DOWNFOLDING RECAST AS A COMPRESSION OF THE ENERGY FUNCTIONAL

Theory

Suppose we start with a quantum system with Hamiltonian H and Hilbert space $\mathcal{H}$.

Definition 1. $E[\Psi] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$

Definition 2. *Let $\mathcal{H}$ be a Hilbert space. Then $\mathcal{LE}(H, N)$ is a subset of $\mathcal{H}$ spanned by N vectors given by the lowest energy solutions to $H|\Phi_i\rangle = E_i\Phi_i$.*

Definition 3. *H_{eff} is an operator on the Hilbert space $\mathcal{LE}(\mathcal{H},\mathcal{N})$.* **LKW: Does this need to be linear?**

Definition 4. *The effective model $E_{eff}[\Psi] = \frac{\langle\Psi|H_{eff}|\Psi\rangle}{\langle\Psi|\Psi\rangle}$ is a functional from $\mathcal{LE} \to \mathbb{R}$*

Theorem 1. *$E[\Psi]$ has a critical point only where Ψ is an eigenstate of H.*

Proof. This has been proven already by **LKW: find citation** □

Theorem 2. *If $E_{eff}[\Psi] = E[\Psi], \forall\,|\Psi\rangle \in \mathcal{LE}$, then $H_{eff}|\Phi_i\rangle = E_i|\Phi_i\rangle$ for all eigenstates $|\Phi_i\rangle \in \mathcal{LE}$.*

Proof. Suppose that $|\Phi_i\rangle$ is an eigenstate of H. Then

$$\left.\frac{\partial E[\Psi]}{\partial\Psi}\right|_{\Psi=\Phi_i} = 0 \tag{1}$$

LKW: We have to project the derivative into the low-energy subspace. If the functional derivative of E is zero at a point, then certainly the functional derivative of E_{eff} is zero. Then

$$\left.\frac{\partial E_{eff}[\Psi]}{\partial\Psi}\right|_{\Psi=\Phi_i} = 0 \tag{2}$$

for $|\Psi\rangle \in \mathcal{LE}$. Using Theorem 1, $H_{eff}|\Phi_i\rangle = E_i|\Phi_i\rangle$. Similarly, if the derivative is not zero, then the wave function must not be an eigenstate. □

We have thus reduced the problem of finding an effective Hamiltonian H_{eff} that reproduces the low-energy spectrum of H to matching the corresponding energy functionals $E[\Psi]$ and $E_{eff}[\Psi]$. An important result of this is that it is not necessary to diagonalize either of the Hamiltonians; one must only be able to select wave functions from the low-energy space $\mathcal{LE}$. As we shall see, this can be substantially easier than attaining full eigenstates.

The theory presented above maps coarse-graining into a functional approximation problem. This is still rather intimidating, since even supposing one can generate wave functions in the low-energy space, they are still complicated objects in a very large space. An effective way to accomplish this is through the use of descriptors, $d_i[\Psi]$, which map from $\mathcal{H} \to \mathbb{R}$. Then we can approximate the energy functional as follows

$$E_{eff}[\Psi] \simeq \sum_i f_i(d_i[\Psi]), \tag{3}$$

where f_i are some parameterized functions. **LKW: This is a compression operation.**

An example

LKW: Simple example: Hubbard → Heisenberg?