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

=> issue : A_λ is a nonlocal op. (A_λ generates U_λ)

-> cannot be implemented in the lab

Q: can we find a good local approximation?

recall : def of gauge pot.

$$\partial_\lambda H + i[A_\lambda, H] = -M_\lambda$$

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

unknown op.

=> 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

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

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

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

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

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

→ calculate:

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

$$M_\lambda = \sum_n \left(\partial_\lambda E_n\right) |n\rangle\langle n|$$

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

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

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

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

→ 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: $\frac{\delta S[X]}{\delta X} \overset{!}{=} 0$

exchange: $m \leftrightarrow n$

$$\frac{\delta S}{\delta X_{ij}} \underset{\text{using einsum}}{=} \frac{\delta}{\delta X_{ij}} \left(G_{nm} G_{mn}\right) = \frac{\delta G_{nm}}{\delta X_{ij}} G_{mn} + G_{nm} \frac{\delta G_{mn}}{\delta X_{ij}}$$

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

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

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

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

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

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

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

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

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

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

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

<u>ansatz</u>: $$X_\lambda = \sum_n \alpha_n(\lambda)\,\mathcal{O}_n$$

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

some operators (educated guess)

- respect <u>locality</u> ✓
- 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 $\mathcal{X} = \sum \alpha_n \mathcal{O}_n$

– consider $H(\lambda)$ real-valued:

$\Rightarrow U^\dagger H U = \text{diag}$: U is real-valued

$\Rightarrow A_\lambda = i(\partial_\lambda U) U^\dagger$ is purely imaginary (e.g. σ^y)

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

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

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

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

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

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

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

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

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

def:

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

subtracts off-diag. matrix elts.

$\Rightarrow$ ansatz for gauge pot.

$$\mathcal{X}_\lambda = \sum_k \underset{\substack{\uparrow \\ \text{variational} \\ \text{coefficients}}}{\alpha_{2k+1}} \underbrace{[H, \ldots, [H}_{2k+1 \text{ times}}, \partial_\lambda H]]$$

<u>examples</u>:

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

<u>ansatz</u>: $\mathcal{X}_\lambda = \alpha \sigma^x + \beta \sigma^y + \gamma \sigma^z$

(all possible operators)

<u>need</u>: $\partial_\alpha S$, $\partial_\beta S$, $\partial_\gamma S$

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

$$\begin{aligned}
G[\mathcal{X}] &= \partial_\lambda H + i [\mathcal{X}, H] \\
&= \sigma^x + i [\alpha \sigma^x + \beta \sigma^y + \gamma \sigma^z, \Delta \sigma^z + \lambda \sigma^x] \\
&= \sigma^x + 2 (\alpha \Delta \sigma^y - \beta \Delta \sigma^x + \beta \lambda \sigma^z - \gamma \lambda \sigma^y) \\
&= (1 - 2\beta\Delta) \sigma^x + 2(\alpha\Delta - \gamma\lambda)\sigma^y + 2\beta\lambda\sigma^z
\end{aligned}$$

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

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

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

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

$$\Rightarrow \begin{cases} \alpha\Delta = \gamma\lambda \quad \leftarrow \text{relation btw } \alpha,\gamma \quad (*) \\ -2\Delta + 4\beta(\Delta^2+\lambda^2) = 0 \quad \Rightarrow \beta = \frac{1}{2}\frac{\Delta}{\Delta^2+\lambda^2} \end{cases}$$

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

$$= A_\lambda + \frac{\alpha}{\lambda}\underbrace{(\Delta\sigma^z + \lambda\sigma^x)}_{=H(\lambda)} \quad \checkmark$$

2) Quantum XY model

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

exchange couplings

external field

anisotropy

re-parametrize: $J_x = \frac{1+\gamma}{2}J$

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

exchange scale

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

- consider rotating $\tilde{H}$ about z-axis at angle $\phi/2$

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

$$\Rightarrow \quad H(\gamma, \phi, h) = U_\phi^\dagger \tilde{H}(\gamma, h) U_\phi$$

- 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:

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

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

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

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

$\to$ 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 contain 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) $O_\ell := 2i \sum_j c_j^\dagger c_{j+\ell}^\dagger - c_{j+\ell} c_j$

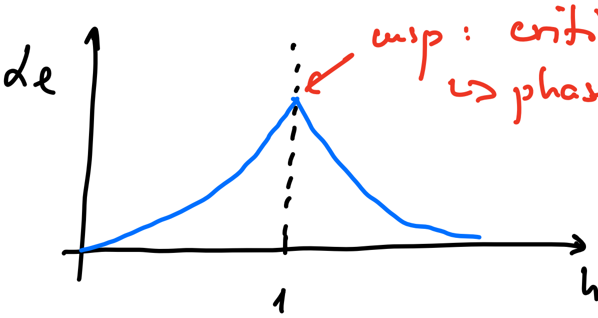
$$\overset{\text{inv. JW}}{=} \sum_j \sigma_j^x \underbrace{\sigma_{j+1}^z \cdots \sigma_{j+\ell-1}^z}_{\text{non-local}} \sigma_{j+\ell}^y + \sigma_j^y \underbrace{\sigma_{j+1}^z \cdots \sigma_{j+\ell-1}^z}_{\text{Pauli strings}} \sigma_{j+\ell}^x$$

then $A_h = \sum_\ell \alpha_\ell O_\ell$

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

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

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



cusp: critical point
↳ phase transition

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

→ away from critical point, truncate:

$$A_\lambda \approx \alpha_1 O_1 + \alpha_2 O_2$$

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

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

local approximation