Building Model Hamiltonians via an Evolutionary Approach

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PLEASE!

Interrupt me
Ask questions
Make comments
Respond to questions
Evolutionary approach for determining first-principles hamiltonians

Genesis of crystal structures

Genetic algorithms prove useful to distil a complex quantum mechanical calculation of interatomic interactions down to its simplest mathematical expression. This makes it possible to predict the structure of new compounds from first principles.

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LETTERS

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The argument for “fancy”

Goal: A fast, but quantitatively accurate, Hamiltonian

- Such models are complex, almost by definition—generally not even the “shape” of the model is simple
- That is, the value of parameters is not the issue, which parameters to use in the model (or even how many!) is essentially unguessable

Fancy or not, we need an approach that “works”
An Illustration:
Cluster expansion (Ising)

\[ Z = J_0 + J_1 \sum_i \hat{S}_i + \sum_{i<j} J_{ij} \hat{S}_i \hat{S}_j + \sum_{i<j<k} J_{ijk} \hat{S}_i \hat{S}_j \hat{S}_k + \ldots \]

where:

- \( Z \) is any configurational-dependent quantity
- \( \{J\} \) are "interaction parameters" (to be fitted)
- \( \{S\} \) are the site variables (\( S = \pm 1 \))

Formally exact but useless unless sums can be truncated
An Illustration: Cluster expansion (Ising)

\[ Z = J_0 + J_1 \sum_i \hat{S}_i + \sum_{i<j} J_{ij} \hat{S}_i \hat{S}_j + \sum_{i<j<k} J_{ijk} \hat{S}_i \hat{S}_j \hat{S}_k + \ldots \]

Approach:
Determine \( Z \) for a “few” structures via DFT
Use fitting to find values for \( \{ J \} \)
Predict \( Z \) for new structures, check against DFT
Add new structures to your computed set of \( Z \)'s
Iterate until we have a universal set of \( J \)'s

Result: a robust, extremely fast, model Hamiltonian

(millions of atoms, millions of configurations)
How do we truncate?

Determine the model’s “shape?”

\[ Z = J_0 + J_1 \sum_i \hat{S}_i + \sum_{i<j} J_{ij} \hat{S}_i \hat{S}_j + \sum_{i<j<k} J_{ijk} \hat{S}_i \hat{S}_j \hat{S}_k + \ldots \]

Can be handled efficiently by a constrained, k-space fit

But truncating the multi-body interaction types (MBITs) is hard (Why?)
Selecting the multi-body interaction types (MBITs)

Very rapid increase in the number of MBITs as a function of distance! (Too many choices!)

\[ Z = J_0 + J_1 \sum_i \hat{S}_i + \sum_{i < j} \]

b.c.c. many-body figures
Selecting the multi-body interaction types (MBITs)

- Optimization (search) problem:
  
  Out of $\left( \begin{array}{c} 50-100 \\ 5-10 \end{array} \right)$ possibilities...

  ...find (one of) the best model
(Actually, the problem is even worse for surfaces...)

\[ \binom{400}{20} \approx 10^{33} \]
How to pick the terms

- By physics “intuition”—dangerous (and physics shouldn’t be an “art”)
- Formal hierarchy (converges way too slow to be practical)
- Simulated annealing (didn’t work—highly correlated problem)
- Systematic “guessing”—hierarchal approach
- Something “fancier” (anything that works!)
“Physical” choices aren’t obvious
How to pick the terms

- By “physics” intuition—dangerous (and physics shouldn’t be an “art”)
- Formal hierarchy (converges way too slow to be practical)
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Evolutionary optimization

- Good approach for some highly correlated problems
- Not “too fancy” if it’s the simplest thing that works
Flowchart of a genetic algorithm for choosing the terms to retain in a model hamiltonian. Each candidate model is represented by a series of zeros and ones, a one indicating that the corresponding term is included.
\[ Z = J_0 + J_1 \sum_i \hat{S}_i + \sum_{i<j} J_{ij} \hat{S}_i \hat{S}_j + \sum J_{ijk} \hat{S}_i \hat{S}_j \hat{S}_k + \ldots \]
Flowchart of a genetic algorithm for choosing the terms to retain in a model hamiltonian. Each candidate model is represented by a series of zeros and ones, a one indicating that the corresponding term is included.
But does it work?

Exact case:

\[
\binom{45}{5} = 1.22 \times 10^6
\]

Total solutions explored: 975 (< 0.1%)
But does it work?

Only 0.02% of the solution space is explored by the GA.

Best set of MBITs doesn’t follow a systematic scheme.

\[
\binom{45}{6} = 8.1 \times 10^6
\]
But does it work?

Only 1/30 000 of the solution space is explored by the GA

Different lattice (fcc)
Different chemistry

\[
\binom{58}{7} \approx 3 \times 10^8
\]
Still have problems with local minima...

GA search with lock-out: LDA input data for Mo-Ta
“Lock-out” makes the approach completely robust
Do we really need all this accuracy in the fitting/construction?

Does it really make a difference?!
Now for the fun part...
(Today’s lab)
A simple view of the problem

What string of zeroes and ones will minimize the output?
The specific problem for today

3x3 Lattice
Every site is connected
(9x9-9)/2 connections
Each interaction is different
Compute the energy by summing over occupied “pairs”
Computing the energy

\[ E(\vec{\xi}) = (\xi_1, \xi_2, \cdots, \xi_N) \begin{pmatrix} J_{1,1} & J_{1,2} & \cdots & J_{1,N} \\ J_{2,1} & J_{2,2} & \cdots & J_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ J_{N,1} & J_{N,2} & \cdots & J_{N,N} \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_N \end{pmatrix} \]
Flowchart of a genetic algorithm for choosing the terms to retain in a model hamiltonian. Each candidate model is represented by a series of zeros and ones, a one indicating that the corresponding term is included.