

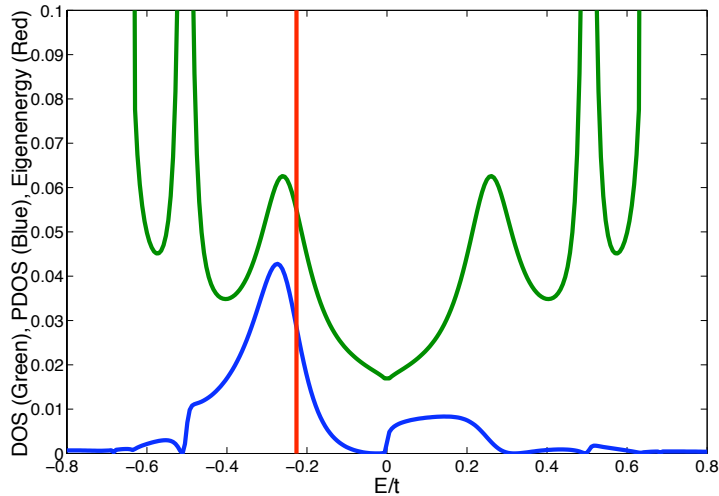
Eigenstate Explorer v2.0: The MidPoint

Douglas Mason

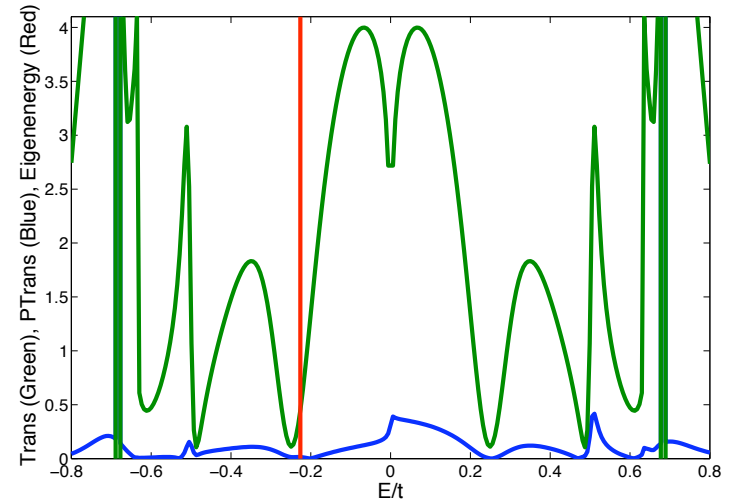
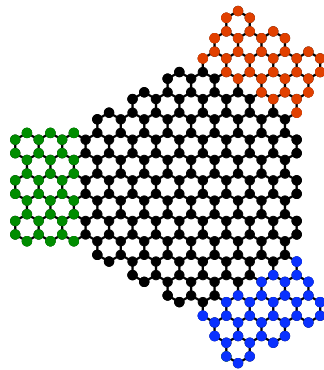
Some Scientific Developments

- Ability to correlate information between eigenstates and electron transmission exciting new development
- Can isolate contribution of an individual state, like a standing wave, to the conductance
- Can predict systems with desirable conductance properties

Partial Transmission

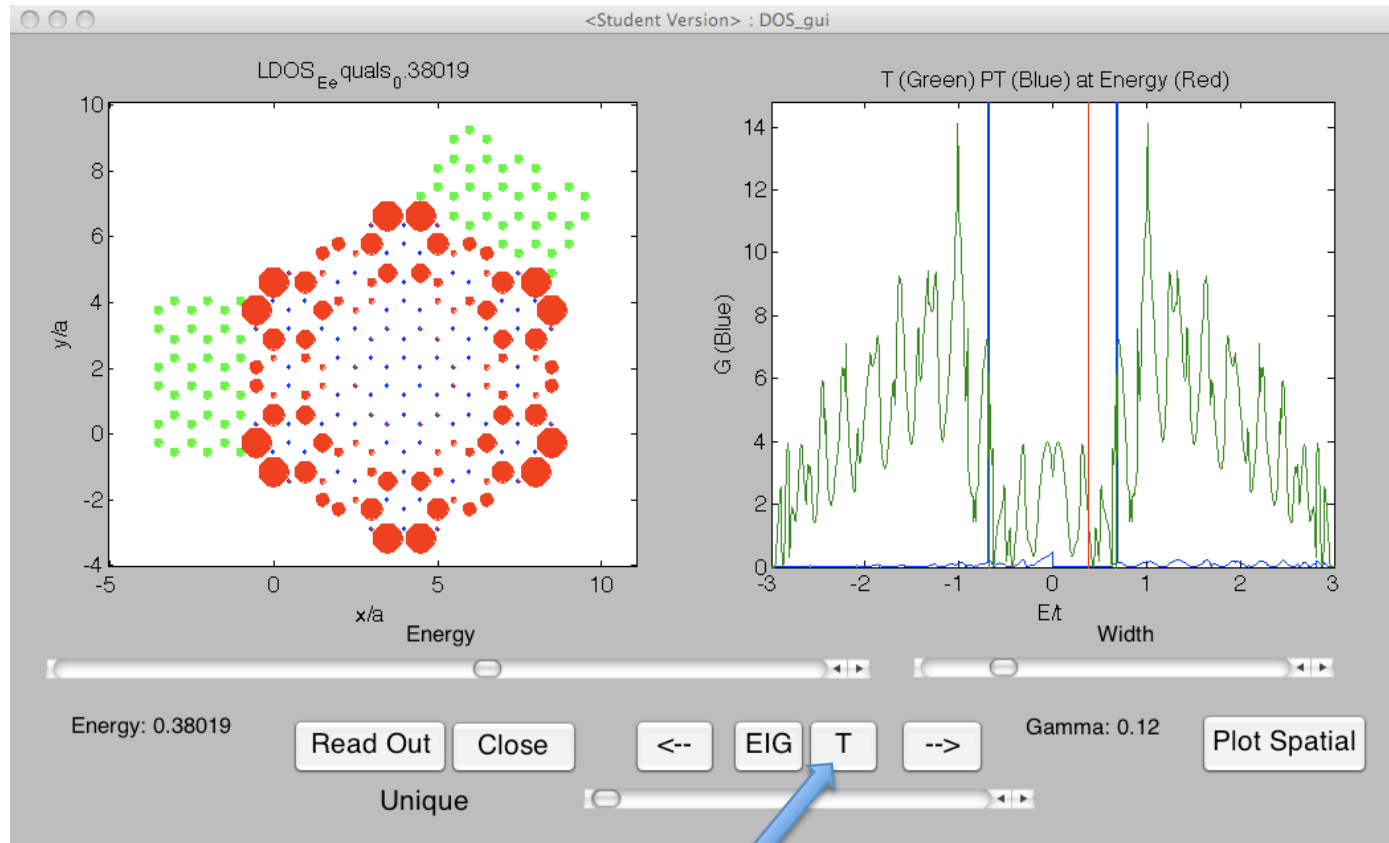


Partial Density of States has been done and gives indication of eigenstate contribution to microscope measurements



Partial Transmission is new and gives indication of eigenstate contribution to conductance measurements

Partial Transmission



Transmission button allows you to switch between DOS and transmission formalism

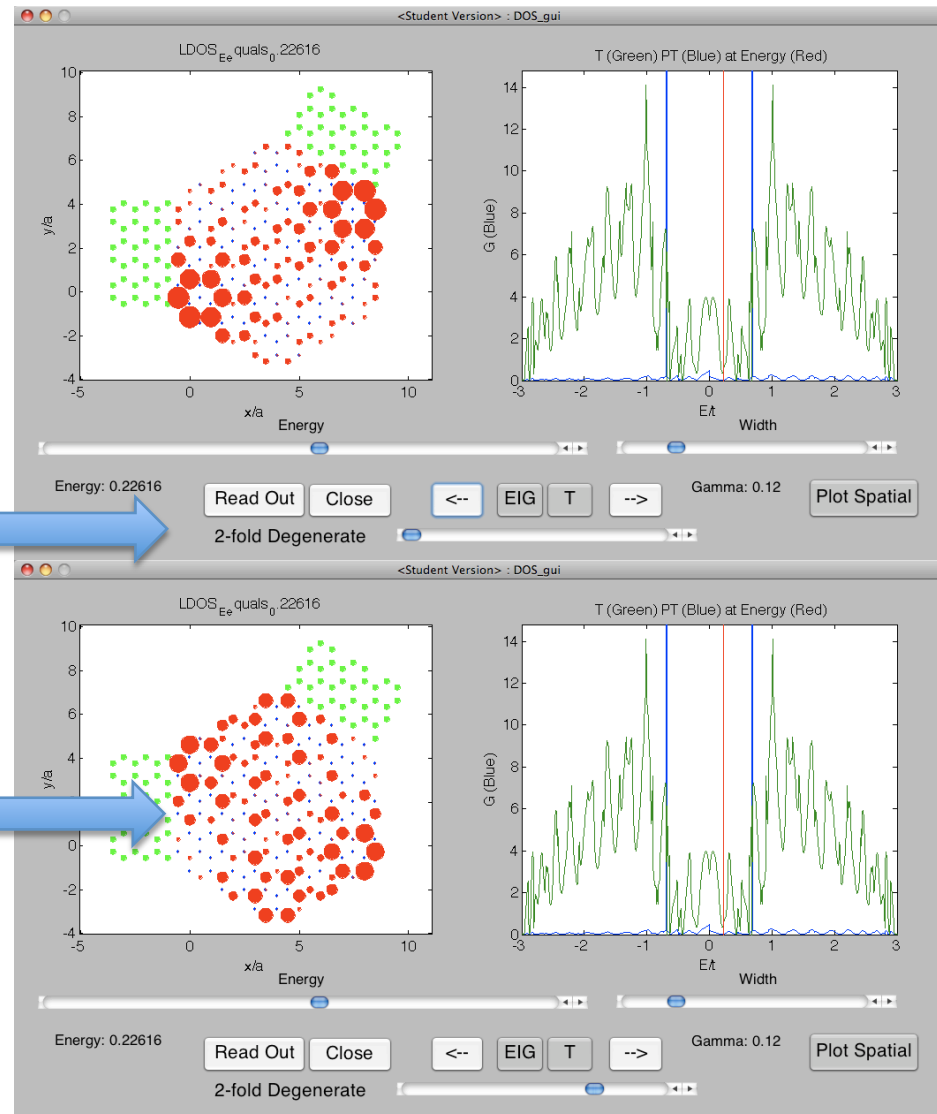
Eigensubspaces

- The contribution of the eigenstate is a deep phenomenon, but is actually a special case
- For a symmetric system, like a hexagon, with 6 axes of symmetry, adding leads reduces and lifts the symmetry
- Eigenstates become eigenspaces which you can rotate within

Rotating in Eigenspace

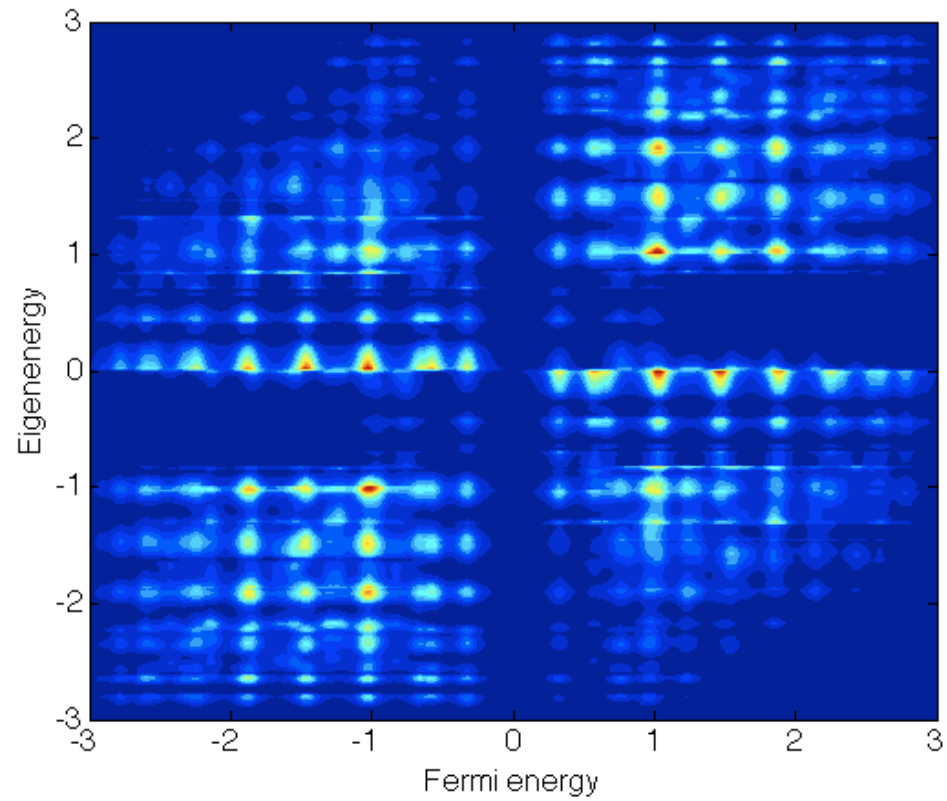
New textfield and slider indicates if an eigenspace is an eigenstate and allows you to rotate between the two principle states

In many cases, the concept of rotation can be literal, but isn't always



2-D Plots

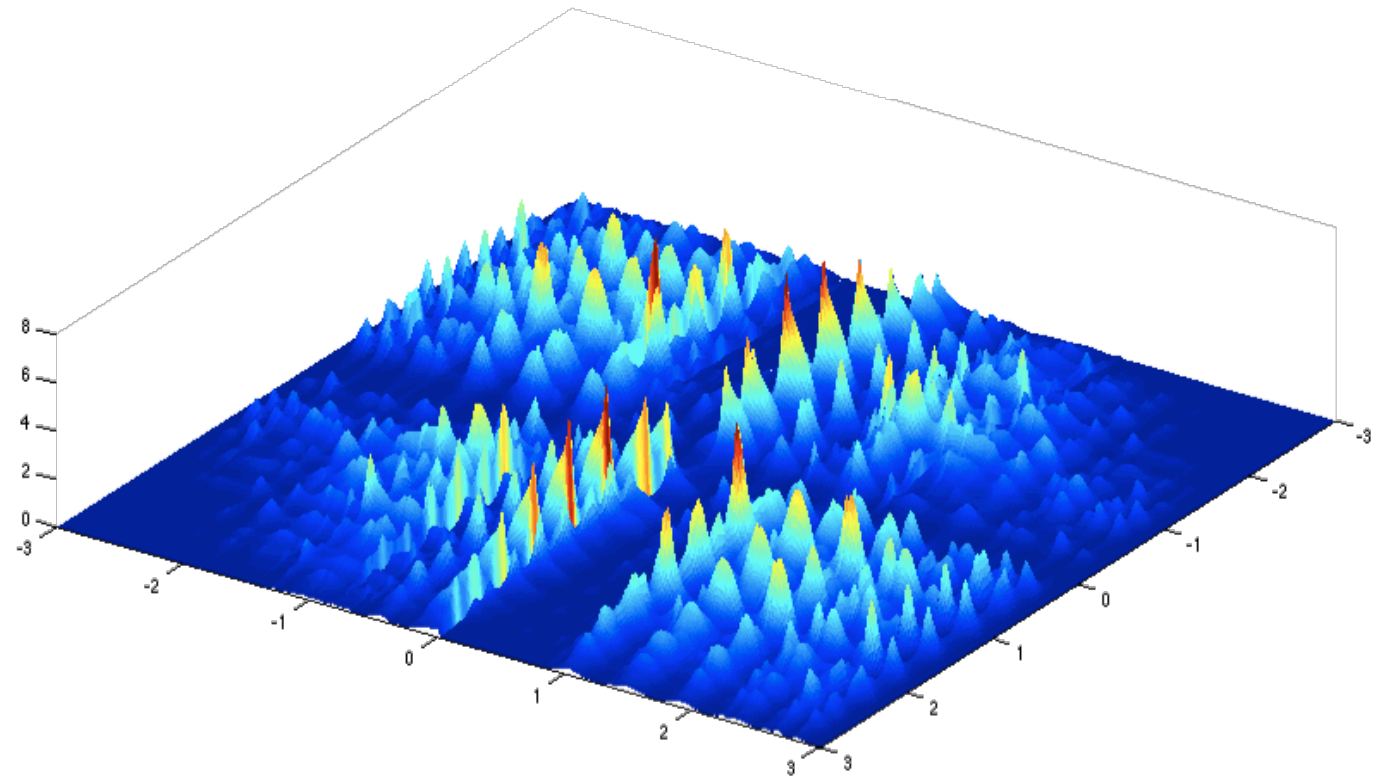
Energy of the test
electron



Weighted superposition of energy of the
eigenstates, weighted

3-D Plots

Energy of the test
electron



Weighted superposition of energy of the
eigenstates, weighted

Where to go from here?

- Still need to optimize and implement scaled multiples of eigenstates in proportion to relative contribution at each energy
- Optimize visualizations via “waterfall” plot – which method produces most visually informative results?
- Self-similarity matrix