Variational CD Driving

recall: $A_\lambda := (i\partial_\lambda U_\lambda)U_\lambda^\dagger$, & $U_\lambda^\dagger H_\lambda U_\lambda$ = diagonal

- for a non-int. many body system, U_λ is generated by a nonlocal operator, e.g. $\sigma^x_j \sigma^z_{j+1} \cdots \sigma^z_{j+\ell-1} \sigma^y_{j+\ell}$

$\Rightarrow$ issue: A_λ is a nonlocal op. (A_λ generates U_λ)

$\to$ cannot be implemented in the lab

Q: can we find a good local approximation?

recall: def of gauge pot.

$$\partial_\lambda H + i[A_\lambda, H] = -M_\lambda \qquad (*)$$

def: $G_\lambda(X) = \partial_\lambda H + i[X, H]$ op.-valued function

unknown op.

$\Rightarrow$ if $G_\lambda(X) + M_\lambda = 0$, then $X = A_\lambda$

idea: cast problem of looking for a sol. to $G_\lambda(X) + M_\lambda = 0$ as optimization problem wrt X

$\to$ since $G_\lambda(X)$ is linear in X, use a quadratic matrix norm (Frobenius norm):

$$d^2(X) := \mathrm{tr}\left[(G_\lambda(X) + M_\lambda)^\dagger (G_\lambda(X) + M_\lambda)\right]$$

$$\overset{\text{hermitian}}{=} \mathrm{tr}\left[(G_\lambda(X) + M_\lambda)^2\right] = \mathrm{tr}\, G_\lambda^2 + \mathrm{tr}\, M_\lambda^2 + 2\,\mathrm{tr}\, M_\lambda G_\lambda$$

$$d^2(X) = 0 \iff G_\lambda = -M_\lambda$$

$$G_\lambda(X) = \partial_\lambda H + i[X, H]$$

→ calculate:

$$\mathrm{tr}\, M_\lambda G_\lambda = \mathrm{tr}\left(M_\lambda \partial_\lambda H\right) + i\, \underbrace{\mathrm{tr}\left(M_\lambda [X, H]\right)}_{= \mathrm{tr}\left(\underbrace{[H, M_\lambda]}_{=0} X\right) = 0} = -\mathrm{tr}\, M_\lambda^2$$

$$M_\lambda = \sum_n \left(\partial_\lambda E_n\right) P_n$$

$$\rightarrow \mathrm{tr}\left(M_\lambda \partial_\lambda H\right) \overset{(*)}{=} \mathrm{tr}\left(M_\lambda \left(-i[A_\lambda, H] - M_\lambda\right)\right)$$

$$= -i\, \mathrm{tr}\left(\underbrace{[H, M_\lambda]}_{=0} A_\lambda\right) - \mathrm{tr}\, M_\lambda^2$$

$$= -\mathrm{tr}\, M_\lambda^2$$

$$\Rightarrow d^2(X) = \mathrm{tr}\left(G_\lambda^2(X)\right) - \underbrace{\mathrm{tr}\left(M_\lambda^2\right)}_{\text{indep. of } X}$$

→ drop w/ changing value of minimum

– define a least action principle for adiabatic gauge pot.

$$S[X] = \mathrm{tr}\, G^2(X) = \mathrm{tr}\left(G^\dagger(X)\, G(X)\right)$$

X: is an op.-valued unknown variable

least action principle: $\dfrac{\delta S[X]}{\delta X} \overset{!}{=} 0$

exchange: $m \leftrightarrow n$

$$\frac{\delta S}{\delta X_{ij}} \overset{\uparrow}{=} \frac{\delta}{\delta X_{ij}}\left(G_{nm} G_{mn}\right) = \frac{\delta G_{nm}}{\delta X_{ij}} G_{mn} + G_{nm} \frac{\delta G_{mn}}{\delta X_{ij}}$$

using einsum

tr

$$= 2\, \frac{\delta G_{nm}}{\delta X_{ij}} G_{mn}$$

$$\frac{\delta G_{nm}}{\delta X_{ij}} = \frac{\delta}{\delta X_{ij}} \Big(\underbrace{\cancel{\partial_\lambda H_{nm}}}_{\text{indep. of } X} + i\left([X, H]\right)_{nm} \Big)$$

$$= i \frac{\delta}{\delta X_{ij}} \left(X_{nl} H_{lm} - H_{nl} X_{lm} \right)$$

$$= i\left(\delta_{in}\, \delta_{jl}\, H_{lm} - \delta_{il}\, \delta_{jm}\, H_{nl}\right)$$

$$-i \frac{\delta G_{nm}}{\delta X_{ij}} G_{nm} = \delta_{in}\, \delta_{jl}\, H_{lm} G_{mn} - \delta_{il}\, \delta_{jm}\, H_{nl}\, G_{mn}$$

$$= H_{jm} G_{mi} - G_{jn} H_{ni}$$

$$= \left([H, G]\right)_{ji}$$

$$\Rightarrow \quad \frac{\delta S}{\delta X} \overset{!}{=} 0 \quad \Leftrightarrow \quad [H, G] \overset{!}{=} 0$$

$$\Rightarrow [H, \partial_\lambda H + i[X, H]] \overset{!}{=} 0$$

defining eq. for A_λ, solved by $X = A_\lambda + D$

- least action principle allows us to cast the problem of finding A_λ as a variational optimization problem:

ansatz : $X_\lambda = \sum_n \alpha_n(\lambda)\, O_n$

variational coefficients → to be found by minimizing action $S[X]$

some operators (educated guess)

- respect locality
- can be implemented in lab
- ...

$S[X] = S(\{\alpha_n\})$

goal: find $\alpha_n(\lambda)$, s.t. $\mathcal{X}_\lambda \approx A_\lambda$
in the sense of d^2

procedure: i) $\frac{\partial S[\mathcal{X}]}{\partial \alpha_n} \overset{!}{=} 0$

ii) solve for α_n

iii) write down $\mathcal{X} = \sum \alpha_n O_n$

– var'l. ansatz for Kato AGP:

$\Rightarrow \langle n | A_\lambda^K | n \rangle = 0$: diag. elements vanish

recall: $\langle n | A_\lambda^K | m \rangle = -i \frac{\langle n | \partial_\lambda H | m \rangle}{E_n - E_m}$

$$= \frac{\langle n | \partial_\lambda H | m \rangle}{i(E_n - E_m)} = \lim_{\varepsilon \to 0^+} \frac{\langle n | \partial_\lambda H | m \rangle}{\varepsilon + i(E_n - E_m)}$$

$$= \lim_{\varepsilon \to 0^+} \int_0^\infty dt\, e^{-\varepsilon t} e^{-i(E_n - E_m)t} \langle n | \partial_\lambda H | m \rangle$$

$$= \lim_{\varepsilon \to 0^+} \int_0^\infty dt\, e^{-\varepsilon t} \langle n | \underbrace{e^{-iHt} \partial_\lambda H e^{+iHt}}_{\overset{BCH}{=} \sum_{k=0}^\infty \frac{(it)^k}{k!} \underbrace{[H, [H, \ldots, [H,}_{k\text{-fold}} \partial_\lambda H] \ldots]} | m \rangle$$

– started w/ $\frac{1}{E_n - E_m}$ odd fn of $(E_n - E_m)$

whereas $\langle m | \underbrace{[H, [H, \ldots, [H,}_{\text{even number}} \partial_\lambda H] \ldots] | n \rangle \sim (E_m - E_n)^{2k}$

$\Rightarrow \langle m |$ even # comm. $| n \rangle = 0$

$$\langle n | A_\lambda^K | m \rangle = \lim_{\varepsilon \to 0^+} \int_0^\infty dt\, e^{-\varepsilon t} \sum_{k=0}^{\infty} \frac{(-it)^{2k+1}}{(2k+1)!} \langle n | \underbrace{[[H, \ldots, [H, \partial_\lambda H]]}_{\text{odd},\, 2k+1} | m \rangle$$

$\Rightarrow$

$$A_\lambda^K = \lim_{\varepsilon \to 0^+} \int_0^\infty dt\, e^{-\varepsilon t} \sum_k \frac{(-it)^{2k+1}}{(2k+1)!} \underbrace{[[H, \ldots, [H, \partial_\lambda H]]}_{2k+1}$$

$\Rightarrow$ var. ansatz for Kato gauge pot.

$$X_\lambda^K = \sum_k \underset{\substack{\uparrow \\ \text{variational} \\ \text{coefficients, unknown}}}{\alpha_{2k+1}} \underbrace{[H, \ldots, [H}_{2k+1 \text{ times}}, \partial_\lambda H]] \text{, known structure}$$

examples:

1) 2LS revisited: $H(\lambda) = \Delta \sigma^z + \lambda \sigma^x$

ansatz: $X_\lambda = \alpha \sigma^x + \beta \sigma^y + \gamma \sigma^z$

(all possible operators)

need: $\partial_\alpha S$, $\partial_\beta S$, $\partial_\gamma S$

i) compute: $S[X] = \mathrm{tr}\, G^2(X)$

$$G[X] = \partial_\lambda H + i[X, H]$$

$$= \sigma^x + i[\alpha \sigma^x + \beta \sigma^y + \gamma \sigma^z, \Delta \sigma^z + \lambda \sigma^x]$$

$$= \sigma^x + 2(\alpha \Delta \sigma^y - \beta \Delta \sigma^x + \beta \lambda \sigma^z - \gamma \lambda \sigma^y)$$

$$= (1 - 2\beta\Delta)\sigma^x + 2(\alpha\Delta - \gamma\lambda)\sigma^y + 2\beta\lambda\sigma^z$$

$$G^2(X) = (1-2\beta\Delta)^2 + 4(\alpha\Delta-\gamma\lambda)^2 + 4(\beta\lambda)^2 + \sum_i f_i(\dots)\underbrace{\sigma^i}_{\xrightarrow{tr}\, 0}$$

$$S = tr\, G^2(X) = \underbrace{2}_{=tr\mathbb{1}}\left[(1-2\beta\Delta)^2 + 4(\alpha\Delta-\gamma\lambda)^2 + 4(\beta\lambda)^2\right]$$

ii) minimize action $S(\alpha,\beta,\gamma)$:

$$\begin{cases} \partial_\alpha S \propto \Delta(\alpha\Delta-\gamma\lambda) \overset{!}{=} 0 \\ \partial_\beta S \propto -2\Delta(1-2\beta\Delta) + 4\lambda^2\beta \overset{!}{=} 0 \\ \partial_\gamma S \propto -\lambda(\alpha\Delta-\gamma\lambda) \overset{!}{=} 0 \end{cases} \quad (*)$$

$$\Rightarrow \begin{cases} \alpha\Delta = \gamma\lambda \\ -2\Delta + 4\beta(\Delta^2+\lambda^2) = 0 \end{cases} \Rightarrow \beta = \frac{1}{2}\frac{\Delta}{\Delta^2+\lambda^2}$$

$\leftarrow$ relation btw α, γ $(*)$

$$\Rightarrow X_\lambda = \frac{1}{2}\frac{\Delta}{\Delta^2+\lambda^2}\sigma^y + \alpha\sigma^x \overset{(*)}{+} \alpha\frac{\Delta}{\lambda}\sigma^z$$

$$= A^K_\lambda + \frac{\alpha}{\lambda}\underbrace{(\Delta\sigma^z + \lambda\sigma^x)}_{=H(\lambda)}$$

due to $U(1)$ gauge freedom

Q: procedure to recover Kato potential?

yes, use Moore-Penrose pseudo-inverse to solve $(*)$

$$[H, G(A)] = 0$$

$$\Rightarrow i[H, i[H,A] - \partial_\lambda H] = 0$$

def: $\mathcal{L}(\cdot) := i[H,\cdot]$

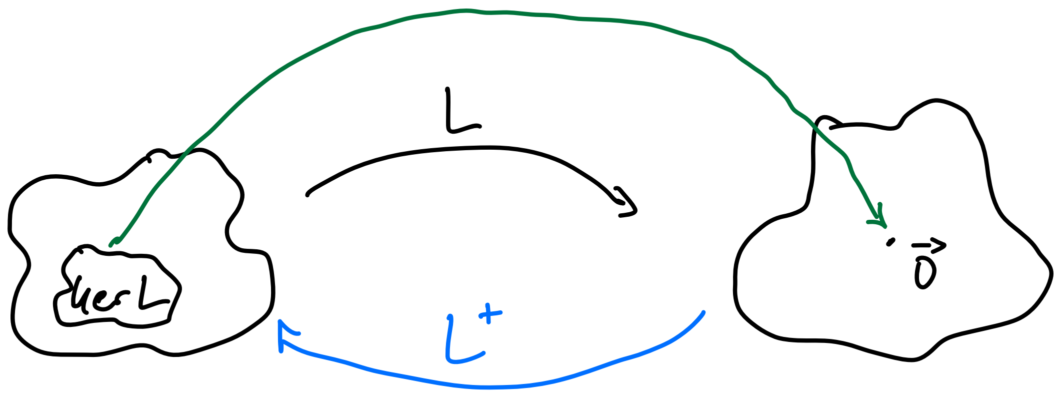
$$\Rightarrow \mathcal{L}(\mathcal{L}(A) - \partial_\lambda H) = 0 \text{ implicit eq. for } A$$

def: Moore-Penrose pseudo-inverse

overdetermined linear system: $L\vec{x} = \vec{b}$,

cannot invert L, since $\dim(\ker(L)) > 0$!

however: can invert L everywhere else:



define via SVD:

$L = UDV^\dagger \Rightarrow L^+ := V D^+ U^\dagger$, where $D^+_{ii} = \begin{cases} \frac{1}{D_{ii}} & \text{if } D_{ii} \neq 0 \\ 0 & \text{if } D_{ii} = 0 \end{cases}$

can show: $L^+ L L^+ = L^+ \overset{L^+ = L}{\Longrightarrow} L L L^+ = L$

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claim: $A^+ := \mathcal{L}^+(\partial_\lambda H) = A^K$ is the Kato AGP

check:

$$\mathcal{L}(\mathcal{L}(A^+) - \partial_\lambda H) = \underbrace{\mathcal{L}\mathcal{L}\mathcal{L}^+}_{=\mathcal{L}}(\partial_\lambda H) - \mathcal{L}(\partial_\lambda H) = 0 \checkmark$$

$\Rightarrow A^+$ is a valid AGP

- consider $\mathcal{L}(\cdot) = i[H, \cdot]$
  - $\ker(\mathcal{L})$ = {all operators that commute w/ H}
    = {all op's. that share same diagonal projectors}
    $[H, \sum d_n P_n] = 0$
  - $\mathcal{L}^+$ maps on complement $\ker(\mathcal{L})^\perp \Rightarrow A^+ \perp \ker(\mathcal{L})$
    $\Rightarrow A^+$ has no diag. elements ∎

example: back to (*):

$$\begin{pmatrix} \Delta & 0 & -\lambda \\ 0 & 2(\Delta^2+\lambda^2) & 0 \\ \cancel{-\Delta} & \cancel{0} & \cancel{\lambda} \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \begin{pmatrix} 0 \\ \Delta \\ 0 \end{pmatrix} \quad \Rightarrow \quad L = \begin{pmatrix} \Delta & 0 & -\lambda \\ 0 & 2(\Delta^2+\lambda^2) & 0 \end{pmatrix}$$

- compute MP pseudo inverse:

$$L^+ = L^\dagger (L L^\dagger)^{-1} = \frac{1}{\Delta^2+\lambda^2}\begin{pmatrix} \Delta & 0 \\ 0 & 1/2 \\ -\lambda & 0 \end{pmatrix}$$

- compute Kato AGP:

$$A^+ = L^+ \begin{pmatrix} 0 \\ \Delta \\ 0 \end{pmatrix} = \frac{\Delta}{2(\Delta^2+\lambda^2)}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\Rightarrow \quad A_r = A^+ = \frac{1}{2}\frac{\Delta}{\Delta^2+\lambda^2}\sigma^y \quad \checkmark$$

2) Quantum XY model

$$H' = -\sum_{j=1}^{L} J_x \sigma^x_{j+1}\sigma^x_j + J_y \sigma^y_{j+1}\sigma^y_j + h\,\sigma^z_j$$

exchange couplings

external field

re-parametrize:

$$J_x = \frac{1+\gamma}{2} J$$

$$J_y = \frac{1-\gamma}{2} J$$

anisotropy

exchange scale (set $J = 1$ to fix energy scale)

- consider rotating H' about z-axis at angle $\phi/2$

$$U_\phi = \prod_j e^{-i \phi/2 \frac{\sigma_j^z}{2}}$$

$$\Rightarrow \quad H(\gamma, \phi, h) = U_\phi^\dagger H'(\gamma, h) U_\phi$$

- symmetries: i) $H(\gamma) = H(-\gamma) \Rightarrow$ restrict to $\gamma \geq 0$
  ii) $H(\phi) = H(\phi + \pi)$: $\sigma^x \to \sigma^y$, $\sigma^y \to -\sigma^x$

- apply Jordan-Wigner transformation:

$$\sigma_j^z \sim 1 - c_j^\dagger c_j \quad , \quad \sigma^+ \sim \prod_{i<j} \sigma_i^z \, c_j^\dagger$$

& go to momentum space:

$$H = \sum_{k \in BZ} \psi_k^\dagger H_k \psi_k \quad , \qquad H_k = -\begin{pmatrix} h - \cos k & \gamma \sin k \, e^{-i\phi} \\ \gamma \sin k \, e^{+i\phi} & -(h - \cos k) \end{pmatrix}$$

Nambu spinor $\psi_k = (c_k^\dagger, c_{-k})$

Hamiltonian reduces to a collection of independent 2LS's, one for each momentum mode k, described by $H_k(\gamma, \phi, h)$

- 3 parameters to tune: $\vec{\lambda} = (\gamma, \phi, h)$

- want gauge potential wrt γ, ϕ, h

$\Rightarrow$ make ansatz for var'l gauge pot.:

$$\mathcal{X}_k(\vec{\lambda}) = \frac{1}{2}\left(\alpha_k^x(\vec{\lambda}) \sigma^x + \alpha_k^y(\vec{\lambda}) \sigma^y + \alpha_k^z(\vec{\lambda}) \sigma^z \right)$$

$\Rightarrow$ compute:

$$i[\mathcal{X}_k, H_k] = \left(\alpha^y(h-\cos k) - \alpha^z\gamma\sin k\sin\phi\right)\sigma^x$$
$$+\left(\alpha^z\gamma\sin k\cos\phi - \alpha^x(h-\cos k)\right)\sigma^y$$
$$+\gamma\sin k\left(\alpha^x\sin\phi - \alpha^y\cos\phi\right)\sigma^z$$

– action: for A_h : $G_{\substack{h\\ \gamma\\ \phi}}(\vec{\alpha}) = \partial_{\substack{h\\ \gamma\\ \phi}} H_k + i[\mathcal{X}_k, H_k]$

$$\frac{1}{2}S_h[\mathcal{X}] = \left(-1 + \alpha^x\gamma\sin k\sin\phi - \alpha^y\gamma\sin k\cos\phi\right)^2$$
$$+\left(\alpha^y(h-\cos k) - \alpha^z\gamma\sin k\sin\phi\right)^2$$
$$+\left(\alpha^z\gamma\sin k\cos\phi - \alpha^x(h-\cos k)\right)^2$$

→ minimizing action S_h wrt $\alpha^{x/y/z}$ gives:

$$\alpha_k^x = \frac{\gamma\sin k\sin\phi}{\gamma\sin^2 k + (h-\cos k)^2}$$

$$\alpha_k^y = -\frac{\gamma\sin k\cos\phi}{\gamma\sin^2 k + (h-\cos k)^2}$$

$$\alpha_k^z = 0$$

→ read off gauge pot.:

$$A_h = \frac{1}{2}\sum_k \frac{\gamma\sin k}{(\cos k-h)^2+\gamma^2\sin^2 k}\,\psi_k^\dagger\left(\sin\phi\,\sigma^x - \cos\phi\,\sigma^y\right)\psi_k$$

→ similarly for A_γ, A_ϕ

Rmks:

→ gauge potentials look simple in momentum space but can be non-local (long-range) in real space

→ gauge potential contains long strings of Pauli op's when written in terms of the original spin op's (inverting JW transf.)

to see this: fix $\gamma = 1$, $\phi = 0$

$$A_h = -\frac{1}{2}\sum_k \frac{\sin k}{(\cos k - h)^2 + \sin^2 k}\, \psi_k^\dagger \sigma^y \psi_k$$

<u>use</u>: 1) $\psi_k^\dagger \sigma^y \psi_k = \frac{1}{L}\sum_\ell \sin(\ell k) \sum_j i\left(c_j^\dagger c_{j+\ell}^\dagger - c_{j+\ell} c_j\right)$

2) $\mathcal{O}_\ell := 2i \sum_j c_j^\dagger c_{j+\ell}^\dagger - c_{j+\ell} c_j$

$$\overset{\text{inv. JW}}{\simeq} \sum_j \sigma_j^x \underbrace{\sigma_{j+1}^z \cdots \sigma_{j+\ell-1}^z} \sigma_{j+\ell}^y + \sigma_j^y \underbrace{\sigma_{j+1}^z \cdots \sigma_{j+\ell-1}^z} \sigma_{j+\ell}^x$$

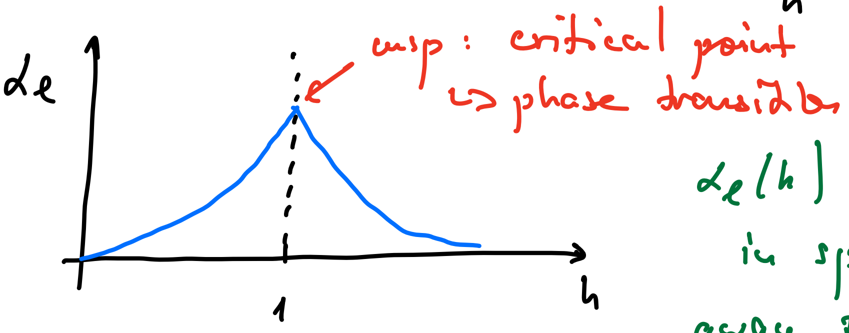
non-local Pauli strings

then $A_h = \sum_\ell \alpha_\ell \mathcal{O}_\ell$

where $$\alpha_\ell = -\frac{1}{4L}\sum_{k\in BZ} \frac{\sin(\ell k)\sin k}{(\cos k - h)^2 + \sin^2 k}$$

$$\xrightarrow[L\to\infty]{\text{TD limit}} -\frac{1}{4\pi}\int_{-\pi}^{\pi} dk\, \frac{\sin(\ell k)\sin k}{(\cos k - h)^2 + \sin^2 k}$$

$$= -\frac{1}{8}\begin{cases} h^{\ell-1}, & |h| \le 1 \\ \frac{1}{h^{\ell+1}}, & |h| \ge 1 \end{cases}$$



$\alpha_\ell(h)$ decays exponentially in in space (i.e. in ℓ) away from critical pt. at $h_c = 1$

→ away from critical point, truncate:

$$A_\lambda \approx \alpha_1 \mathcal{O}_1 + \alpha_2 \mathcal{O}_2$$

$$= \alpha_1 \sum_j \sigma_j^x \sigma_{j+1}^y + \sigma_j^y \sigma_{j+1}^x$$

$$+ \alpha_2 \sum_j \sigma_j^x \sigma_{j+1}^z \sigma_{j+2}^y + \sigma_j^y \sigma_{j+1}^z \sigma_{j+2}^x$$

local approximation