

MDPH480/PHYS480/ASTR480/MAPH480 Research Projects 2009

Project Title: Extracting a parametrized Hamiltonian from first-principles calculations

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Abstract of the Proposed Research (use this page only)

In recent years it has become possible to do quite accurate first-principles calculations of the energy levels of lanthanide and actinide ions embedded in various materials. However, comparing these calculations with experimental data can be difficult. This is because hundreds of energy levels can be observed, and deciding whether the calculation is a “good fit” to experiment can be difficult.

Instead of doing first-principles calculations it is possible to fit the energy levels using a small set of parameters. This is the usual starting point for analysing the experimental data.

Recently we have been exploring the mathematics of extracting a parametrized Hamiltonian from first-principles calculations (which is primarily an exercise in linear algebra) and we have done some small “proof of principle” calculations. There are now two directions that require further development:

1. Doing some larger calculations with first-principles codes and investigating the trends in the parameters that emerge, and how they compare with experiment.
2. Developing the technique itself so that it can be applied to other physical situations. Our current technique is quite specific to localised states. It is also of interest to consider other systems, such as those with extended states (e.g. conduction-band states) and how best to extract a parametrized Hamiltonian in those cases.

The first direction would be interesting for a student who wanted to develop computational and data-analysis skills. The second direction would be interesting for a student who wanted to do something of a more mathematical nature.