping the weather and climate on Earth, by modulating winds, temperature and precipitation, and by transferring energy across different latitudes and longitudes. It is thus critical to accurately assess the waves’ response to human activity. However, previous studies have analyzed the changes in atmospheric waves by pooling across all waves scales, thus not accounting for the fact that the climate impacts of the waves’ response to anthropogenic emission might be scale dependent. In this project, the student will investigate the recent spectral changes in atmospheric waves in order to elucidate how waves with different wavelengths have changed over recent decades.

Eran Bouchbinder

Yael Kiro

1 - Modeling groundwater flow fields and seawater circulation in coastal aquifers, focusing on superposition of different mechanisms with different spatial and temporal scales

2 - Reactive-transport modeling along a flowpath of seawater in coastal aquifers, using a geochemical model (PHREEQC, USGS), studying the effect of adsorption-desorption, redox and precipitation and dissolution processes on major and trace elements in coastal groundwater.

Amit Finkler

**Quantum sensing using single spins**