

Speaker: Dan Dix

Title: Genericity and Holonomy for Eigenvalue Crossings in the Molecular Hamiltonian Operator

Abstract: The molecular Hamiltonian operator acts in a Hilbert space for multi-electron wavefunctions, and depends on the positions of the nuclei as parameters. As those parameters are varied, energy eigenvalues can cross (coincide). Most of the understanding of this phenomenon assumes that the crossing is ‘generic’. We will examine what this means and what would be required to prove that a particular crossing is generic in the nuclear position space. We will also discuss how, under the genericity assumption on the crossing, the eigenfunctions belonging to the two eigenvalues behave near the crossing. This is related to the concept of holonomy in vector bundles.