IV Exact diagonalization

From now on we will work with some discrete representation of phys systems using second quantization:

$\mathcal{H}_j \hat{=}$ Hilbert space of local degree of freedom "j". Also refered to as: lattice sites, orbitals..

$$\mathcal{H}^L = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_L$$

$\hat{=}$ Hilbert space of L local degrees of freedom

$$\mathcal{H}^L_N \subseteq \mathcal{H}^L$$

$\hat{=}$ subspace describing N occupied local degrees of freedom

Let $\hat{H}: \mathcal{H}^L \to \mathcal{H}^L$ be the Hamiltonian of a system of L sites/orbitals. How do we efficiently solve the eigenvalue problem of $\hat{H}$?

IV.1 Quadratic Hamiltonians

Denote by $\{\hat{O}_j^\alpha\}_{\alpha \in \mathbb{N}}$ the set of local operators acting on $\mathcal{H}_j$ with dimension $\dim(\mathcal{H}_j) = d$ such, that $\{\hat{O}_j^\alpha\}$ is a complete basis of operators acting on $\mathcal{H}_j$.

In second quantization we distinguish between:

(i) Occupation number operators satisfying

(a) $\hat{O}_j^\alpha$ is hermitian

(b) Eigenstates $|\sigma_j\rangle$ of $\hat{O}_j^\alpha$ span a complete ONB

(ii) Ladder operators satisfying:

(a) $\hat{O}_j^\alpha |\sigma_j\rangle \propto |\sigma_j - 1\rangle$ or zero

(b) $(\hat{O}_j^\alpha)^\dagger |\sigma_j\rangle \propto |\sigma_j + 1\rangle$ or zero

(c) $[\hat{O}_i^\alpha, (\hat{O}_j^\alpha)^\dagger]_\pm = \delta_{ij}$ ($\pm$ for commutators/anticommutators)

(d) $\left(\hat{O}_j^\alpha\right)^\dagger \left(\hat{O}_j^\alpha\right) \propto \hat{O}_j^\beta$ with $\hat{O}_j^\beta$ an occupation number operator.

Examples

(i) Spinless Fermions ($d=2$):

Basis of local operators given by $\mathbb{1}_j, \hat{c}_j, \hat{c}_j^\dagger, \hat{n}_j$

and

$$\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij} \, , \quad \hat{n}_j = \hat{c}_j^\dagger \hat{c}_j$$

(ii) Spin-$\frac{1}{2}$ ($d=2$):

Basis of local operators given by $\mathbb{1}_j, \hat{S}_j^+, \hat{S}_j^-, \hat{S}_j^z$

and

$$[\hat{S}_i^-, \hat{S}_j^+] = \delta_{ij} \, , \quad \hat{S}_j^z = \frac{1}{2}\left(\mathbb{1}_j - 2\hat{S}_j^+\hat{S}_j^-\right)$$

In general, Hamiltonians are of the form

$$\hat{H} = \underbrace{\sum_j \sum_\alpha h_j^\alpha \hat{O}_j^\alpha}_{\text{linear in } \hat{O}_j^\alpha} + \underbrace{\sum_{i,j} \sum_{\alpha,\beta} h_{ij}^{\alpha\beta} \hat{O}_i^\alpha \hat{O}_j^\beta}_{\text{quadr. in } \hat{O}_j^\alpha} + \ldots$$

Consider now an important case:

If $\hat{H}$ is quadratic in fermionic ladder operators, we can find its eigenvalues & states by diagonalizing a matrix scaling linear in L!

Let $\hat{c}_j^\dagger$, $\hat{c}_j$ be the fermionic ladder operators & consider quadr. Hamiltonian:

$$\hat{H} = \sum_{i,j} \left(h_{ij} \hat{c}_i^\dagger \hat{c}_j + \Gamma_{ij} \hat{c}_i \hat{c}_j - \Gamma_{ij}^* \hat{c}_i^\dagger \hat{c}_j^\dagger \right)$$

with $h_{ij}^* = h_{ji}$.

We introduce operator-valued fields:

$$\underline{\hat{\Psi}}^\dagger = \left(\hat{c}_1^\dagger \; \hat{c}_2^\dagger \; \dots \; \hat{c}_L^\dagger \right), \quad \underline{\hat{\Psi}} = \begin{pmatrix} \hat{c}_1 \\ \hat{c}_2 \\ \vdots \\ \hat{c}_L \end{pmatrix}$$

Then, $\hat{H}$ can be written as formal bilinear form:

$$\hat{H} = \left(\underline{\hat{\psi}}^{\dagger} \ \underline{\hat{\psi}}^{t} \right) \underbrace{\begin{pmatrix} \underline{\underline{h}} & -\underline{\underline{\Gamma}}^{*} \\ \underline{\underline{\Gamma}} & -\underline{\underline{h}} \end{pmatrix}}_{\doteq \underline{\underline{H}}} \begin{pmatrix} \underline{\hat{\psi}} \\ \underline{\hat{\psi}}^{*} \end{pmatrix} \quad \text{with } \underline{\hat{\psi}}^{*} = \left(\underline{\hat{\psi}}^{\dagger} \right)^{t}$$

&

$$\underline{\underline{h}} \doteq \begin{pmatrix} h_{11} & h_{12} & \cdots & h_{1L} \\ \vdots & & & \\ h_{L1} & \cdots & & h_{LL} \end{pmatrix}, \quad \underline{\underline{\Gamma}} \doteq \begin{pmatrix} \Gamma_{11} & \cdots & \Gamma_{1L} \\ \vdots & & \\ \Gamma_{L1} & \cdots & \Gamma_{LL} \end{pmatrix}$$

Since $\underline{\underline{H}}$ is hermitian, it can be diagonalized.
Denote by ϵ_α the eigenvalues & $\underline{v}_\alpha$ the corresponding eigenvectors of $\underline{\underline{H}}$.

It then follows:

$$\hat{H} = \left(\underline{\hat{\psi}}^{\dagger} \ \underline{\hat{\psi}}^{t} \right) \begin{pmatrix} | & & | \\ \underline{v}_1 & \cdots & \underline{v}_{2L} \\ | & & | \end{pmatrix} \begin{pmatrix} \epsilon_1 & & 0 \\ & \ddots & \\ 0 & & \epsilon_{2L} \end{pmatrix} \begin{pmatrix} - & \underline{v}_1^{*} & - \\ & \vdots & \\ - & \underline{v}_{2L}^{*} & - \end{pmatrix} \begin{pmatrix} \underline{\hat{\psi}} \\ \underline{\hat{\psi}}^{*} \end{pmatrix}$$

We split the components of the $\underline{v}_\alpha$'s:

$$\underline{V}_\alpha = \begin{pmatrix} V^+_{1\alpha} \\ \vdots \\ V^+_{L\alpha} \\ V^-_{1\alpha} \\ \vdots \\ V^-_{L\alpha} \end{pmatrix} \Rightarrow \left(\underline{\hat{\psi}}^+ \; \underline{\hat{\psi}}^t\right) \cdot \underline{V}_\alpha = \sum_{j=1}^{L} \left(\hat{c}^+_j V^+_{j\alpha} + \hat{c}_j V^-_{j\alpha} \right)$$

so that:

$$\hat{H} = \sum_{\alpha=1}^{2L} \sum_{\beta=1}^{2L} \left\{ \sum_{j=1}^{L} \left(V^+_{j\alpha} \hat{c}^+_j + V^-_{j\alpha} \hat{c}_j \right) \right\} \delta_{\alpha\beta} \epsilon_\alpha \left\{ \sum_{m=1}^{L} \left(\bar{V}^+_{m\beta} \hat{c}_m + \bar{V}^-_{m\beta} \hat{c}^+_m \right) \right\}$$

$$= \sum_{\alpha=1}^{2L} \epsilon_\alpha \sum_{j=1}^{L} \left(V^+_{j\alpha} \hat{c}^+_j + V^-_{j\alpha} \hat{c}_j \right) \sum_{m=1}^{L} \left(\bar{V}^+_{m\beta} \hat{c}_m + \bar{V}^-_{m\beta} \hat{c}^+_m \right)$$

Let us define:

$$\hat{\varphi}^+_{\alpha,+} = \sum_{j=1}^{L} V^+_{j\alpha} \hat{c}^+_j , \qquad \hat{\varphi}^+_{\alpha,-} = \sum_{j=1}^{L} V^-_{j\alpha} \hat{c}_j$$

$$\Rightarrow \hat{H} = \sum_{\alpha} \epsilon_\alpha \left(\hat{\varphi}^+_{\alpha,+} + \hat{\varphi}^+_{\alpha,-} \right) \left(\hat{\varphi}_{\alpha,+} + \hat{\varphi}_{\alpha,-} \right)$$

Now let us deduce an important property of $\underline{\underline{H}}$ from the fact that $\hat{H}$ is quadratic.

Consider the particle-hole transformation:

$$\hat{c}^+_j \mapsto \hat{c}_j \quad , \quad \hat{c}_j \mapsto -\hat{c}^+_j$$

$$\Rightarrow \hat{H} \mapsto \hat{H} = -\sum_{i,j} h_{ij}\, \hat{c}_i \hat{c}_j^\dagger + \sum_{i,j} \left(\Gamma_{ij}\, \hat{c}_i^\dagger \hat{c}_j^\dagger - \Gamma_{ij}^* \hat{c}_i \hat{c}_j \right)$$

$$= \begin{pmatrix} \underline{\hat{\psi}}^t & \underline{\hat{\psi}}^\dagger \end{pmatrix} \begin{pmatrix} -\underline{\underline{h}} & -\underline{\underline{\Gamma}}^* \\ \underline{\underline{\Gamma}} & \underline{\underline{h}} \end{pmatrix} \begin{pmatrix} \underline{\hat{\psi}}^* \\ \underline{\hat{\psi}} \end{pmatrix}$$

$$\overset{!}{=} \begin{pmatrix} -\underline{\hat{\psi}}^\dagger & \underline{\hat{\psi}}^t \end{pmatrix} \begin{pmatrix} -\underline{\underline{h}} & -\underline{\underline{\Gamma}}^* \\ \underline{\underline{\Gamma}} & \underline{\underline{h}} \end{pmatrix} \begin{pmatrix} \underline{\hat{\psi}} \\ -\underline{\hat{\psi}}^* \end{pmatrix}$$

$$= \begin{pmatrix} \underline{\hat{\psi}}^\dagger & \underline{\hat{\psi}}^t \end{pmatrix} \begin{pmatrix} \underline{\underline{h}} & -\underline{\underline{\Gamma}}^* \\ \underline{\underline{\Gamma}} & -\underline{\underline{h}} \end{pmatrix} \begin{pmatrix} \underline{\hat{\psi}} \\ \underline{\hat{\psi}}^* \end{pmatrix}$$

$\Rightarrow$ $\underline{\underline{H}}$ invariant under P-H-transformation.

$\Rightarrow$ Eigenvalues of $\underline{\underline{H}}$ come in pairs with ϵ_α eigenvalue, then $-\epsilon_\alpha$ eigenvalue, too!

Proof: $|v_\alpha)$ eigenvector with eigenvalue ϵ_α, then $\underline{\underline{U}}_{PH} |v_\alpha)$ is eigenvector, too. Since $\underline{\underline{U}}_{PH}^2 = \mathbb{1}$ it is $\underline{\underline{U}}_{PH}\, \underline{\underline{\hat{H}}}\, |v_\alpha) = e^{i\varphi_\alpha} \epsilon_\alpha |v_\alpha)$ & from $\mathrm{Tr}\, \underline{\underline{H}} = 0$ we have $\varphi_\alpha = \pi$.

Furthermore, $\underline{\underline{H}}$ can be block-diagonalized!

We can already read-off the block-diagonal form:

$$\hat{H} = \sum_{\alpha} \left(\epsilon_\alpha \hat{\varphi}^\dagger_{\alpha,+} \hat{\varphi}_{\alpha,+} - \epsilon_\alpha \hat{\varphi}^\dagger_{\alpha,-} \hat{\varphi}_{\alpha,-} \right)$$

We check the anti-commutators:

$$\left\{ \hat{\varphi}_{\alpha,\pm} ; \hat{\varphi}^\dagger_{\alpha,\pm} \right\} = \sum_{j,m} V^{\pm}_{j,\alpha} \bar{V}^{\pm}_{m,\alpha} \left\{ \hat{c}_j , \hat{c}^\dagger_m \right\}$$

$$= \sum_j V^{\pm}_{j,\alpha} \bar{V}^{\pm}_{j,\alpha} = \underline{1}$$

Thus, the $\hat{\varphi}^\dagger_{\alpha,\pm}$ create eigenstates of $\hat{H}$!

Then for any set $(n_{1,+} \dots n_{L,-})$ with $n_{\alpha,\mu} \in \{0,1\}$ the product state:

$$\prod_{\alpha=1}^{L} \left(\hat{\varphi}^\dagger_{\alpha,+} \right)^{n_{\alpha,+}} \left(\hat{\varphi}^\dagger_{\alpha,-} \right)^{n_{\alpha,-}} |\emptyset\rangle$$

is eigenstate of $\hat{H}$ with energy $\sum_{\alpha,\mu} (-1)^{\mu} \epsilon_\alpha$.

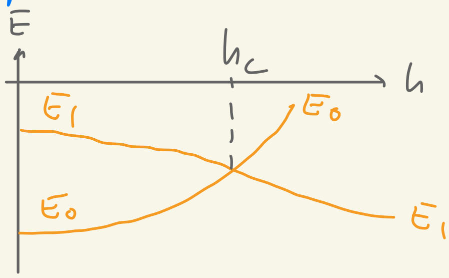
Interlude: Finite size effects @ quantum phase transitions

Quantum phase transitions can be characterized by a gap-closing/opening. What happens in such "critical" systems at finite system sizes?

Consider a critical system, i.e. the energy difference between ground state E_0 & first excited state E_1 satisfy:

$$\lim_{L\to\infty} E_1 - E_0 \to 0$$

Typical situation: Level crossing! Let system be parametrized by parameter h (e.g. magnetic field)



$\Rightarrow$ Expand E_0 around h_c:

$$E_0(h)|_{h_c} = E_0(h_c) + \begin{cases} \frac{\partial E}{\partial h}\Big|_{h \nearrow h_c} (h-h_c) + \mathcal{O}((h-h_c)^2) \\ \frac{\partial E}{\partial h}\Big|_{h \searrow h_c} (h-h_c) + \mathcal{O}((h-h_c)^2) \end{cases}$$

$\lim_{h \searrow h_c}$ & $\lim_{h \nearrow h_c}$ symmetric in typical systems

$$= E_0(h_c) + \left|\frac{\partial E}{\partial h}\right|_{h=h_c} |h-h_c| + \mathcal{O}((h-h_c)^2)$$

This linear spectrum near h_c has important consequences! In particular, order parameters are described by:

$$O \sim \begin{cases} (h-h_c)^{-\beta} & h < h_c \\ 0 & h > h_c \end{cases} \qquad (*)$$

in thermodynamic limit. On the other hand we have:

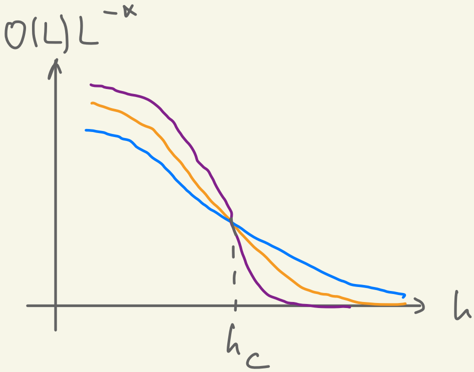
$$O = \sum_n' \langle E_n | \hat{O} | E_n \rangle$$

$$= \sum_n' \sum_m' |\langle E_n | O_m \rangle|^2 O_m \qquad \text{with } \hat{O}|O_m\rangle = O_m|O_m\rangle.$$

A non-analyticity $(*)$ can only arise if $L \to \infty$! However, at finite system sizes O as a function of L can be written as (no proof here):

$$O(L) = L^{-\alpha} f(L^{-\gamma}(h-h_c))$$

We can thus plot $O(L) \cdot L^{\alpha}$ over $h - h_c$ & identify h_c by the point where these lines cross:



IV.2 Krylov space methods

Problem in exact diagonalization:

Operators represented as matrices grow $\sim d^{2L}$!

But most operators are sparse! Can we use this fact to reach larger system sizes?

Answer: Yes, if we are happy with only a few eigenstates! ... which is mostly sufficient!

But first some more precise notation:

- Rep. of tensor product basis

Let $\{|0\rangle, |1\rangle, \dots |d-1\rangle\}$ be basis of one site/orbital

We represent states in the tensor product Hilbert space $\mathcal{H}_L$ in terms of basis states $|\underline{n}\rangle = |n_1\rangle \otimes |n_2\rangle \otimes \dots \otimes |n_L\rangle$

The $\underline{n}$'th basis state is given by the unit vector $\underline{e}_{F(\underline{n})}$ with:

$$F(\underline{n}) = \sum_{j=1}^{L} n_j \cdot d^{(j-1)}$$

$$\Rightarrow \underline{e}_{F(\underline{n})} = (0 \; 0 \; \dots \; 0 \; 1 \; 0 \; \dots \; 0)$$

element $F(\underline{n})$

- An operator $\hat{H}$ on $\mathcal{H}_L$ with

$$\hat{H} = \sum_{\underline{n},\underline{m}} \langle \underline{n} | \hat{H} | \underline{m} \rangle \, |\underline{n}\rangle\langle \underline{m}|$$

maps basis states: $\underline{e}_{F(\underline{m})} \longmapsto \langle \underline{n} | \hat{H} | \underline{m} \rangle \, \underline{e}_{F(\underline{n})}$

- For sparse operators, the number of non-vanishing matrix elements $\langle \underline{n} | \hat{H} | \underline{m} \rangle \neq 0$ scales polynomially in L:

$$\mathcal{N}(L) = \left| \{ |\underline{n}\rangle, |\underline{m}\rangle \in \mathcal{H}_L \mid \langle \underline{n} | \hat{H} | \underline{m} \rangle \neq 0 \} \right| \sim \mathcal{O}(L^a)$$

Consider the expansion of $\hat{H}$ in terms of k-point couplings:

$$\hat{H} = \sum_j \sum_\alpha h_j^\alpha \hat{O}_j^\alpha + \sum_{i,j} \sum_{\alpha,\beta} h_{ij}^{\alpha\beta} \hat{O}_i^\alpha \hat{O}_j^\beta + \dots$$

$$\equiv \hat{H}^{(1)} + \hat{H}^{(2)} + \dots$$

where $\hat{O}_j^\alpha$ denote local operators (in 2^{nd} quantization).

$\Rightarrow \mathcal{N}(\hat{H}^{(1)}) \sim \mathcal{O}(L)$, $\mathcal{N}(\hat{H}^{(2)}) \sim \mathcal{O}(L^2)$, …, $\mathcal{N}(\hat{H}^{(k)}) \sim \mathcal{O}(L^k)$

$\Rightarrow$ Operators with "local", i.e. $k \ll L$, coupling terms are always sparse!

We conclude:

Using sparsity, the action of an operator to a state can be evaluated with costs $\sim \mathcal{O}(L^k)$!

Question: Can we construct a basis such that only sparse operator applications are required to find eigenvalues/-vectors?

The Lanczos method

Consider the eigenvalue problem:

$$\hat{H}|\psi\rangle = E|\psi\rangle \text{ for hermitian } \hat{H}.$$

Solving this for the ground state is equivalent to find $|\psi_0\rangle$ via minimization of the Rayleigh-Ritz quotient:

$$|\psi_0\rangle = \underset{|\psi\rangle\in\mathcal{H}_L}{\arg\min} \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$$

Let $|\psi\rangle = \sum_n c_n |\varphi_n\rangle$ for a basis set $\{|\varphi_n\rangle\}_{n=1\ldots K}$

with $K \leq \dim(\mathcal{H}_L) = d^L$. Then minimization means to find $\nabla_{\underline{c}} \langle\psi|\hat{H}|\psi\rangle = 0$ under the constraint $\langle\psi|\psi\rangle = 1$. Introducing Lagrange multiplier α we get:

$$\nabla_{\underline{c}} \left(\langle\psi|\hat{H}|\psi\rangle - \alpha \left(\langle\psi|\psi\rangle - 1 \right) \right) \overset{!}{=} 0$$

Using $\langle\psi|\hat{H}|\psi\rangle = \sum_{n,m} \langle\varphi_n|\hat{H}|\varphi_m\rangle c_n^* c_m$

$$\doteq (c_1^* \cdots c_K^*) \begin{pmatrix} h_{11} & \cdots & h_{1K} \\ \vdots & & \vdots \\ h_{K1} & \cdots & h_{KK} \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_K \end{pmatrix}$$

as well as $\langle\psi|\psi\rangle = \sum_n |c_n|^2 = (c_1^* \cdots c_K^*) \begin{pmatrix} c_1 \\ \vdots \\ c_K \end{pmatrix}$

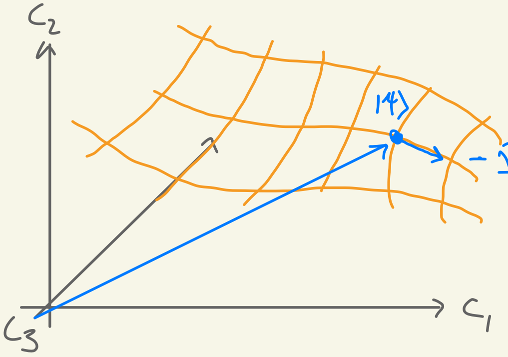
we find:

$$\nabla_{\underline{c}^*} \langle\psi|\hat{H}|\psi\rangle = \sum_{j=1}^{K} \sum_{m=1}^{K} \underline{e}_j \, h_{jm} c_m \doteq \hat{H}|\psi\rangle$$

$$\nabla_{\underline{c}^*} \langle\psi|\psi\rangle = \sum_{j=1}^{K} \underline{e}_j \, c_j \doteq |\psi\rangle$$

$$\Rightarrow \nabla_{\underline{c}} \left(\langle\psi|\hat{H}|\psi\rangle - \alpha \left(\langle\psi|\psi\rangle - 1 \right) \right) = \hat{H}|\psi\rangle - \alpha|\psi\rangle$$

Thus, $-(\hat{H}|\psi\rangle - \alpha|\psi\rangle)$ gives the "direction" in which $\langle\psi|\hat{H}|\psi\rangle$ can be reduced most efficiently (steepest decent):



Let us use this to construct a basis starting from some guess $|\varphi_1\rangle$ with $\langle\varphi_1|\varphi_1\rangle = 1$:

$$|v_1\rangle = \hat{H}|\varphi_1\rangle - \alpha|\varphi_1\rangle$$

From linear algebra we know that optimal α is such that $\langle v_1|\varphi_1\rangle = 0$ (projection into tangent space)

$$\Rightarrow \quad \langle\varphi_1|v_1\rangle = \langle\varphi_1|\hat{H}|\varphi_1\rangle - \alpha \overset{!}{=} 0 \quad \Rightarrow \quad \alpha = \langle\varphi_1|\hat{H}|\varphi_1\rangle$$

Finally define $|\varphi_2\rangle = \dfrac{|v_1\rangle}{\sqrt{\langle v_1|v_1\rangle}}$ for normalization.

Note that $|\varphi_2\rangle \in \text{span}\{|\varphi_1\rangle, \hat{H}|\varphi_1\rangle\}$.

Now express $\hat{H}$ in that basis:

$$\hat{H}^{(1)} \doteq \begin{pmatrix} \langle\varphi_1|\hat{H}|\varphi_1\rangle & \langle\varphi_1|\hat{H}|\varphi_2\rangle \\ \langle\varphi_2|\hat{H}|\varphi_1\rangle & \langle\varphi_2|\hat{H}|\varphi_2\rangle \end{pmatrix} = \begin{pmatrix} \alpha_1 & \beta \\ \beta^* & \alpha_2 \end{pmatrix}$$

with

$$\beta = \langle\varphi_1|\hat{H}|\varphi_2\rangle = \left(\langle v_1| + \alpha^*\langle\varphi_1|\right)|\varphi_2\rangle = \langle v_1|\varphi_2\rangle = \sqrt{\langle v_1|v_1\rangle}$$

Solving the eigenvalue equation for $\hat{H}^{(1)}$ yields an approx. to the solutions of the eigenvalue problem:

$$|\psi^{(1)}\rangle = c_1^{(1)}|\varphi_1\rangle + c_2^{(1)}|\varphi_2\rangle$$

with $\hat{H}^{(1)}|\psi^{(1)}\rangle = E^{(1)}|\psi^{(1)}\rangle$.

Note:

(i) The energy cost-function is convex! There are no local minima!

(ii) Iterating this procedure using $|\psi_0^{(1)}\rangle$ (groundstate of $\hat{H}^{(1)}$) to construct

$$|v_2\rangle = \hat{H}|\psi_0^{(1)}\rangle - \langle\psi_0^{(1)}|\hat{H}|\psi_0^{(1)}\rangle|\psi_0^{(1)}\rangle$$

yields power-method like algorithm

(iii) Defining the residual $\left(\hat{H} - E^{(n)}\right)|\psi_0^{(n)}\rangle \equiv |r^{(n)}\rangle$

we can measure convergence since

$$\langle \underline{r}^{(n)} | \underline{r}^{(n)} \rangle = \langle \Psi_0^{(n)} | (\hat{H} - E^{(n)})^2 | \Psi_0^{(n)} \rangle$$

$$= \mathrm{Var}\left[|\Psi_0^{(n)}\rangle \right]$$