- General setting (stationary)

- Consider family of states $|\Psi_\omega\rangle$ with $\omega \in \Omega$ denoting the variational parameters of the chosen ansatz

- If $|\phi_0\rangle$ is the exact ground state of H ($H|\phi_0\rangle = E_0|\phi_0\rangle$), we have

$$\langle H \rangle_{|\Psi_\omega\rangle} =: E_\omega = \frac{\langle \Psi_\omega | H | \Psi_\omega \rangle}{\langle \Psi_\omega | \Psi_\omega \rangle} \geq E_0 \text{ , since}$$

$$\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_0 \quad \forall_{|\Psi\rangle \in \mathcal{H}} .$$

$\rightsquigarrow$ $|\phi_0\rangle$ is global minimum of the functional

$$|\Psi\rangle \mapsto \langle H \rangle_{|\Psi\rangle} = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} .$$

↳ Necessary condition for minimum in unconstrained Hilbert space:

$$0 \stackrel{!}{=} \delta \langle H \rangle_{|\Psi\rangle} \Leftrightarrow \langle \delta\Psi | H - \langle H \rangle_{|\Psi\rangle} | \Psi \rangle = 0$$

$$\Leftrightarrow |\Psi\rangle \text{ is eigenstate of } H.$$

↳ Apply to variation within variational ansatz:

$$0 \stackrel{!}{=} \delta_\omega \langle H \rangle_{|\Psi_\omega\rangle} \Leftrightarrow \langle \delta_\omega \Psi_\omega | H - \langle H \rangle_{|\Psi_\omega\rangle} | \Psi_\omega \rangle = 0.$$

Variation only within ansatz

Interlude relating back to part A: Mean field approximation for electrons as a variational ansatz.

↳ Consider variational ansatz containing Slater determinants $|\phi_1, \dots, \phi_N\rangle$ of N orthonormal single particle orbitals ϕ_j, where the ϕ_j themselves play the role of variational parameters.

↳ Application of variational principle:

$$\delta \langle \tilde{H} \rangle_{MF} = \delta \left(\langle H \rangle_{MF} - \sum_{i=1}^{N} \varepsilon_i \left(\langle \phi_i | \phi_i \rangle - 1 \right) \right) \overset{!}{=} 0$$

[Lagrange multipliers ensuring normalization]

This yields the standard MF equations (cf. A.4)

Explicitly for N electrons with $H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V(x_i) + \sum_{i>j} \frac{e^2}{|x_i - x_j|}$

we get:

$$\left(-\frac{\hbar^2}{2m}\Delta + V(x)\right)\varphi_i(x) + \int d^3x' \frac{e^2}{|x-x'|}\sum_j \varphi_j^*(x')\Big[\varphi_j(x')\varphi_i(x) - \varphi_j(x)\,\varphi_i(x')\,\underbrace{\delta_{s_i,s_j}}_{\text{exchange term, only for equal spins}}\Big] = \varepsilon_i\,\varphi_i(x).$$

$\boxed{\varphi_i(x) = \langle x|\varphi_i\rangle}$

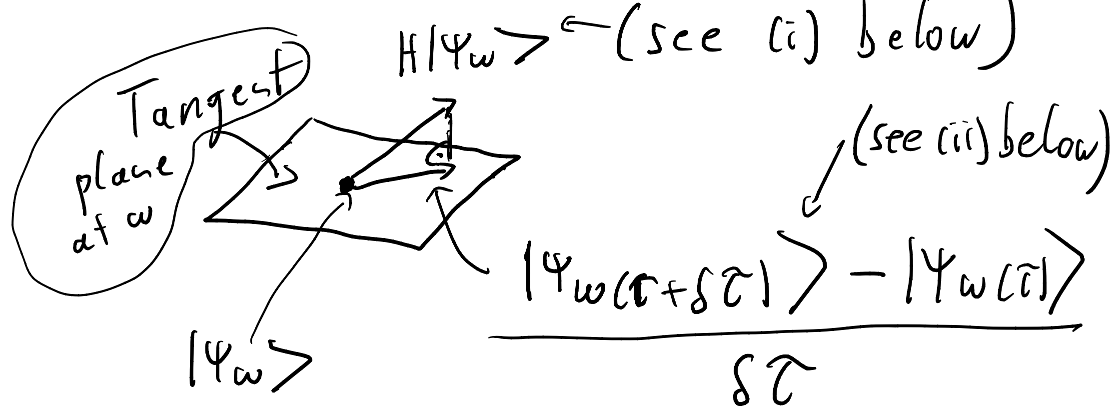
- Practical recipe for minimizing $\langle E\rangle_\omega$ by optimizing ω: Imaginary time propagation projected to the variational state manifold:

Normalization:

$\langle \Psi_\omega(\tau)|\Psi_\omega(\tau)\rangle \overset{!}{=} 1$

at all τ.

τ (imag. time)



$$(i): \quad |\Psi_w(\tau+\delta\tau)\rangle = \frac{e^{-\delta\tau H}|\Psi_w(\tau)\rangle}{\|\quad '' \quad\|} = \frac{(1-H\delta\tau)|\Psi_w(\tau)\rangle}{\|\quad '' \quad\|} + \mathcal{O}(\delta\tau^2)$$

$$= |\Psi_w(\tau)\rangle - \delta\tau\left(1 - |\Psi_w(\tau)\rangle\langle\Psi_w(\tau)|\right) H |\Psi_w(\tau)\rangle + \mathcal{O}(\delta\tau^2)$$

Then $\langle\Psi_w(\tau+\delta\tau)|\Psi_w(\tau+\delta\tau)\rangle = \langle\Psi_w(\tau)|\Psi_w(\tau)\rangle + \mathcal{O}(\delta\tau^2)$

$$(ii): \quad |\Psi_w(\tau+\delta\tau)\rangle = |\Psi_w(\tau)\rangle + \delta\tau \sum_k \dot{w}_k(\tau)\Big[|\partial_{w_k}\Psi_w(\tau)\rangle - |\Psi_w(\tau)\rangle\langle\Psi_w(\tau)|\partial_{w_k}\Psi_w(\tau)\rangle\Big]$$

necessary to maintain norm of the wave-function

$$\boxed{|\Psi_{\omega(\tau+\delta\tau)}\rangle \overset{!}{=} |\Psi_\omega(\tau+\delta\tau)\rangle}$$

corresponds to two sides of: $\partial_\tau|\Psi\rangle = -H|\Psi\rangle$

$$(ii)-(i):\quad 0 \overset{(*)}{=} \delta\tau\left[\sum_k \dot{\omega}_k \left(1-|\Psi_\omega\rangle\langle\Psi_\omega|\right)|\partial_{\omega_k}\Psi_\omega\rangle + \left(1-|\Psi_\omega\rangle\langle\Psi_\omega|\right)H|\Psi_\omega\rangle\right]$$

↳ Problem: $H|\Psi_\omega\rangle$ is in general not within the variational state manifold (see illustration above)

↳ Best approximation: Tangent projection of $(*)$ onto the variational manifold should hold.

↳ Multiplying $(*)$ from the left with $\langle\partial_{\omega_j}\Psi_\omega|\left(1-|\Psi_\omega\rangle\langle\Psi_\omega|\right)$

gives: $\sum_k \dot{\omega}_k\left[\langle\partial_{\omega_j}\Psi|\partial_{\omega_k}\Psi\rangle - \langle\partial_{\omega_j}\Psi|\Psi_\omega\rangle\langle\Psi_\omega|\partial_{\omega_k}\Psi\rangle\right] =$

$$[\quad " \quad] =: (\hat{S})_{jk}$$

$$\underbrace{= -\langle \partial_{w_j} \Psi_w | H | \Psi_w \rangle + \langle \partial_{w_j} \Psi_w | \Psi_w \rangle \langle \Psi_w | H | \Psi_w \rangle}_{=: (\vec{F})_j}, \text{ i.e.}$$

$$\boxed{\hat{S}_w \dot{\vec{w}} = \vec{F}_w}$$

(Dynamical equation of motion for variational parameters w)

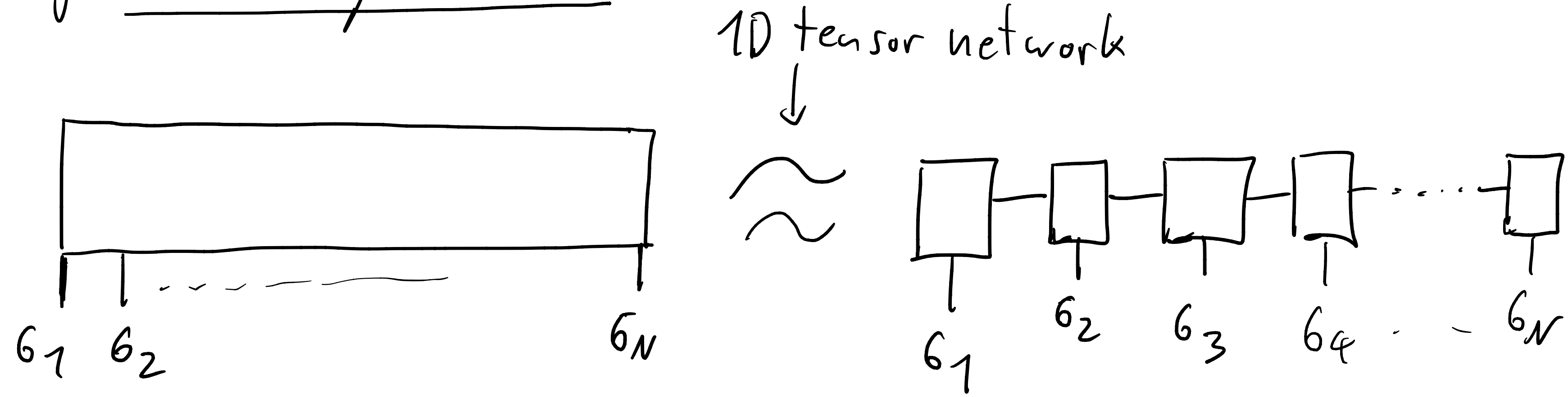
both $\hat{S}$ and $\vec{F}$ depend on w

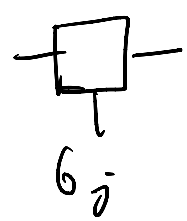
- Generalization to real-time evolution:

simply replace $\tau \to it$, i.e. $\boxed{\hat{S}_w \dot{\vec{w}} = i \vec{F}_w}$

C.1: Basic Notion of Tensor Network States

- Basic idea: Tame exponential complexity of $|\psi\rangle$ by considering only states up to a certain degree of <u>entanglement</u>.



where the tensors 

(in 1D) are variational parameters to be optimized.