

Theory of everything and the role of the kitchen sink

*Supervisory Committee Meeting
December 11, 2009*

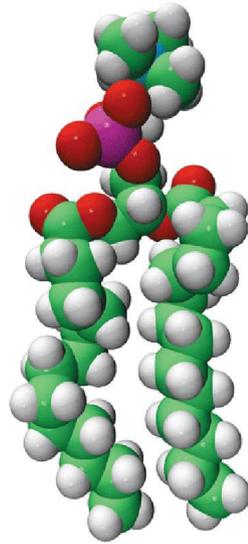
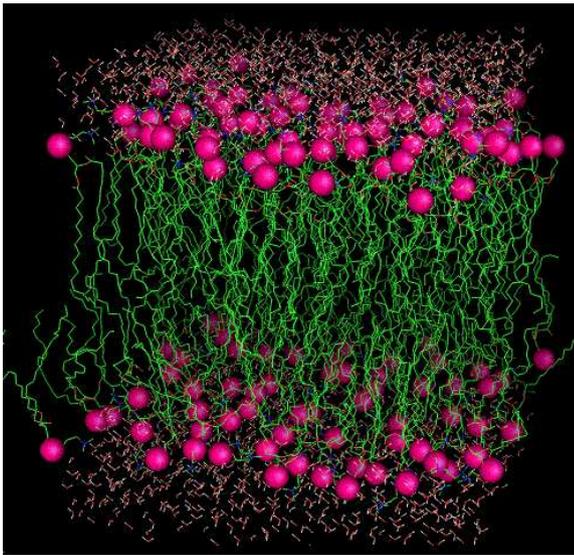
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Outline

- What is my project
- Review of relevant theory and literature
- What have I done so far
- Timeline of what remains
- Conclusions

My project: lipids in membranes



For ^2H -NMR, deuterium (^2H) replaces ^1H on the hydrocarbon chains of lipids

- biological and model membranes are *liquid crystals*, they behave like a 2D fluid.
- mechanical properties of the membrane depend on lipids interactions and motions.

Motions of lipids

The hierarchy of time scales:

- exchange of two equivalent D nuclei
- vibrations of C-D bond (10^{-14} - 10^{-15} s)
- rotations around C-C bond (10^{-10} s)
- kink formation in the C-C-C chain (10^{-9} s)
- whole-lipid rotation around the bilayer normal (10^{-8} s)
- lateral diffusion in the membrane (10^{-7} - 10^{-8} s per lipid spacing)
- flip-flop of a lipid (1 s-1 week)

Theory: Quadrupolar Hamiltonian

$$\hat{H}_Q = eQ\hat{I} \cdot \mathbf{V} \cdot \hat{I}$$

Axial symmetry in the reference frame (PACS) of the C-D bond:

$$\eta_{\text{EFG}} = \frac{V_{XX} - V_{YY}}{V_{ZZ}} = 0, \quad q = \frac{V_{ZZ}}{e}$$

where $V_{ij} = \frac{\partial}{\partial r_i} E_j$ is the Electric Field Gradient (**EFG**) tensor.

So far: Relaxation (not *that* kind)

- $F_m(t)$ has a vanishing average but a non-vanishing autocorrelation:

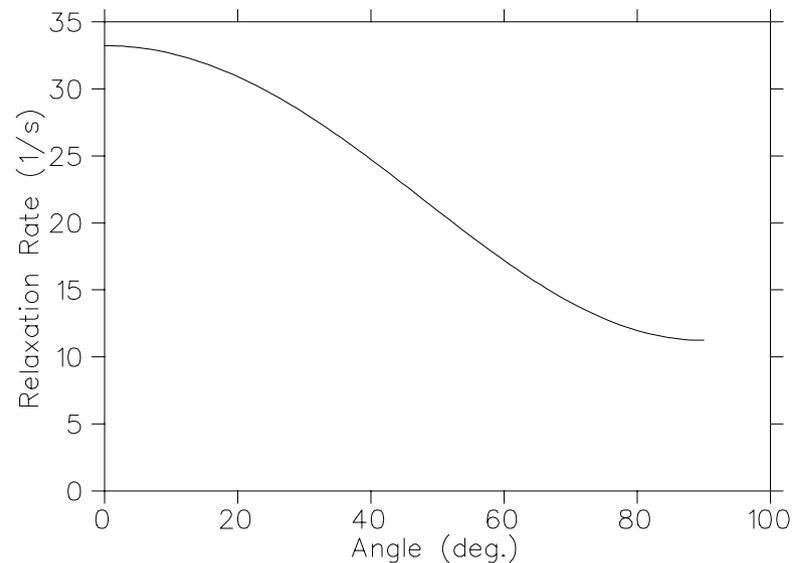
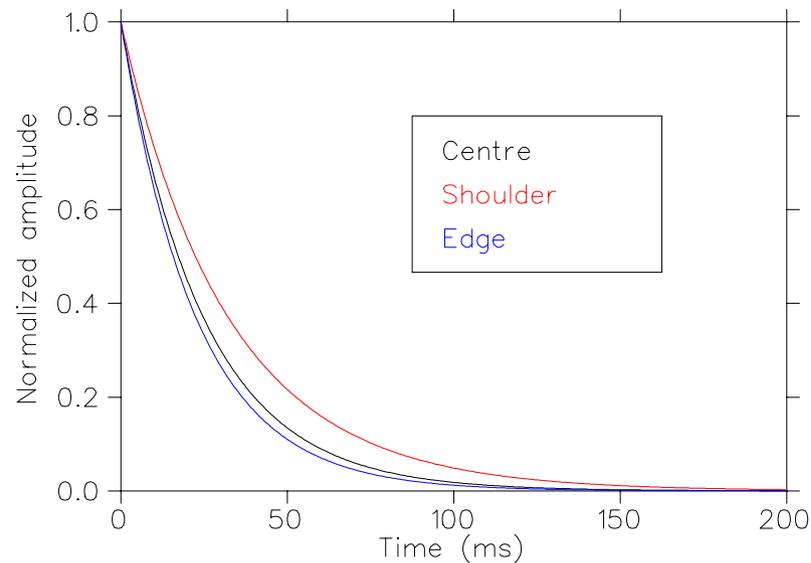
$$G_m(t + \tau, t) = \overline{F_m(t + \tau)F_m^*(t)}$$

- spectral densities are related to the autocorrelations

$$J_m(m\omega_0) = \int_0^{\infty} G_m(\tau) e^{im\omega_0\tau} d\tau$$

Still to do: HMB relaxation

Orientation-dependence of HMB relaxation:



- centre $\rightarrow \beta = 54.7^\circ$
- shoulder $\rightarrow \beta = 90^\circ$
- edge $\rightarrow \beta = 0^\circ$

Conclusion

- obtained relaxation parameters
- experimentally, $S(\omega, 0)$ is not accessible
- despite severe instability, the kitchen sink is the key
- extending to bathroom sink

Timetable

- remaining steps (early June)
- first draft (early August)
- defence (August 26)

The End

Thank you!