From real materials to model lattice Hamiltonians: multi-scale modelling of strongly correlated electronic systems with information from many body wavefunctions

(Dated:)

I. INTRODUCTION TO DOWNFOLDING THE MANY ELECTRON PROBLEM

▷ Why we want interacting models

- Coarse-graining to get to longer length/time scales
- Conceptual understanding
- **LKW: other thoughts?**

▷ Standard methods. DFT-based downfolding, CRPA-based downfolding. **LKW: What is the issue with these methods? Accuracy? Being able to tell if a model is good or not? This will determine what we talk about in the paper. When are these methods good?**

▷ We are presenting a more general solution to this problem:

- can tell us when a model is good/bad, how much.
- can take advantage of many-body wave functions

II. THEORY: COMPRESSION OF THE ENERGY FUNCTIONAL

▷ What principles are important for connecting a problem of many electrons to a problem of few electrons

- Analogy to fitting classical PES
  - Some modes get gapped out (bond stretch in water, for example)
- $E[\Psi]$ is like the classical PES. High energy directions also get gapped out.
- A downfolded or coarse-grained model is a representation of the low-energy $E[\Psi]$ in terms of descriptors $\{d_i[\Psi]\}$

- For many systems, when we choose d_i to be expectation values of density matrices, $E[\Psi]$ is a linear function.

▷ Protocol

- Generate a set of potential descriptors consistent with symmetry and physical knowledge
- Generate a set of wave functions putatively in the low energy space $|\Psi_i\rangle \in \mathcal{LE}$, and evaluate their descriptor and energy expectation values.
- Assessment point:
  - If two descriptors are highly correlated in the samples, either the samples are not sufficient or the descriptor space is overcomplete.
  - If two wave functions have identical or near-identical descriptor sets, then either take the lowest energy (these are approximations to the low energy manifold and the lowest will be the best approximation), or consider expanding the descriptor set.
- Fitting:
  - Choice of norm and avoiding over-fitting: L_1, L_2 or something else?
  - What does the A matrix encode - standard tricks of fitting...
- Iteration: if we can solve the resultant model, does it predict low-lying states that are not in our sample set? Concept of intruder states; one example is simple stretched N_2 models.

▷ Subtleties: Choice of states, issues related to 1 particle basis...

- choice of energy window, data selection, many body states
- Static vs dynamic
- 1 particle basis, localized orbitals
- Specific algorithmic details?

III. REPRESENTATIVE EXAMPLES

A. Three-band Hubbard model to one band Hubbard model at half filling

▷ What is the 3 band model? Why the 3 band model.. relevance etc? **HJC: Hitesh working on this. Example of lattice to lattice downfolding and a concrete SIMPLE example of what it means to downfold. Performing transferability calculation (8+16 site) and more analyses with existing data**

- VERY Brief history and relevance to cuprates
- Simple example of lattice to lattice downfolding, Explain model and parameter set **HJC: In response to LKW: Not worried about whether parameters correspond to cuprate or not... This paper is to explain downfolding... thus I have considered a model only with t_{pd}, Δ and U_d and map it to a 1 band Hubbard with t and U. For pedagogy I have scanned U_d and Δ. I will not use any parameter set you gave me.**

▷ Downfolding 3 band model

- Model we want to map it to ...
- Effective one particle orbitals and "unitary"
- Effective interactions

▷ Results and Discussion

- U/t and t with Ud/tpd.
- Variation with Ep-Ed
- Hybridization parameter
- Transferability?

B. Hydrogen Chain

HJC: Huihuo working on this. Extension to simple ab initio problem. Issue with transferability being resolved LKW: I thought that Kiel was also working on this for long-range V

- ▷ Why hydrogen chain ? One of the simplest ab initio systems...
  - VERY brief intro
  - Simplest ab initio system
- ▷ Downfolding it
  - Models we want to map it to ...
  - Kohn Sham - Wannier
  - Effective interactions
- ▷ Results and Discussion
  - U/t and t
  - Transferability

C. Graphene and hydrogen honeycomb lattice (SHORT section)

HJC: Huihuo + Hitesh.. Role of screening from other orbitals etc. Highlights importance of core and virtual orbitals. More or less in place...

- ▷ Other realistic example..... Role of sigma and pi electrons
  - Set up of graphene and hydrogen-honeycomb (Why this choice)
  - short range Models we want to map it to ...
  - Role of sigma electrons in screening
  - Compare the two to highlight role...

IV. FUTURE PROSPECTS AND NEED FOR MORE WORK IN THE AREA

HJC: Other areas: Magnetism, small energy scales LKW: We already do magnetism with this method, right? It might be worth mentioning that it justifies the method of looking at the Neel state versus the AFM state. HJC: Applications to non QMC methods - coupled cluster, FCI, HCI HJC: Strengths and limitations of effective Hamiltonian approach

- ▷ Strengths and limitations of approach - separation of energy scales etc..
- ▷ Other places where it can be applied
- ▷ Non QMC methods