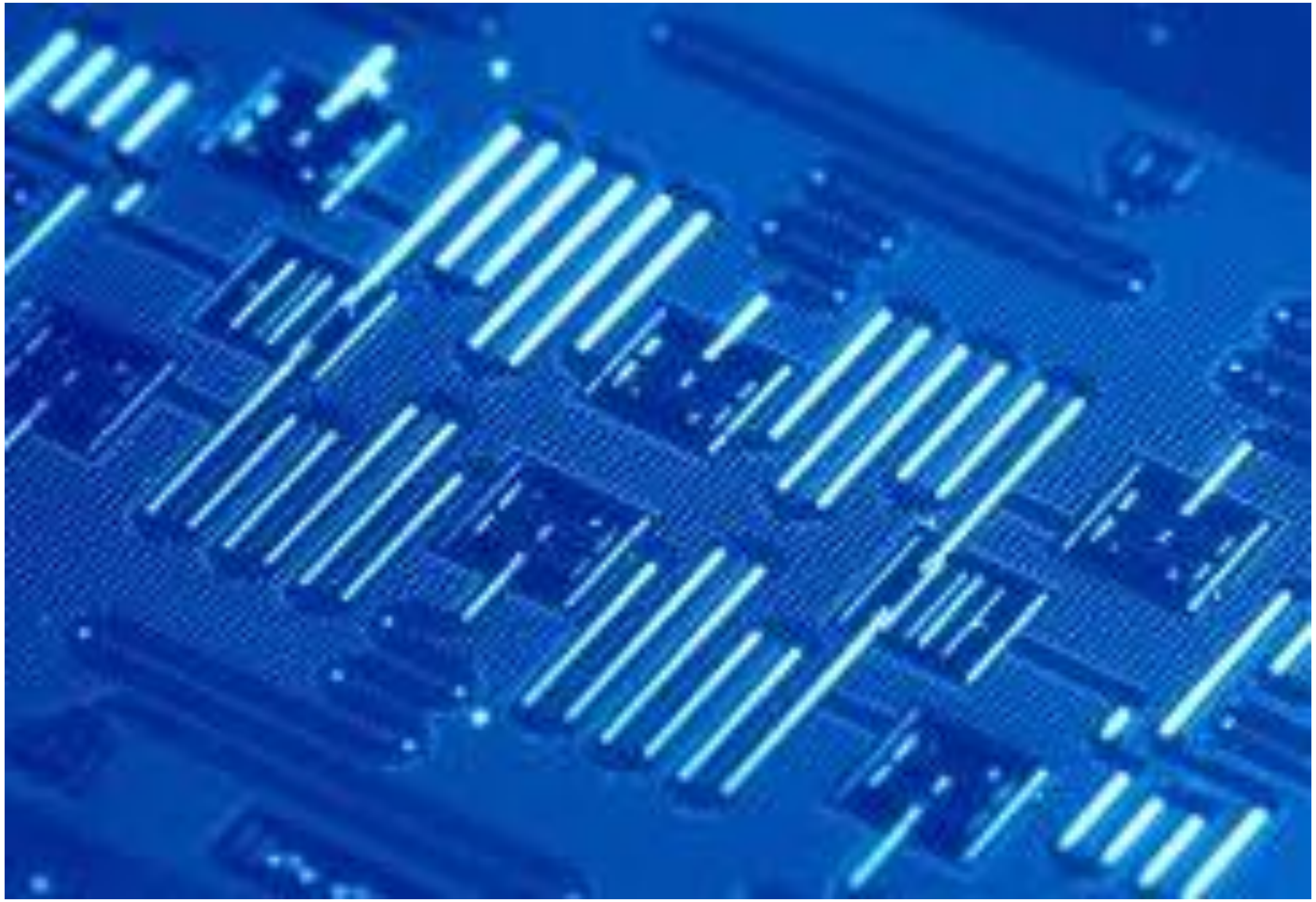
Numerical analysis of protected qubits

TR CONTROL:

Gabriel Vandersippe,
Eliot Delachaux



Source : IBM (via The Quantum Insider)

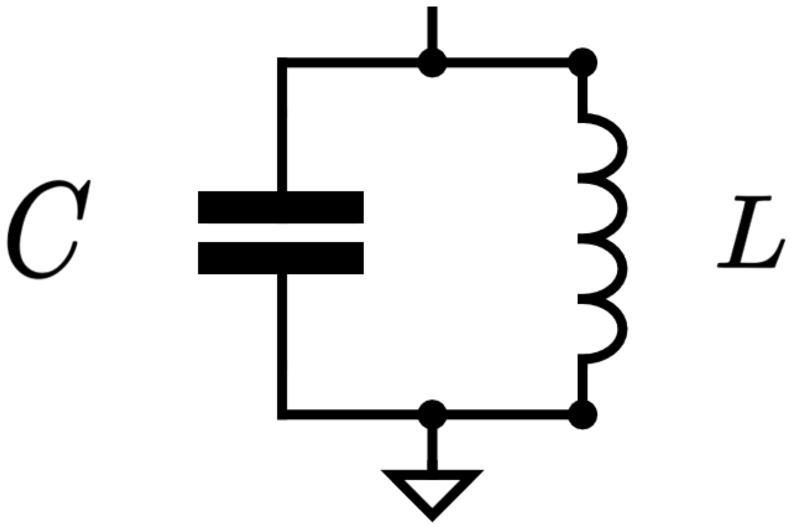
Outline

1. Brief introduction to superconducting circuits
2. Project Motivations
3. Results with Krylov techniques (Eliot)
4. Results with Tensor Networks (Gabriel)

Using Python packages :
NumPy, QuTiP, SCQubits, MatPlotLib, SciPy, JAX, Pandas

Using Julia packages :
ITensors, ITensorMPS, KrylovKit, CairoMakie, LinearAlgebra, HypergeometricFunctions, CSV, DataFrames

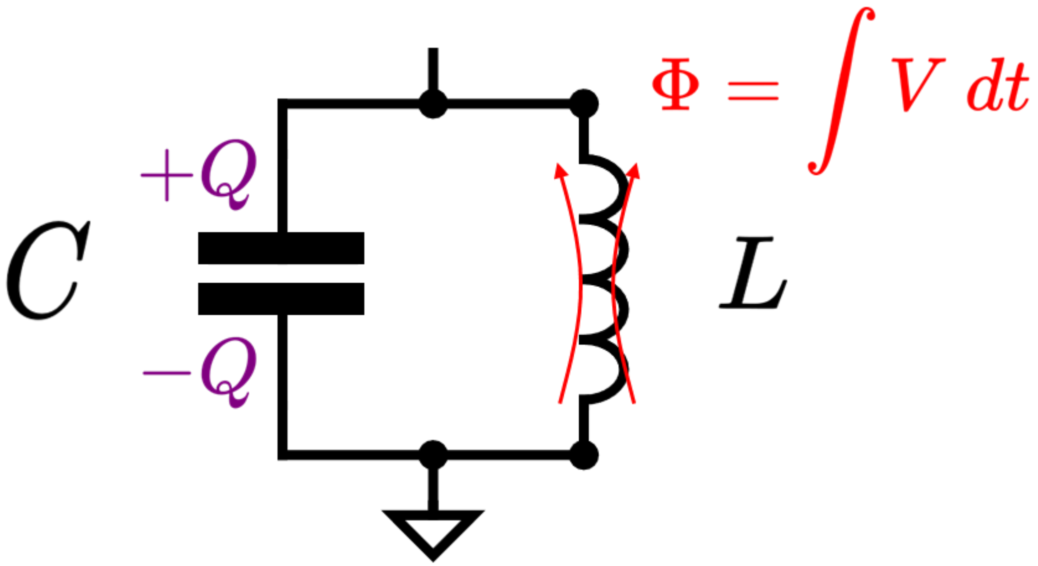
Introduction : Harmonic Oscillator



$$H = \underbrace{\frac{Q^2}{2C}}_{\text{Kinetic}} + \underbrace{\frac{\Phi^2}{2L}}_{\text{Potential}}$$

Blais, *et al.*, *Reviews of Modern Physics* **93 (2)**, 025005 (2021)

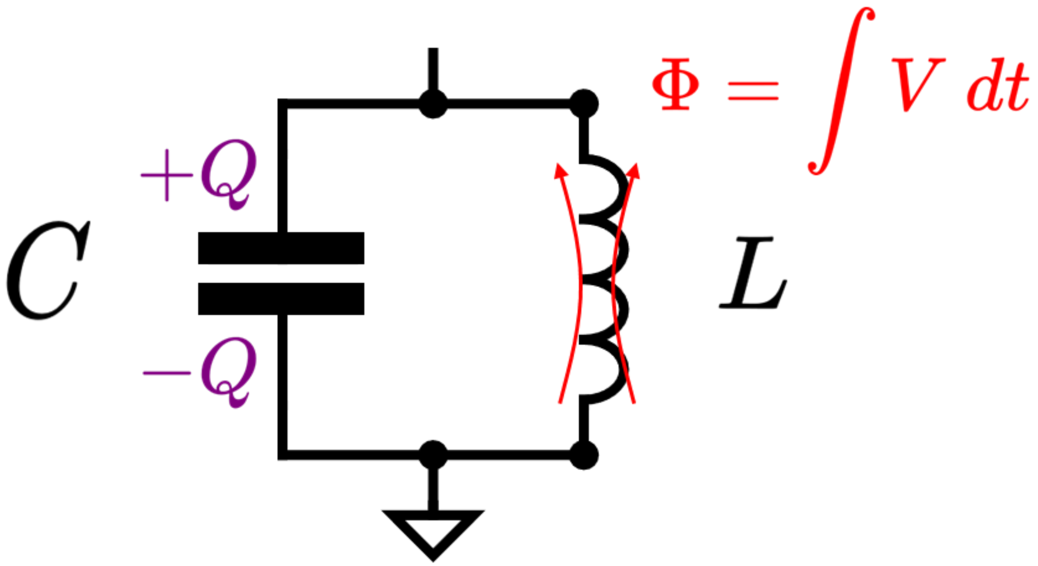
Introduction : Harmonic Oscillator

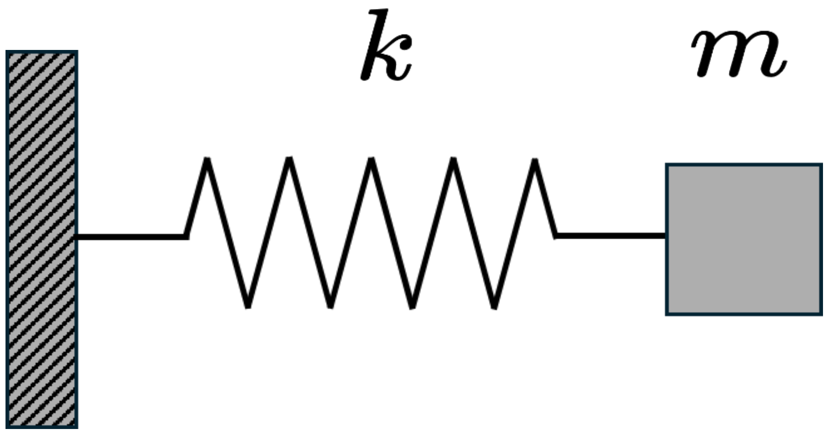


$$H = \underbrace{\frac{Q^2}{2C}}_{\text{Kinetic}} + \underbrace{\frac{\Phi^2}{2L}}_{\text{Potential}}$$

Blais, *et al.*, *Reviews of Modern Physics* **93 (2)**, 025005 (2021)

Introduction : Harmonic Oscillator



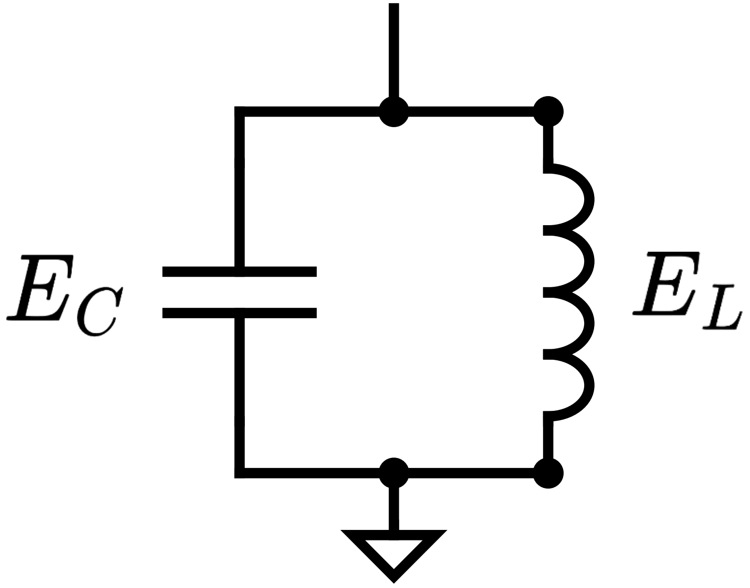


$$H = \underbrace{\frac{Q^2}{2C}}_{\text{Kinetic}} + \underbrace{\frac{\Phi^2}{2L}}_{\text{Potential}}$$

$$H = \underbrace{\frac{1}{2m}p^2}_{\text{Kinetic}} + \underbrace{\frac{k}{2}x^2}_{\text{Potential}}$$

Blais, *et al.*, *Reviews of Modern Physics* **93 (2)**, 025005 (2021)

Quantizing the Harmonic Oscillator



Hamiltonian :

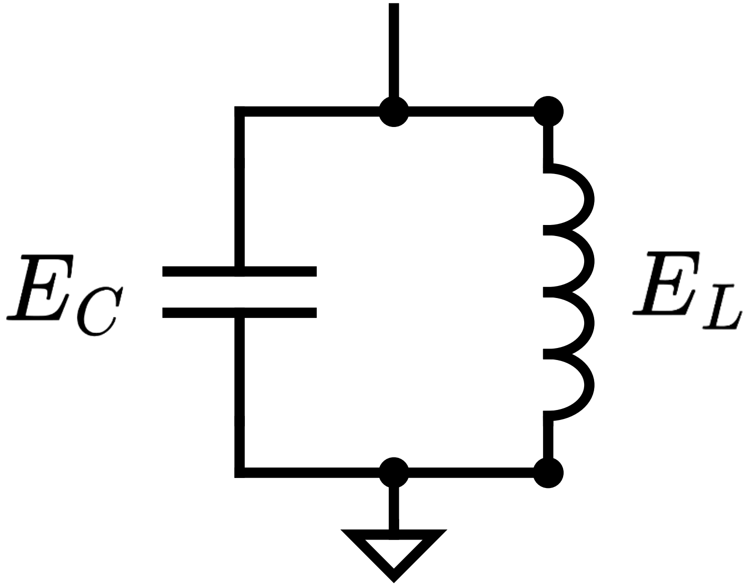
$$H = \underbrace{\frac{Q^2}{2C}}_{\text{Kinetic}} + \underbrace{\frac{\Phi^2}{2L}}_{\text{Potential}}$$

Correspondence principle : $H \rightarrow \hat{H}$ Operator

$$\Rightarrow \quad \hat{H} = 4E_C\hat{n}^2 + \frac{E_L}{2}\hat{\varphi}^2$$

Blais, *et al.*, *Reviews of Modern Physics* **93 (2)**, 025005 (2021)

Quantizing the Harmonic Oscillator



Hamiltonian :

$$H = \underbrace{\frac{Q^2}{2C}}_{\text{Kinetic}} + \underbrace{\frac{\Phi^2}{2L}}_{\text{Potential}}$$

Correspondence principle : $H \to \hat{H}$ Operator

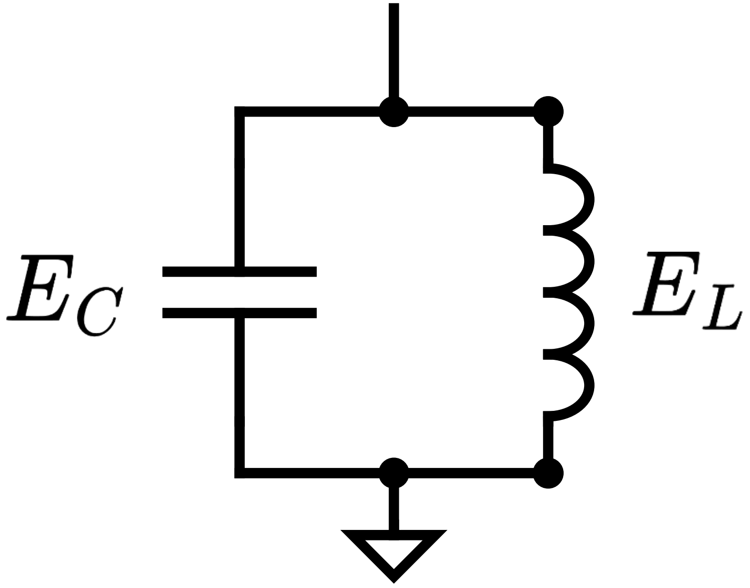
$$\Rightarrow \hat{H} = 4E_C\hat{n}^2 + \frac{E_L}{2}\hat{\varphi}^2$$

$$= \hbar\omega \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Infinite basis : $\{|0\rangle, |1\rangle, \ldots |n\rangle, |n+1\rangle, \ldots\}$

Blais, *et al.*, *Reviews of Modern Physics* **93 (2)**, 025005 (2021)

Quantizing the Harmonic Oscillator



Hamiltonian :

$$H = \underbrace{\frac{Q^2}{2C}}_{\text{Kinetic}} + \underbrace{\frac{\Phi^2}{2L}}_{\text{Potential}}$$

Correspondence principle : $H \to \hat{H}$ Operator

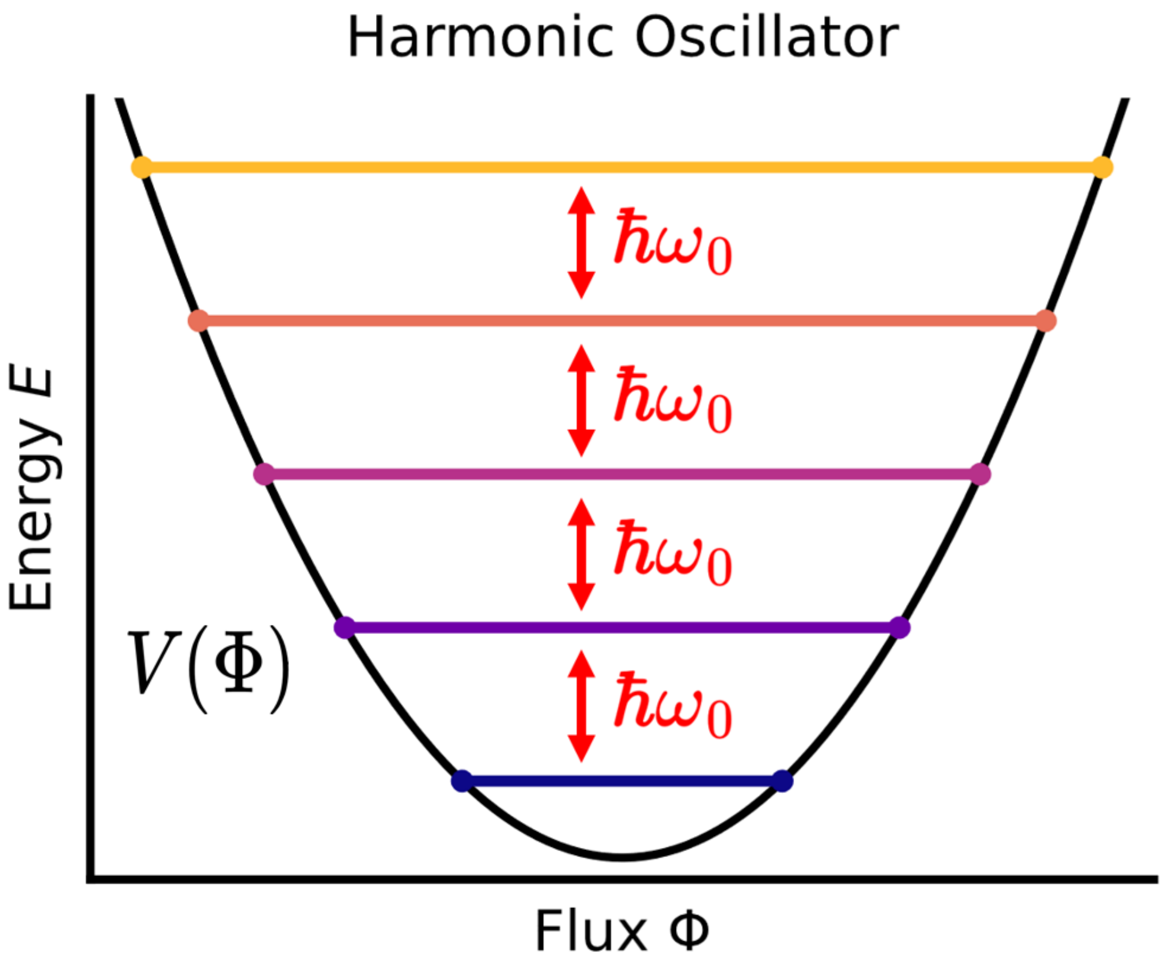
$$\Rightarrow \hat{H} = 4E_C\hat{n}^2 + \frac{E_L}{2}\hat{\varphi}^2$$

$$= \hbar\omega \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

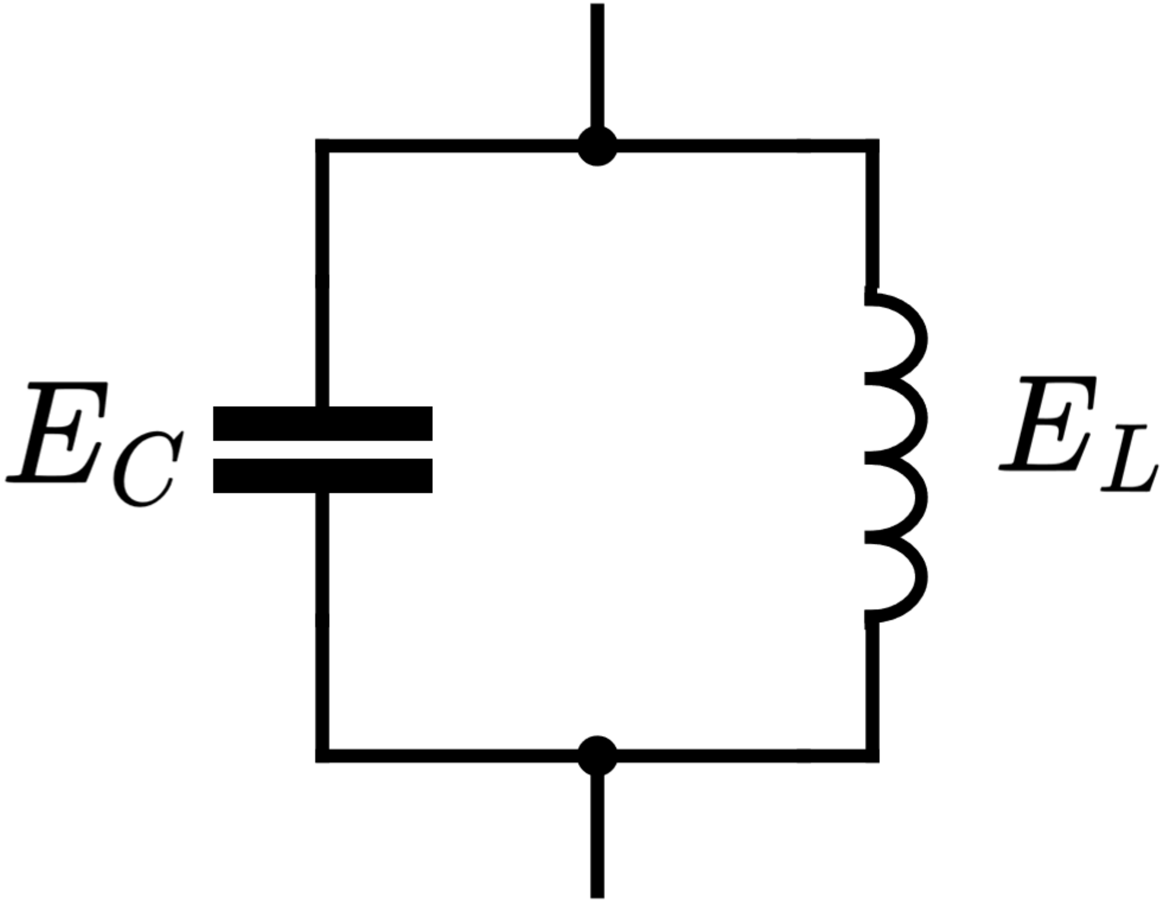
Infinite basis : $\{|0\rangle, |1\rangle, \ldots |n\rangle, |n+1\rangle, \ldots\}$

cutoff

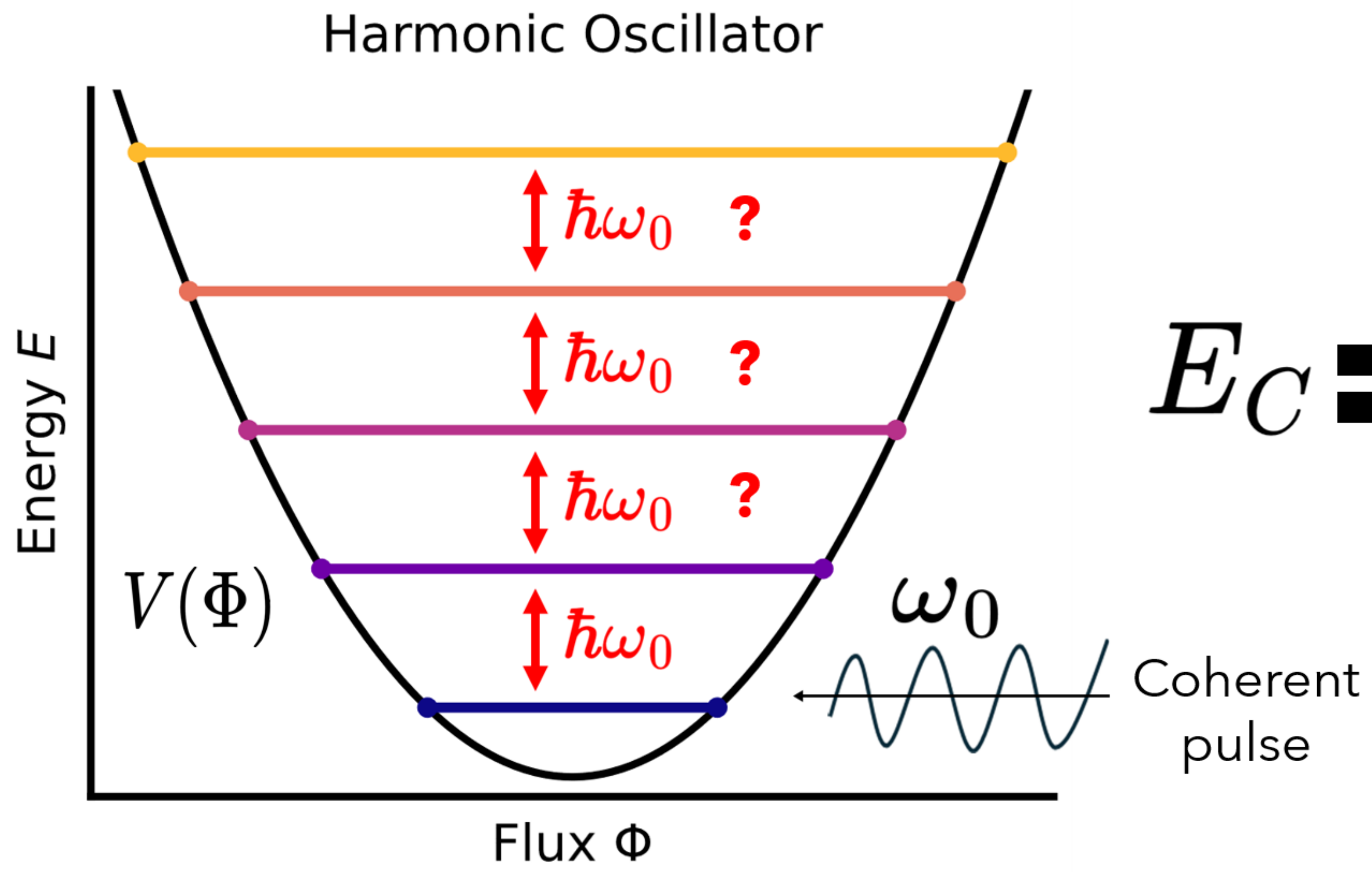
Harmonic oscillator to Qubit



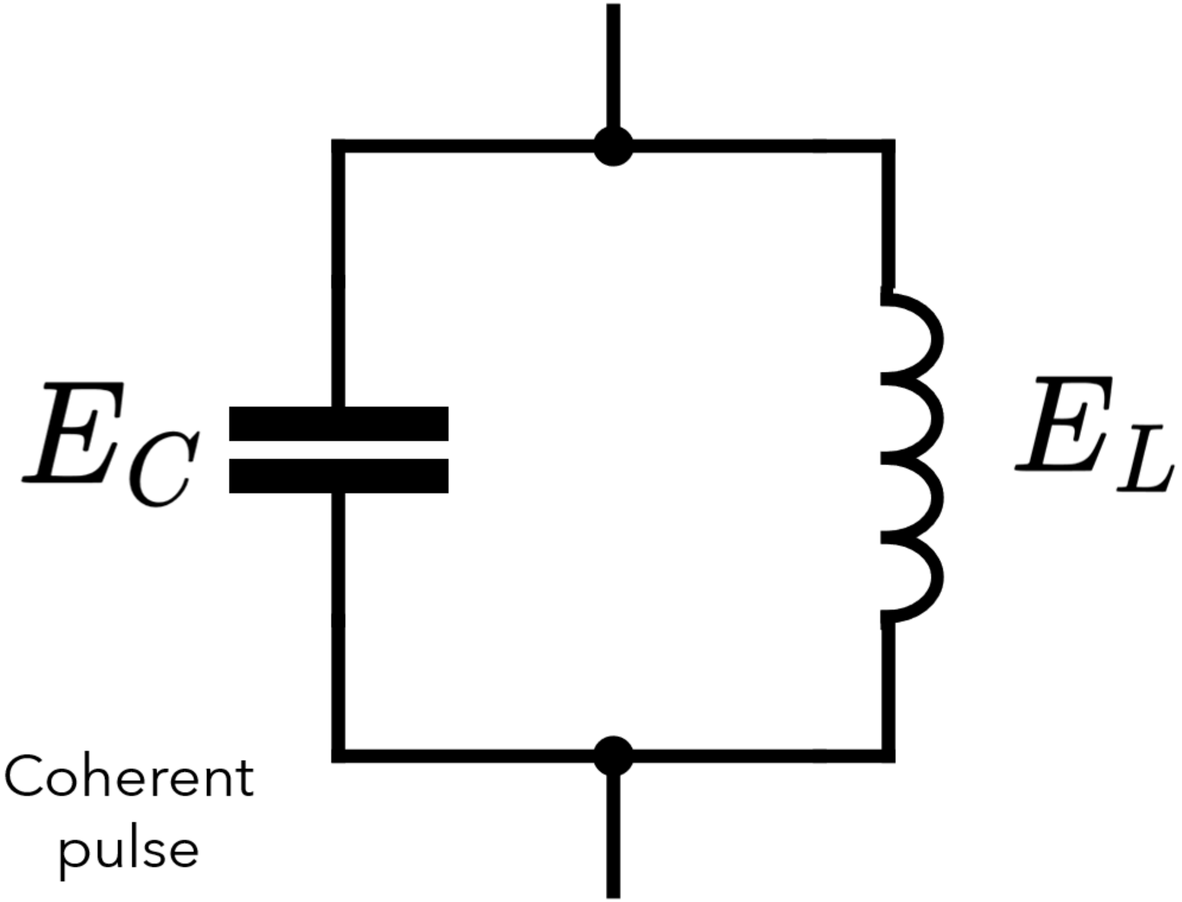
Plotted with scqubits



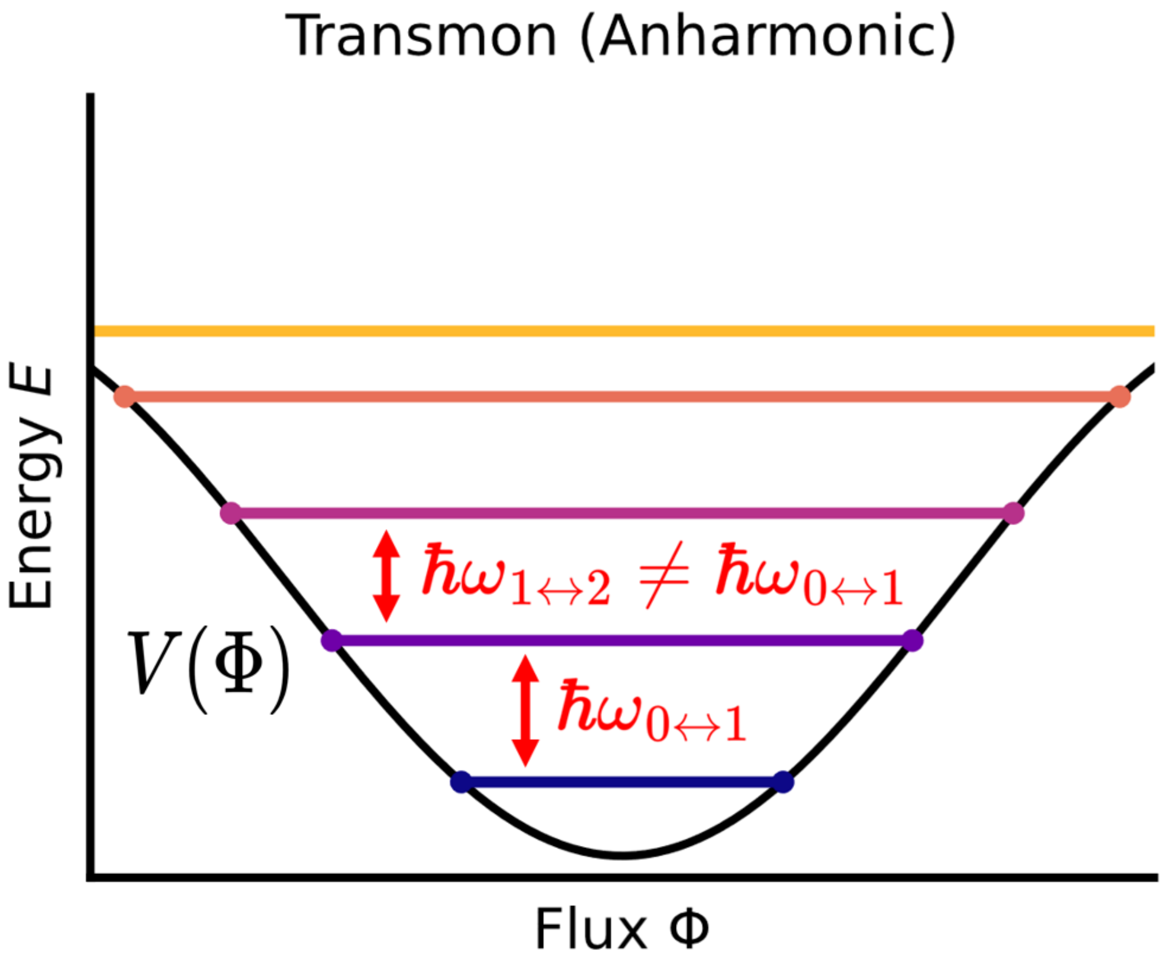
Harmonic oscillator to Qubit



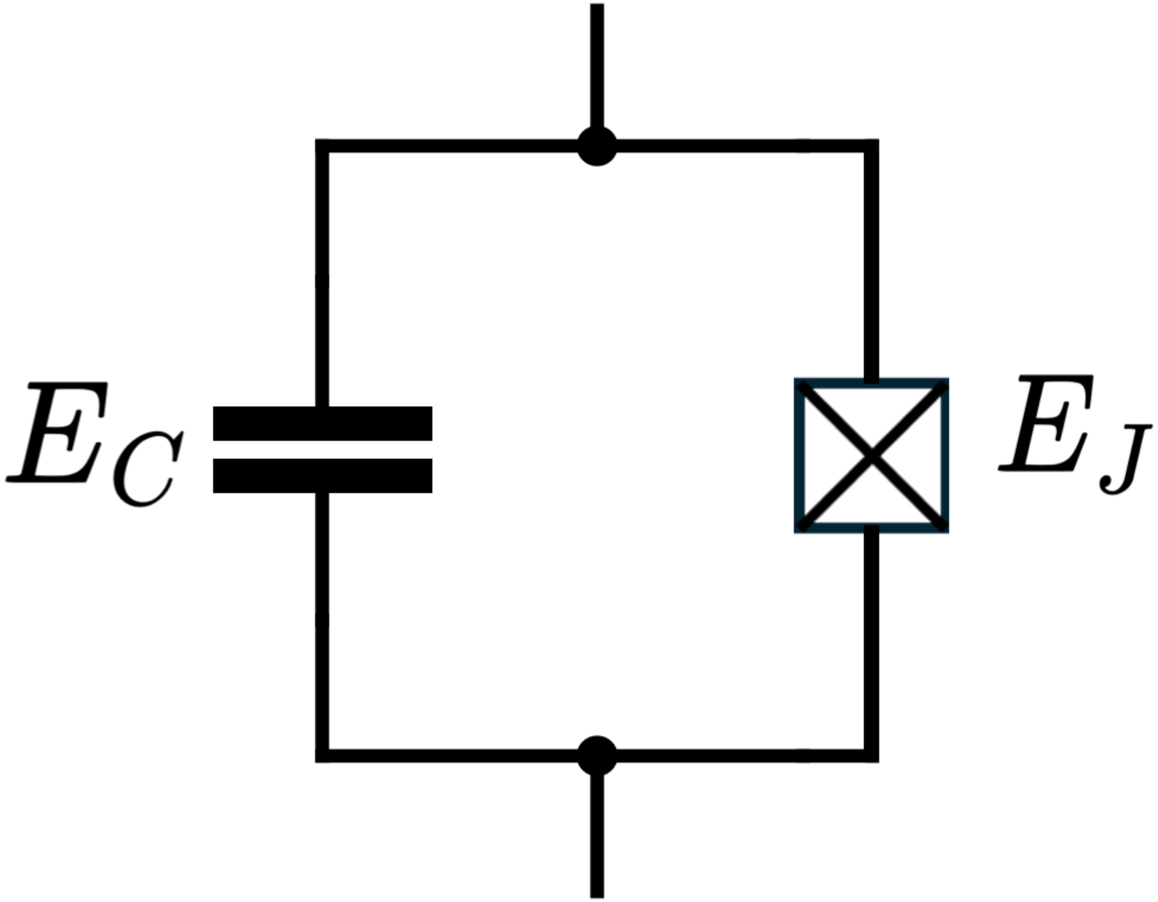
Plotted with scqubits



Harmonic oscillator to Qubit

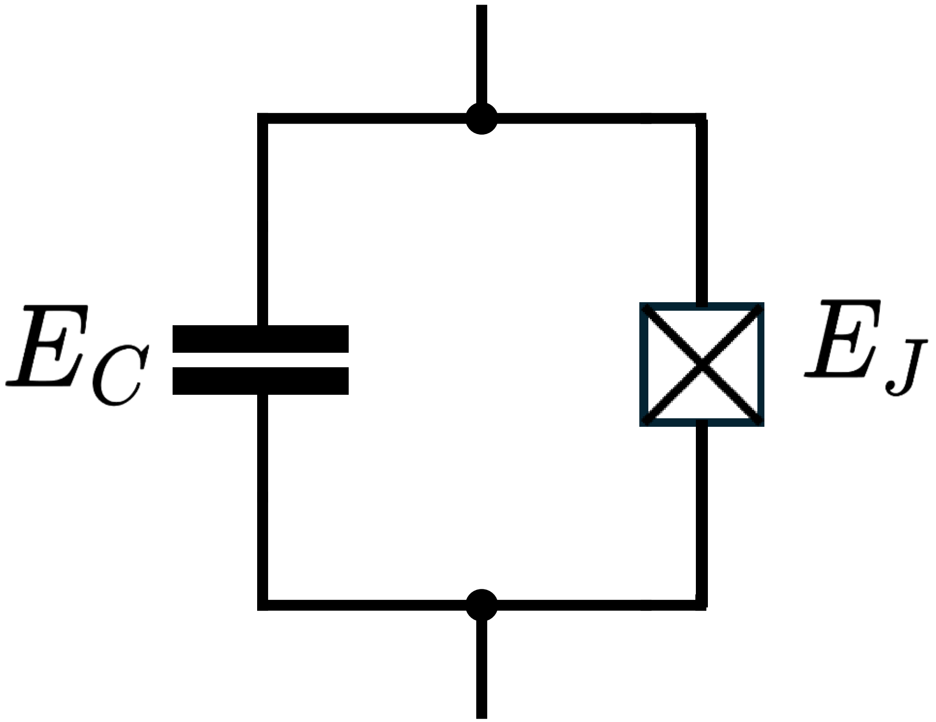


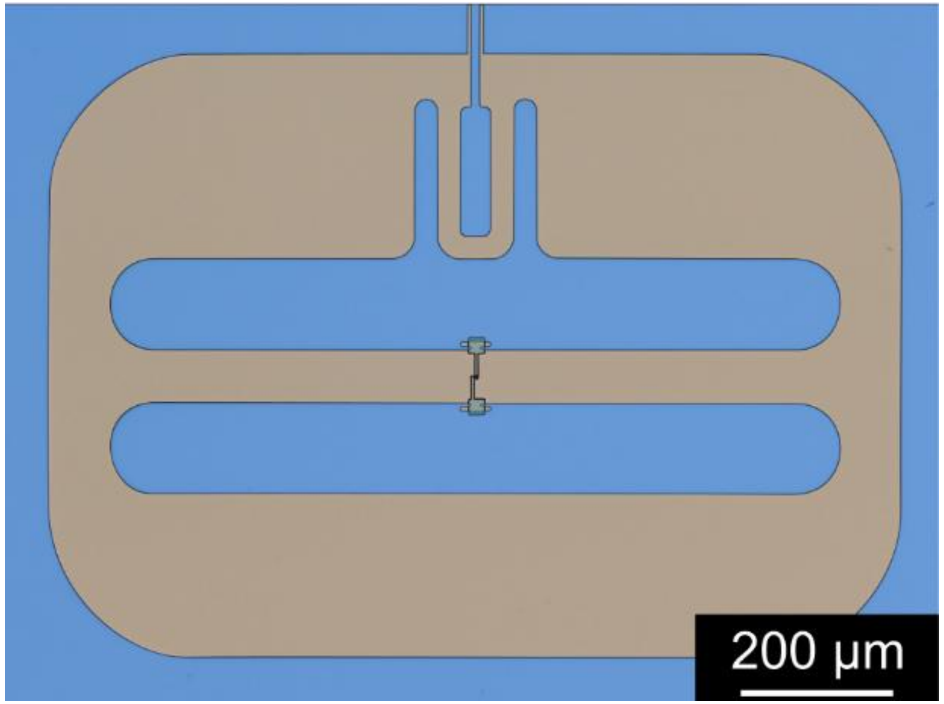
Plotted with scqubits



Koch, *et al.*, *Phys. Rev. A* **76**, 042319 (2007)

Transmon

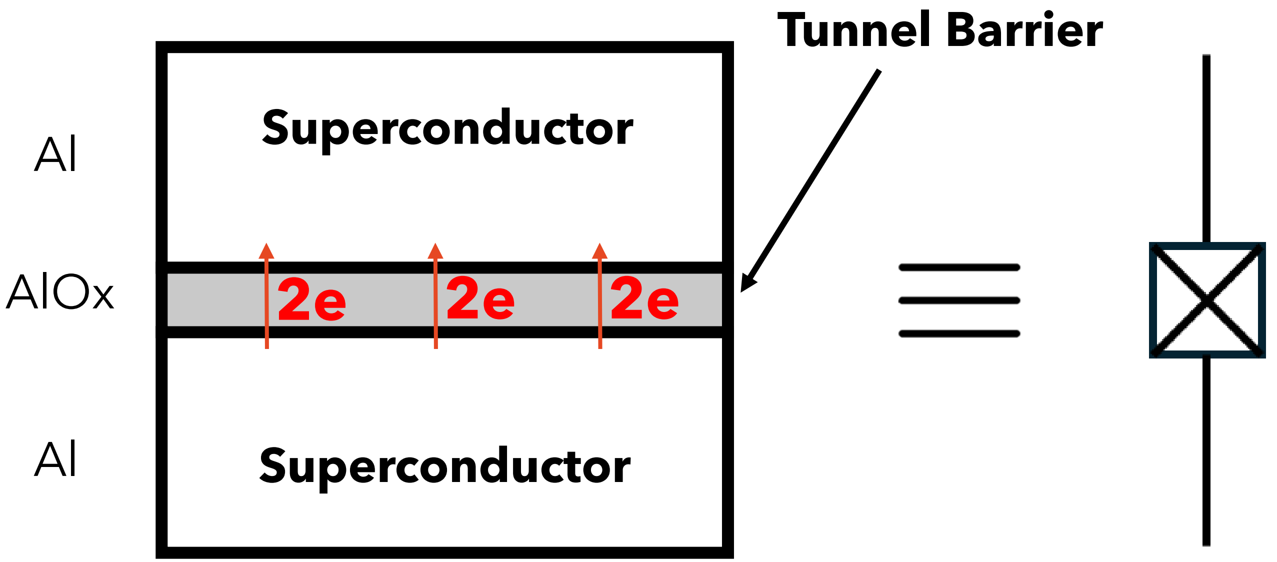


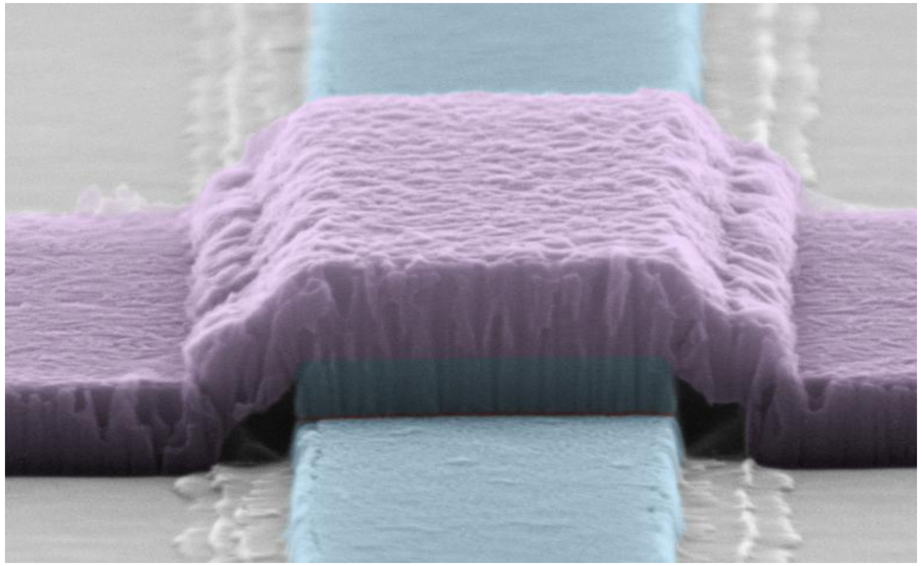


Houck lab arXiv : 2003.00024

Koch, *et al.*, *Phys. Rev. A* **76**, 042319 (2007)

Josephson Junction

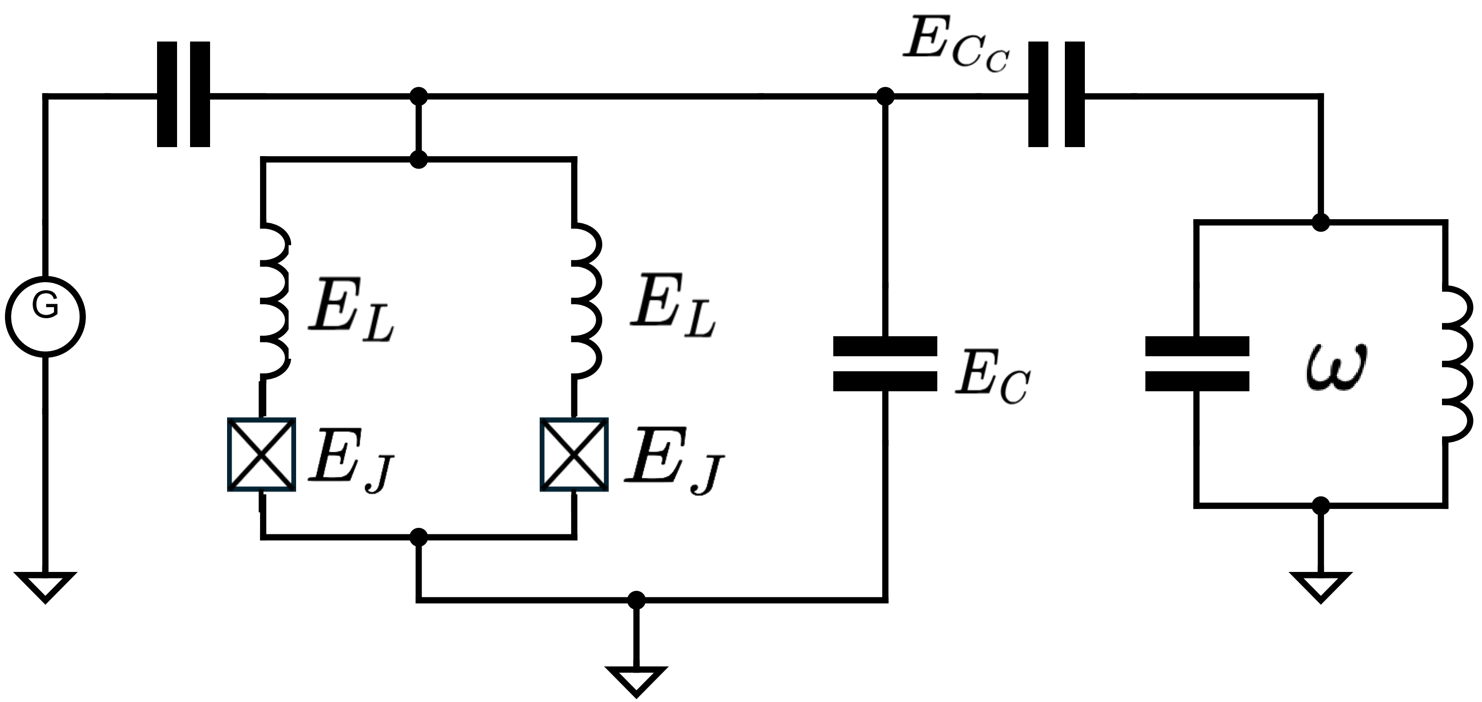




Source : NQISRC

$$H = 4E_C n^2 - E_J \cos(\varphi)$$

Kite Qubit

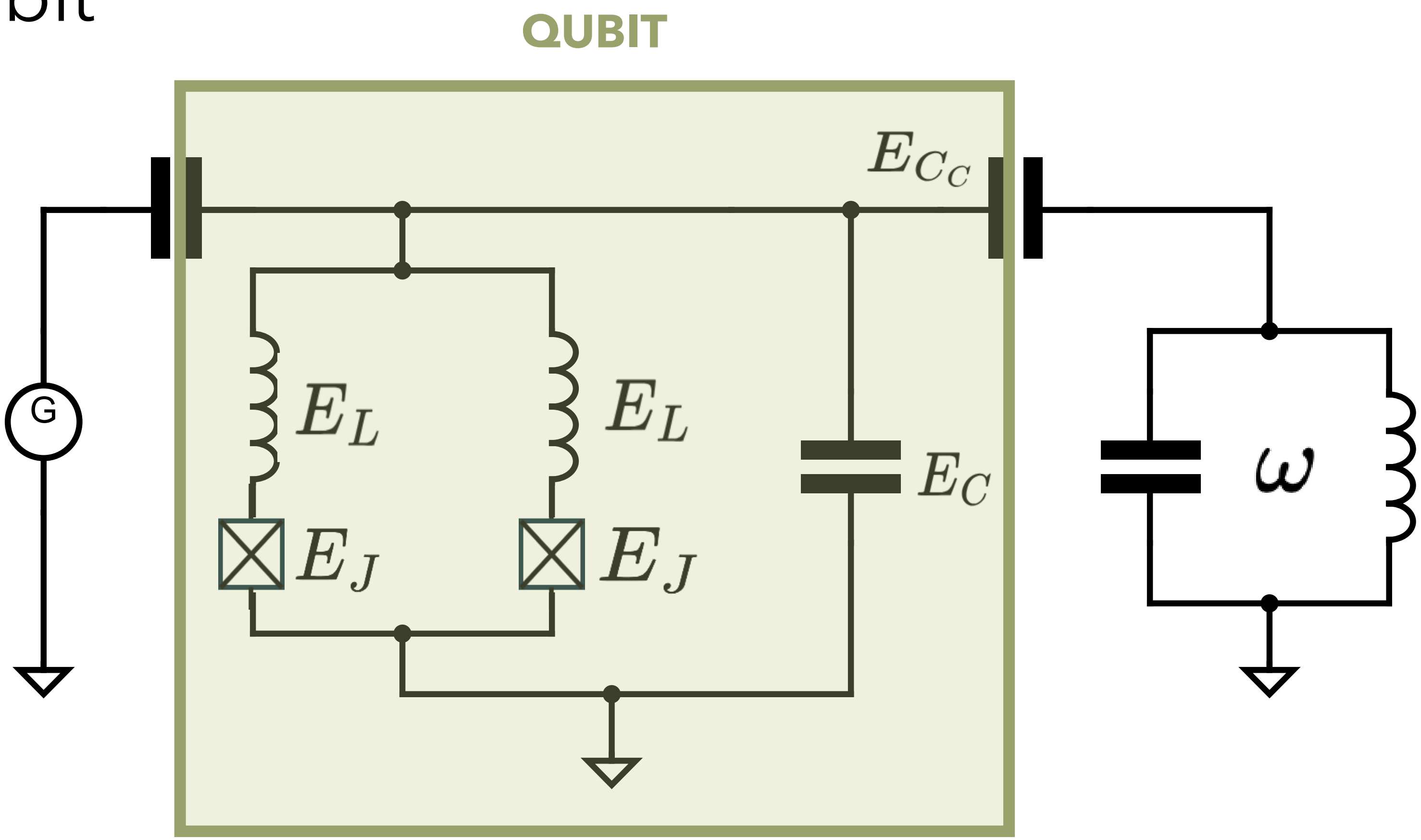


$$\hat{H} =$$

$$d =$$

Smith, *et al.*, *Phys. Rev. X* **12**, 021002 (2022)

Kite Qubit

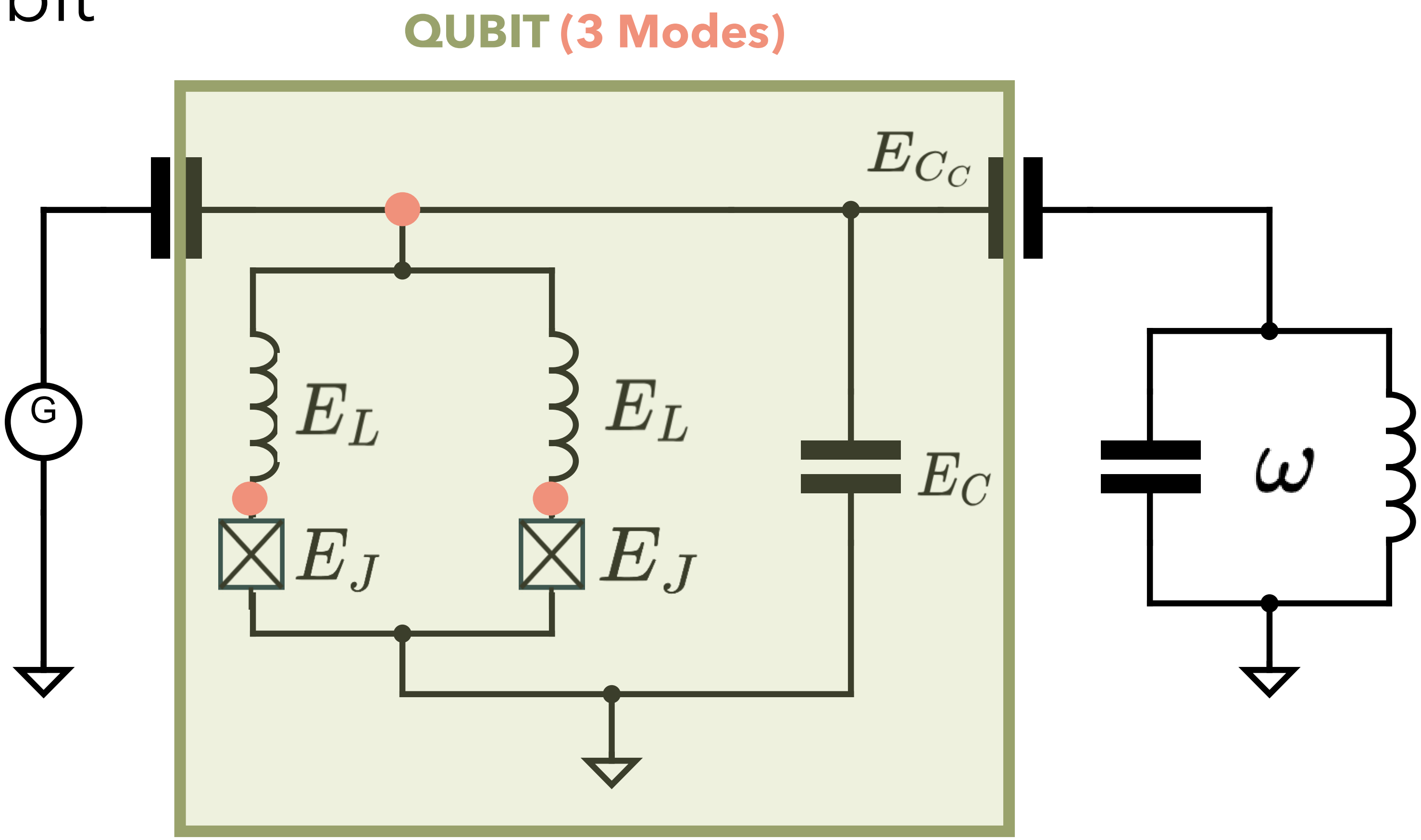


$$\hat{H} = \hat{H}_q$$

$$d = (n_1 * n_2 * n_3)$$

Smith, *et al.*, *Phys. Rev. X* **12**, 021002 (2022)

Kite Qubit

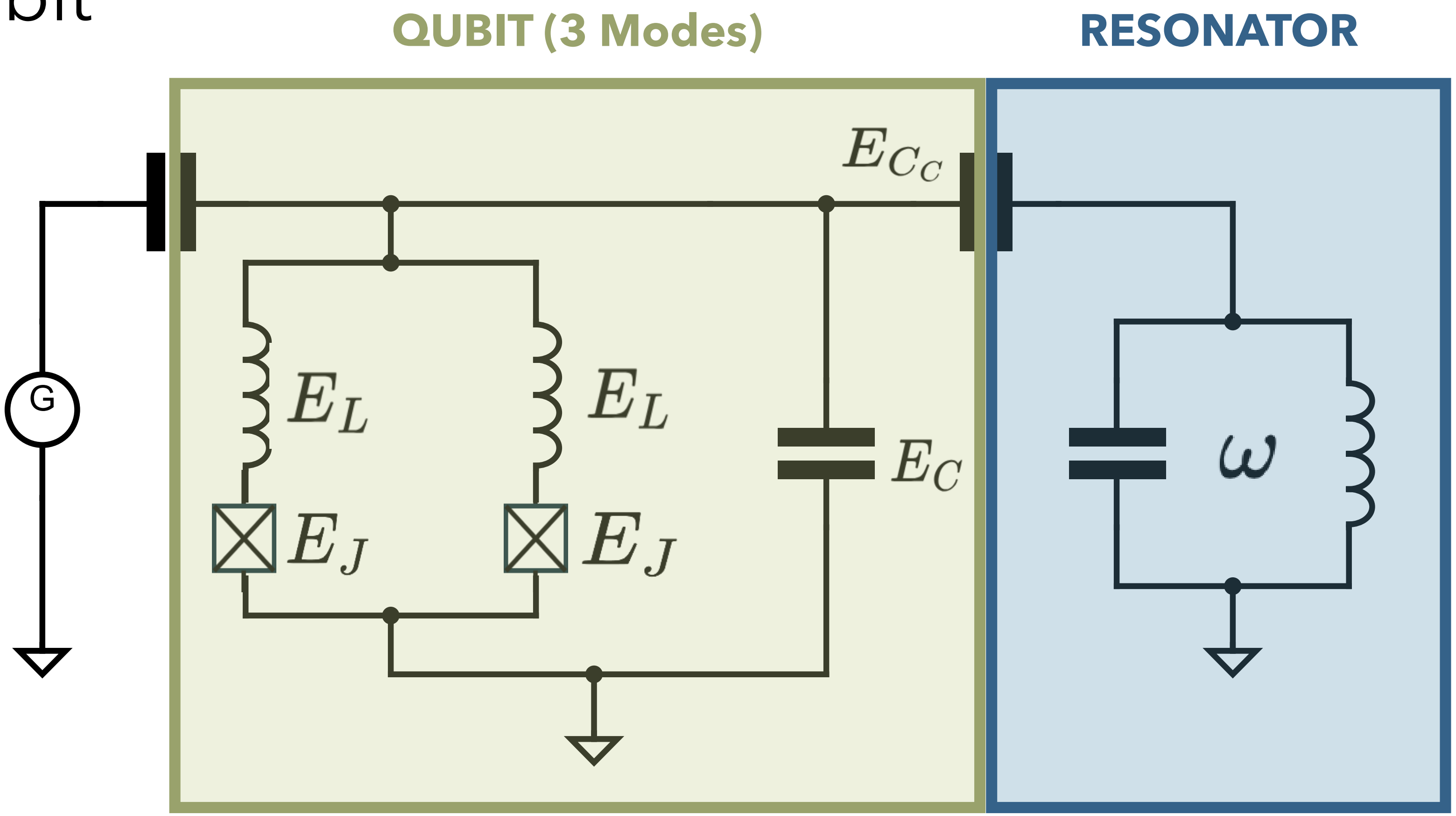


$$\hat{H} = \hat{H}_q$$

$$d = (n_1 * n_2 * n_3)$$

Smith, *et al.*, *Phys. Rev. X* **12**, 021002 (2022)

Kite Qubit

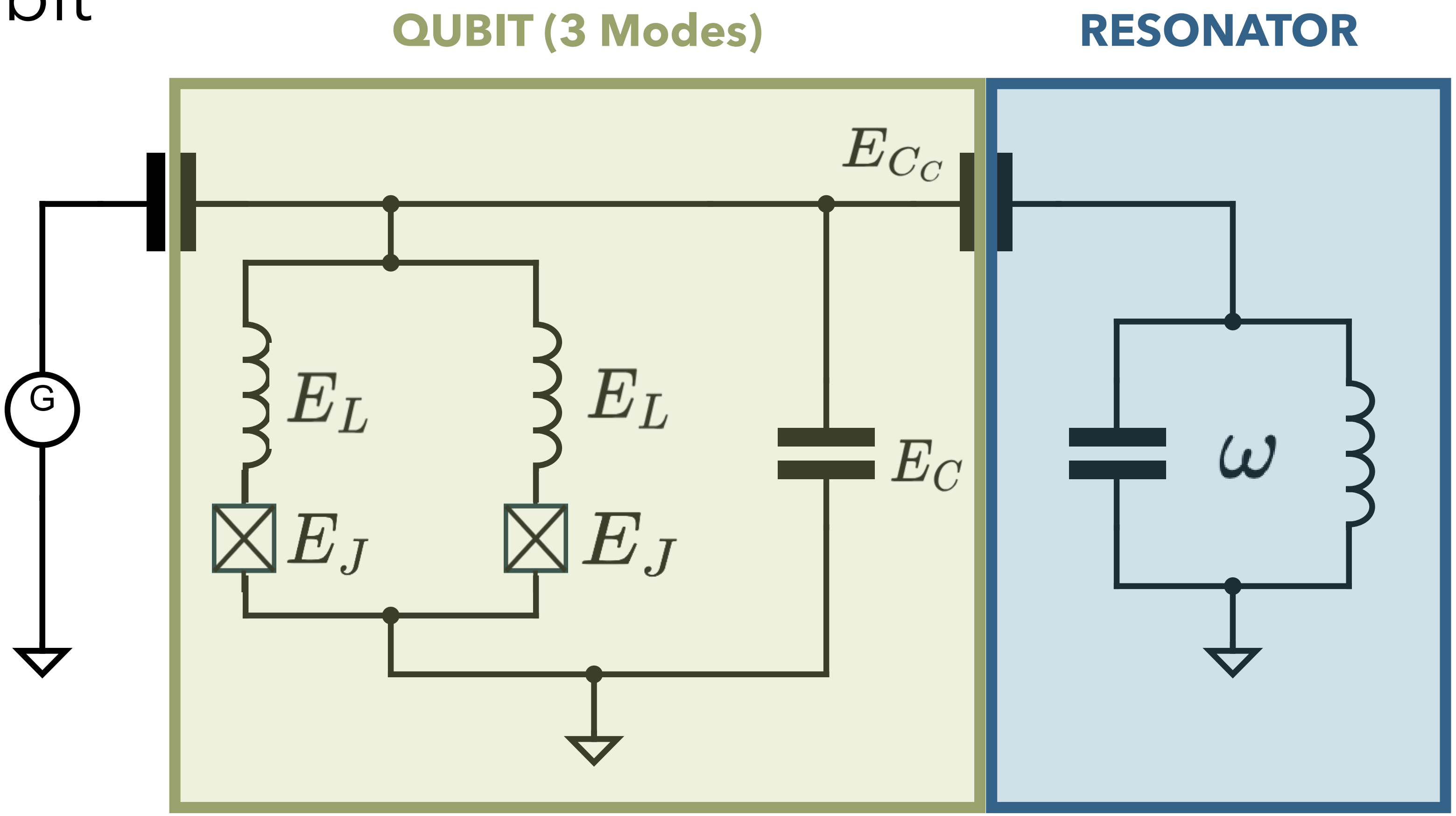


$$\hat{H} = \hat{H}_q + \hat{H}_r$$

$$d = (n_1 * n_2 * n_3) \quad * \quad n_4$$

Smith, *et al.*, *Phys. Rev. X* **12**, 021002 (2022)

Kite Qubit

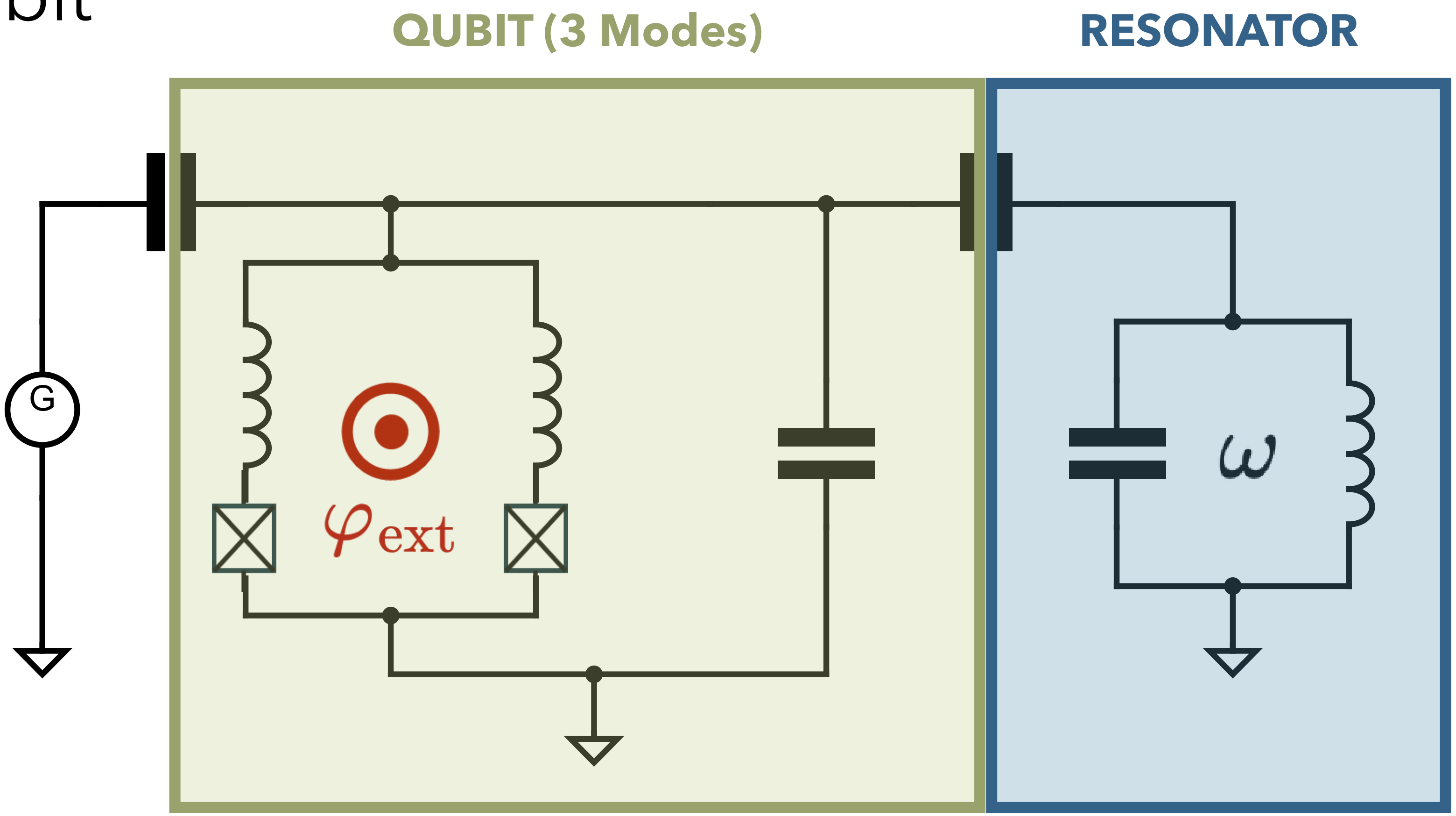


$$\hat{H} = \hat{H}_q + \hat{H}_r - g\,\hat{O}_1\hat{O}_2$$

$$d = (n_1 * n_2 * n_3) \quad * \quad n_4$$

Smith, *et al.*, *Phys. Rev. X* **12**, 021002 (2022)

Kite Qubit



$$\hat{H} = \hat{H}_q + \hat{H}_r - g\,\hat{O}_1\hat{O}_2$$

$$d = (n_1 * n_2 * n_3) \quad * \quad n_4$$

Smith, *et al.*, *Phys. Rev. X* **12**, 021002 (2022)

Motivations

$$\hat{H} = \overbrace{\begin{pmatrix} & \cdots & \\ \vdots & & \vdots \\ & \cdots & \end{pmatrix}}^{n} n$$

Motivations

$$\hat{H} = \begin{array}{cc} n & \\ \begin{pmatrix} & \cdots & \\ \vdots & & \vdots \\ & \cdots & \end{pmatrix} & n \end{array}$$

Exact Diagonalization (ED) :

$$\mathcal{O}\left(n^3\right)$$

Motivations

$$\begin{array}{ccc} & n & \\ \hat{H} = & \begin{pmatrix} & \cdots & \\ \vdots & & \vdots \\ & \cdots & \end{pmatrix} & n \end{array}$$

Exact Diagonalization (ED) :

$$\mathcal{O}\left(n^3\right)$$

Recall that $$n = n_1 * n_2 * n_3 * n_4$$

Motivations

$$\begin{array}{cc} n & \\ \hat{H} = \begin{pmatrix} & \cdots & \\ \vdots & & \vdots \\ & \cdots & \end{pmatrix} & n \end{array}$$

Exact Diagonalization (ED) : $\mathcal{O}\left(n^3\right)$

Recall that $n = n_1 * n_2 * n_3 * n_4$

For example, $n = 19 * 32 * 32 * 5$

$= 97\,280$

Krylov Techniques

The power algorithm : Dominant Eigenspace

$$\text{For a given matrix } \mathbf{A}, \text{ eigenbasis } \{(\lambda_1, |\psi_1\rangle), \ldots, (\lambda_n, |\psi_n\rangle)\}$$
$$\text{with } |\lambda_n| > |\lambda_{n-1}| > \cdots > |\lambda_1|$$

$$\text{For a random vector } |\Psi_0\rangle$$

$$\lim_{k\to\infty} \frac{\mathbf{A}^k|\Psi_0\rangle}{\||\mathbf{A}^k|\Psi_0\rangle\|} = |\psi_n\rangle$$

The power algorithm : Dominant Eigenspace

$$\text{For a given matrix } \mathbf{A}, \ \text{eigenbasis } \{(\lambda_1, |\psi_1\rangle), \ldots, (\lambda_n, |\psi_n\rangle)\}$$
$$\text{with } |\lambda_n| > |\lambda_{n-1}| > \cdots > |\lambda_1|$$

$$\text{For a random vector } |\Psi_0\rangle$$

$$\lim_{k\to\infty} \frac{\mathbf{A}^k|\Psi_0\rangle}{\|\mathbf{A}^k|\Psi_0\rangle\|} = |\psi_n\rangle$$

$$\text{Matrix} \longrightarrow \boxed{\begin{array}{c}\text{Power}\\ \text{algorithm}\end{array}} \longrightarrow (|\psi_n\rangle, \lambda_n)$$

The power algorithm : Dominant Eigenspace

$$\text{For a given matrix } \mathbf{A}, \text{ eigenbasis } \{(\lambda_1, |\psi_1\rangle), \dots, (\lambda_n, |\psi_n\rangle)\}$$
$$\text{with } |\lambda_n| > |\lambda_{n-1}| > \cdots > |\lambda_1|$$

$$\text{For a random vector } |\Psi_0\rangle$$

$$\lim_{k\to\infty} \frac{\mathbf{A}^k|\Psi_0\rangle}{\|\mathbf{A}^k|\Psi_0\rangle\|} = |\psi_n\rangle$$

$$\text{Matrix} \longrightarrow \boxed{\text{Power algorithm}} \longrightarrow (|\psi_n\rangle, \lambda_n)$$

But : More interessed by lower energies

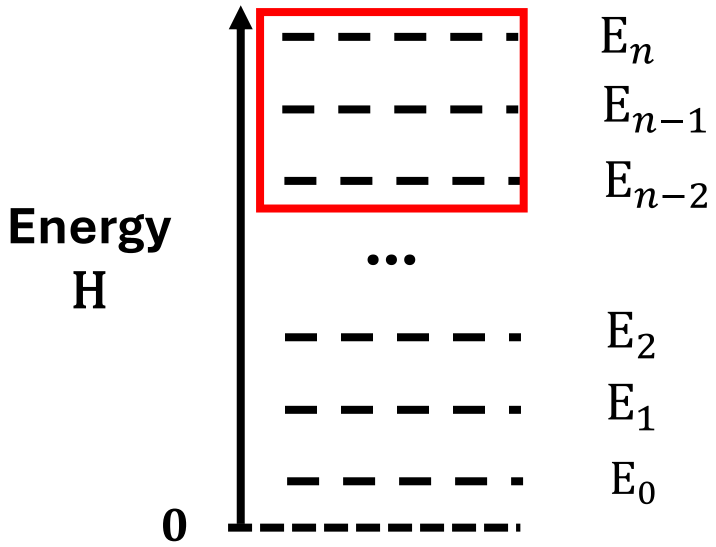
Krylov solver

$$\mathcal{K}_m(H, v) = \underbrace{\mathrm{span}\{v, Hv, H^2 v, \ldots, H^{m-1} v\}}_{\text{Constructed with Matrix}*\text{Vector}}$$

Krylov solver

Dominant Eigenvector

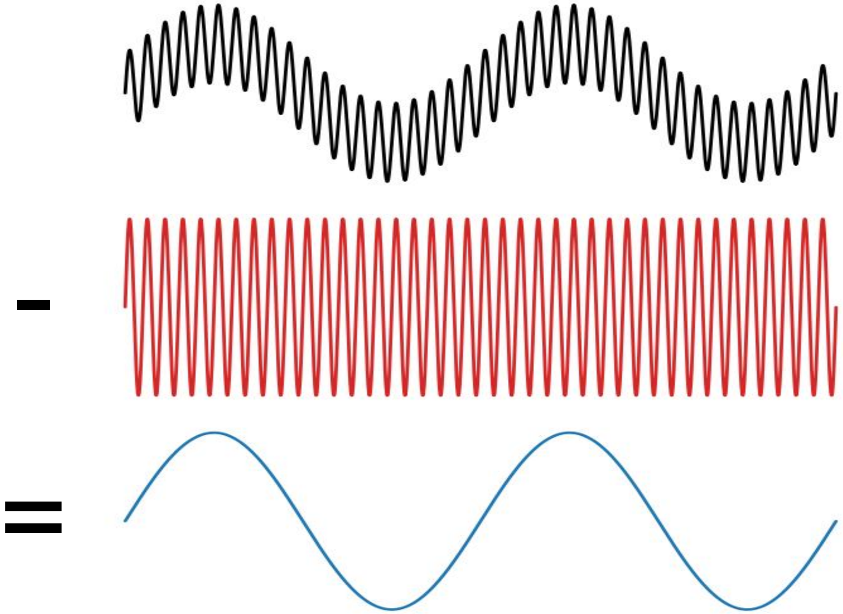
$$\mathcal{K}_m(H, v) = \underbrace{\mathrm{span}\{v, Hv, H^2v, \dots, H^{m-1}v\}}_{\text{Constructed with Matrix}*\text{Vector}}$$

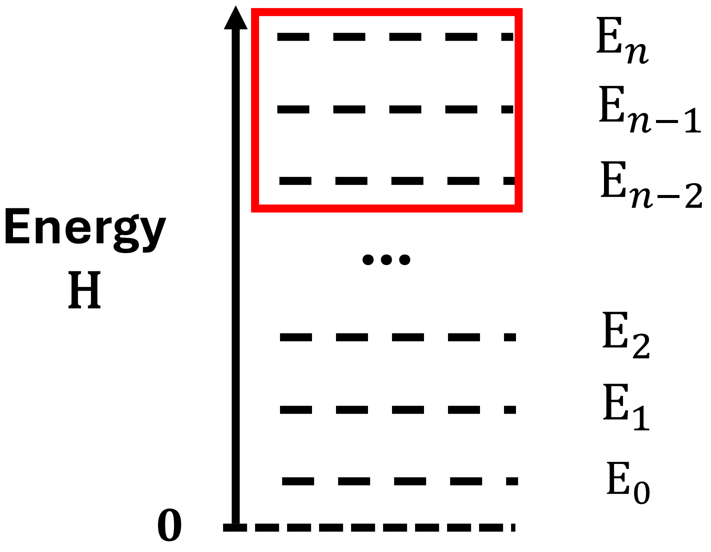


Krylov solver

Dominant Eigenvector

$$\mathcal{K}_m(H, v) = \underbrace{\text{span}\{v, Hv, H^2v, \ldots, H^{m-1}v\}}_{\text{Constructed with Matrix}*\text{Vector}}$$

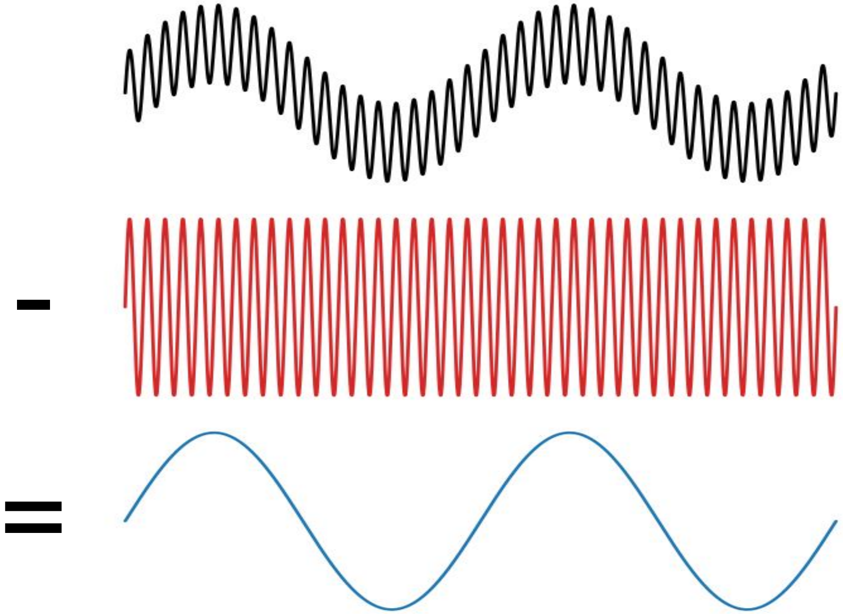


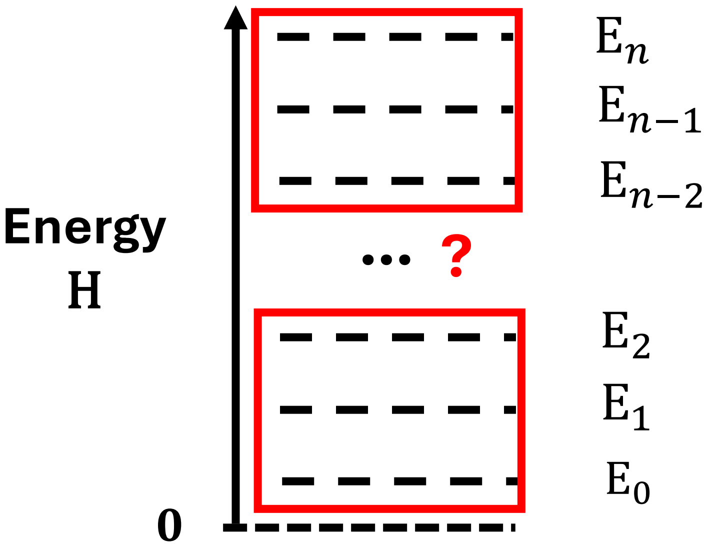


Krylov solver

Dominant Eigenvector

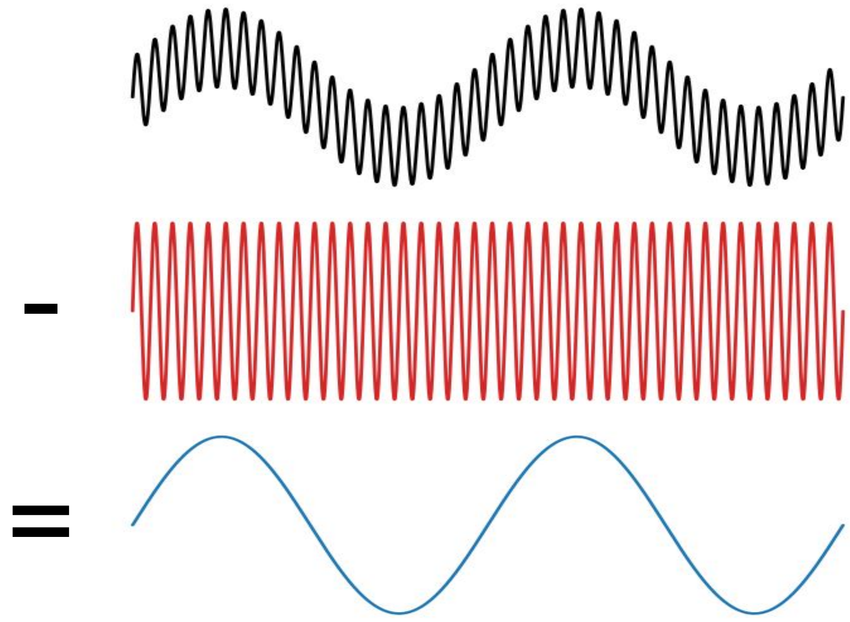
$$\mathcal{K}_m(H,v) = \underbrace{\text{span}\{v, Hv, H^2v, \ldots, \overset{\downarrow}{H^{m-1}v}\}}_{\text{Constructed with Matrix}*\text{Vector}}$$

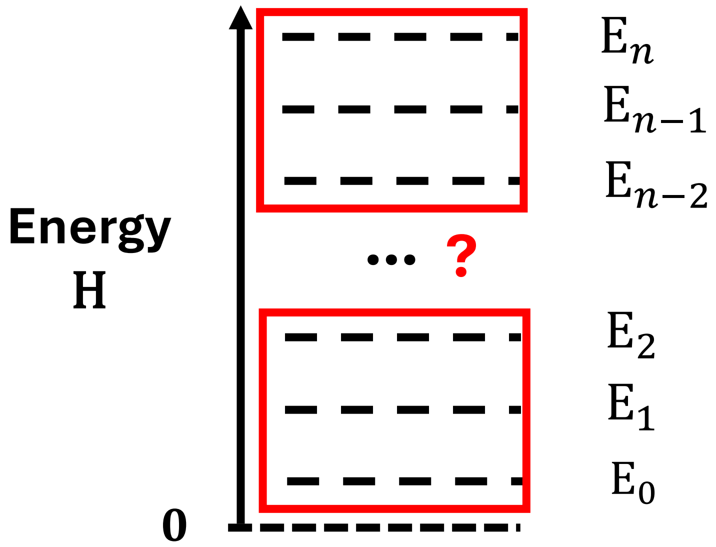




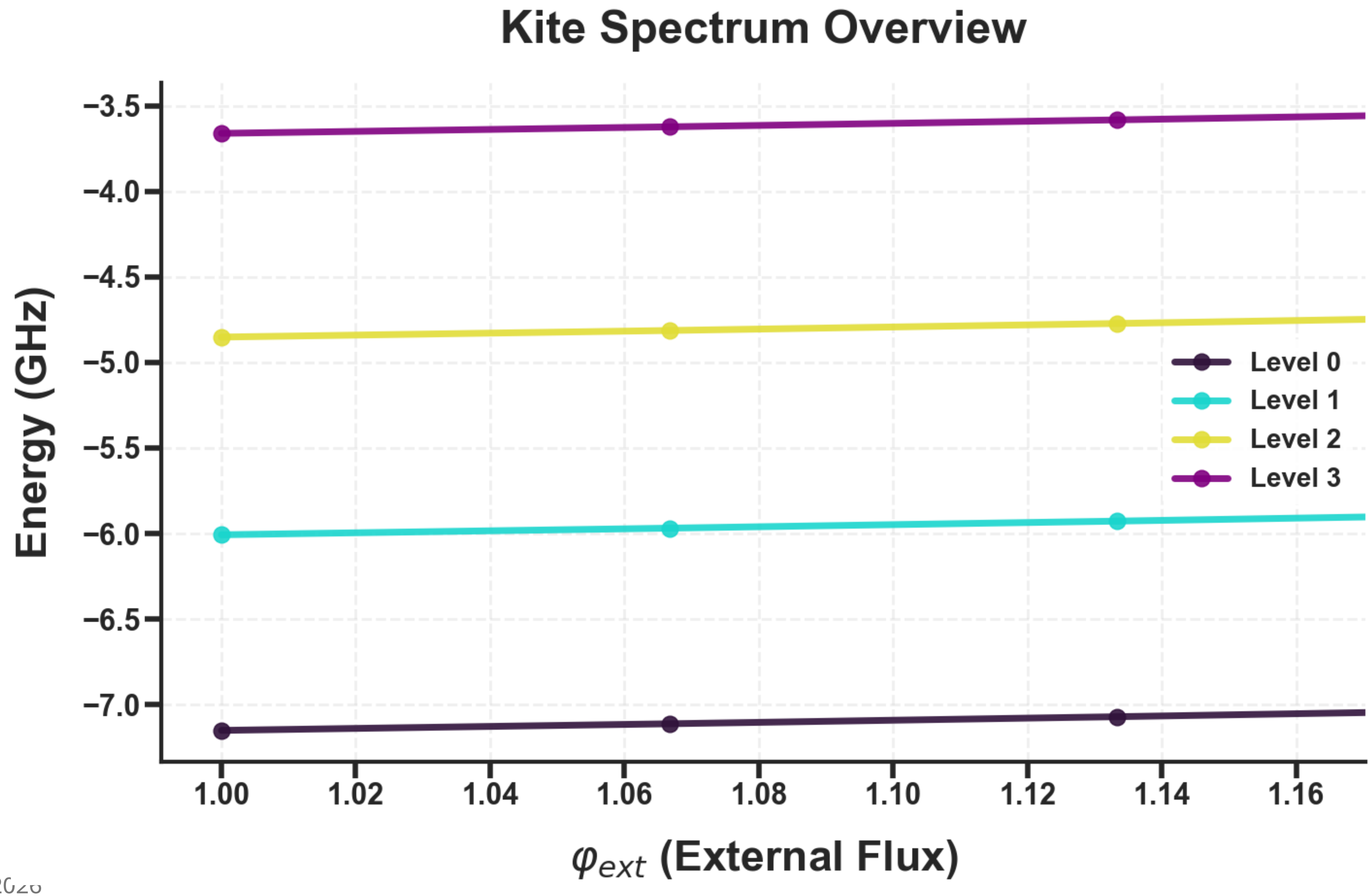
Krylov solver

$$\overset{n}{\hat{H} = \begin{pmatrix} & \cdots & \\ \vdots & & \vdots \\ & \cdots & \end{pmatrix}} \, n \longrightarrow \mathcal{K}_m(H,v) = \underbrace{\mathrm{span}\{v, Hv, H^2v, \ldots, \overset{\substack{\text{Dominant Eigenvector} \\ \downarrow}}{H^{m-1}v}\}}_{\text{Constructed with Matrix}*\text{Vector}} \longrightarrow \overset{m \ll n}{\hat{T} = \begin{pmatrix} & \cdots & \\ \vdots & & \vdots \\ & \cdots & \end{pmatrix}} \, m$$



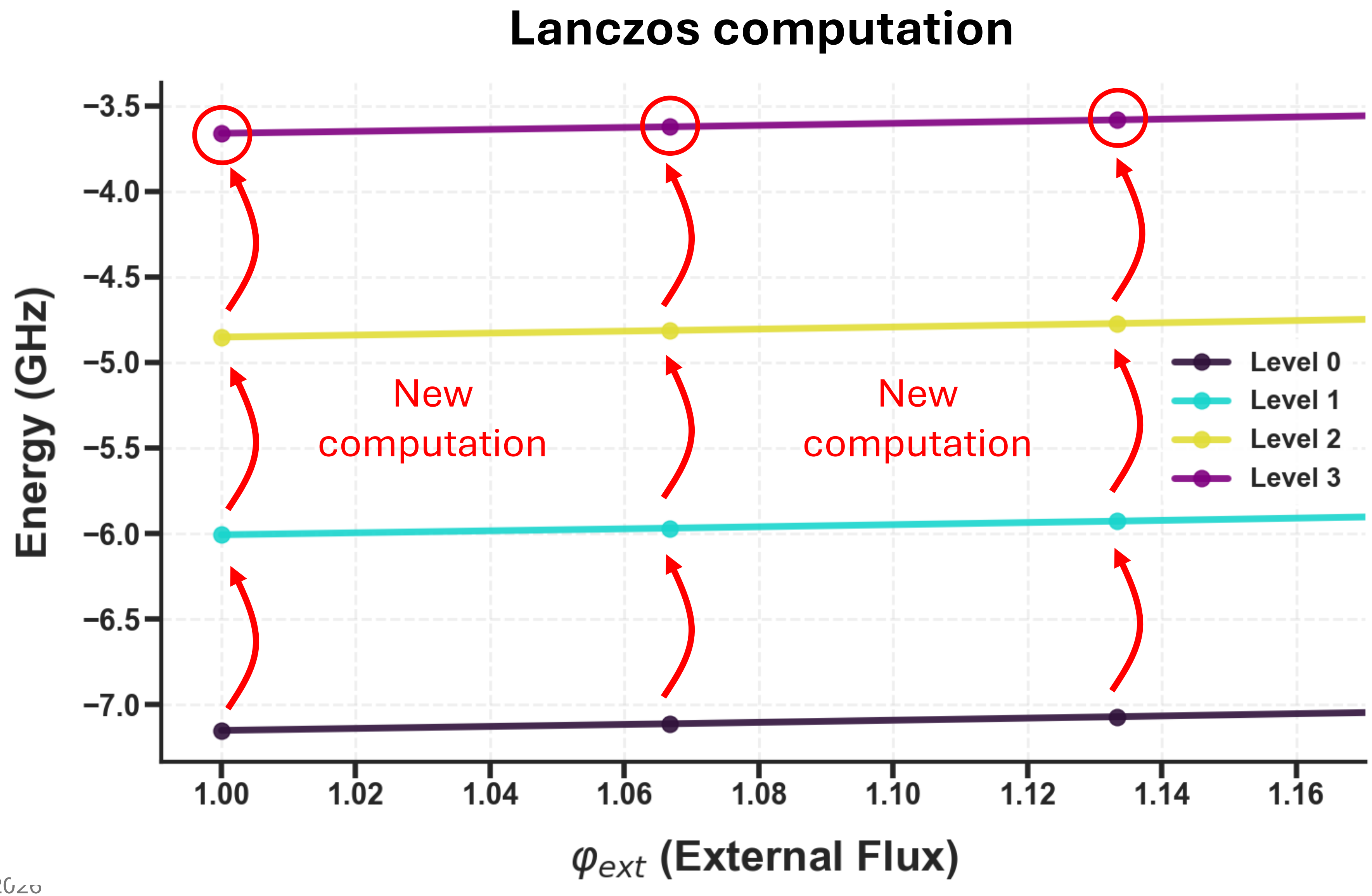


The idea



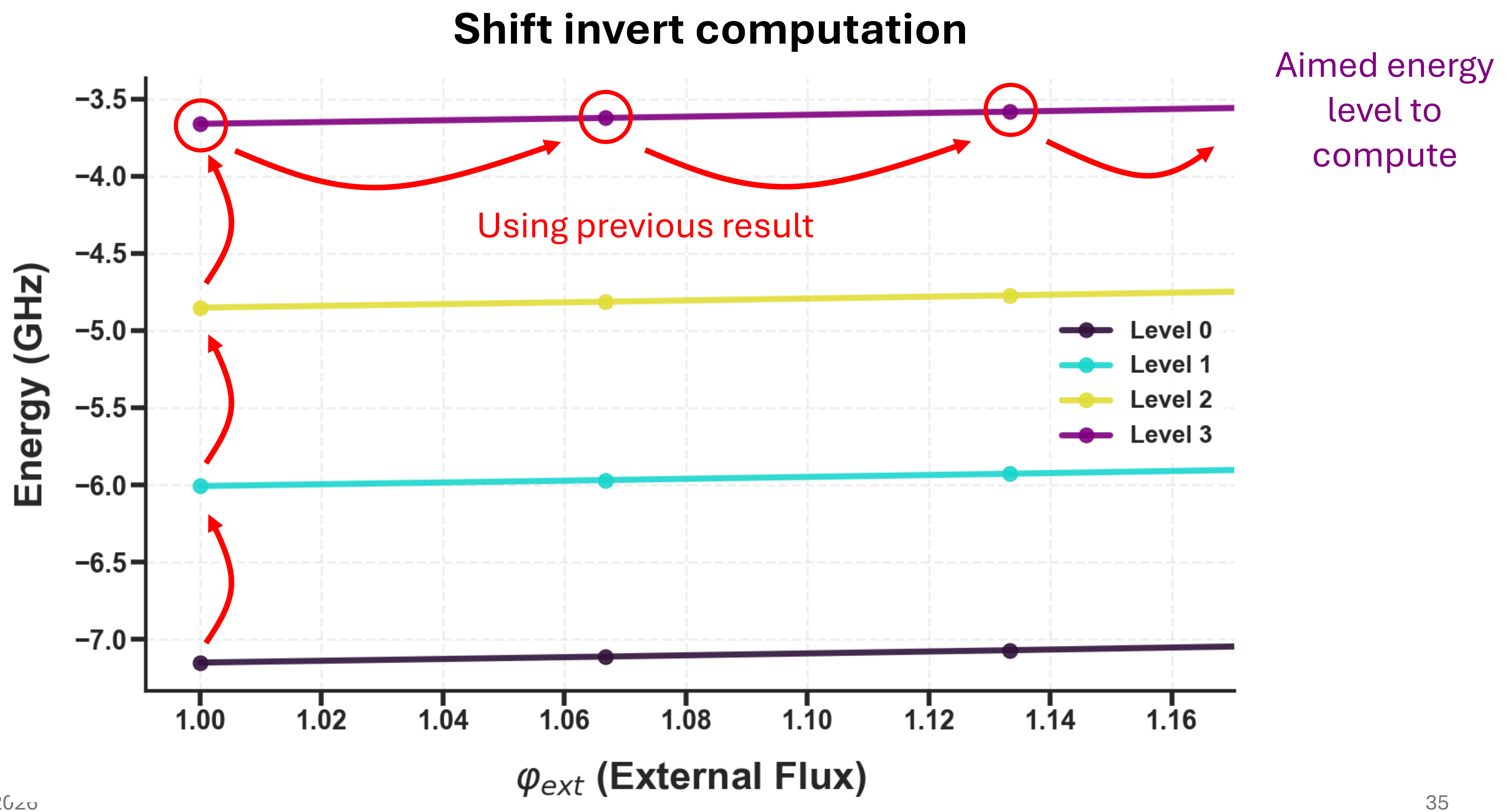
Kite Spectrum Overview
−3.5
−4.0
−4.5
−5.0
−5.5
−6.0
−6.5
−7.0
Energy (GHz)
1.00
1.02
1.04
1.06
1.08
1.10
1.12
1.14
1.16
φext (External Flux)
Level 0
Level 1
Level 2
Level 3

The idea



Aimed energy level to compute

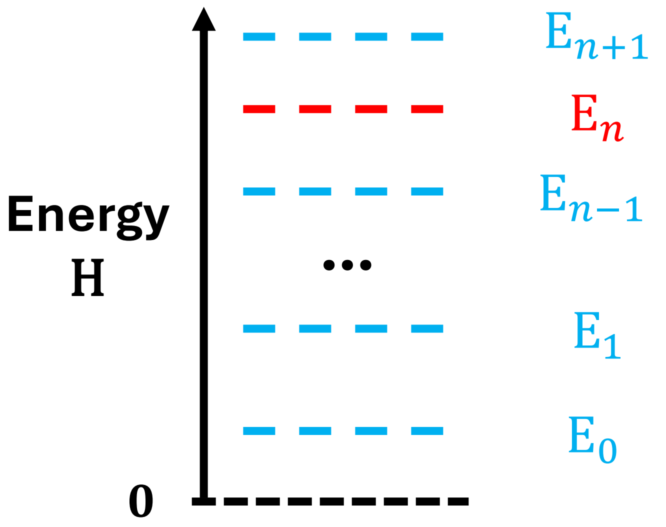
The idea


Shift invert computation
Aimed energy level to compute
Using previous result
Energy (GHz)
−3.5
−4.0
−4.5
−5.0
−5.5
−6.0
−6.5
−7.0
1.00
1.02
1.04
1.06
1.08
1.10
1.12
1.14
1.16
φ_{ext} (External Flux)
Level 0
Level 1
Level 2
Level 3

Shift Invert : conceptually

$E_n \simeq E$: Mixed with other energies → propel it to the top of the spectrum

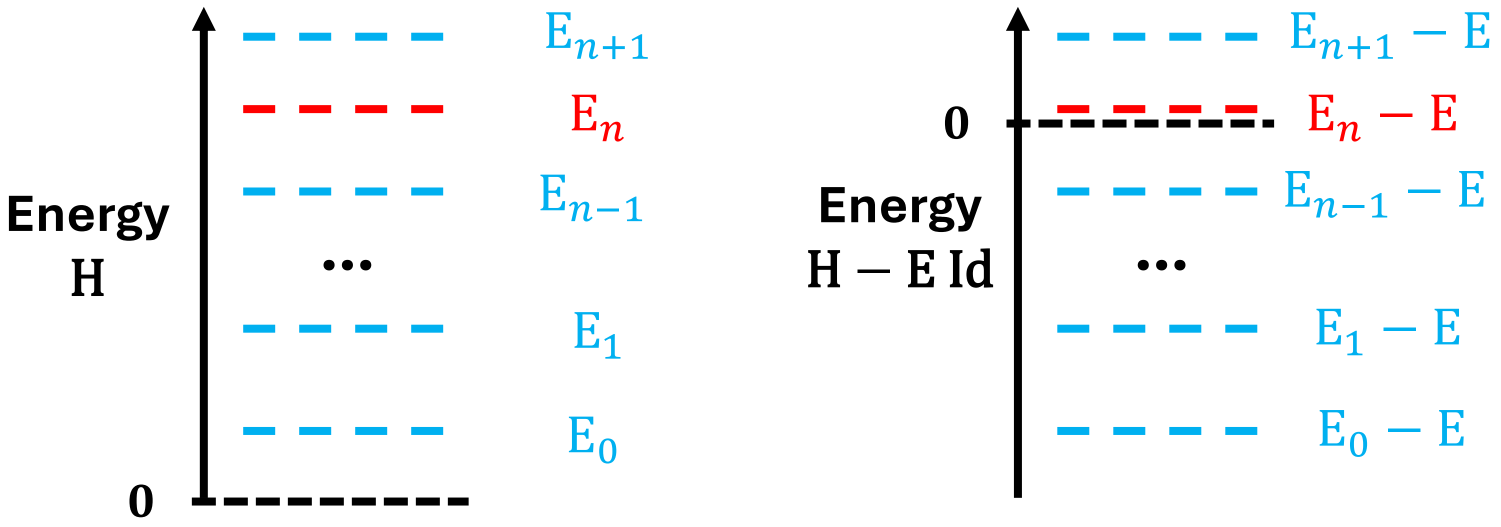
guess



Shift Invert : conceptually

$E_n \simeq E$: Mixed with other energies → propel it to the top of the spectrum

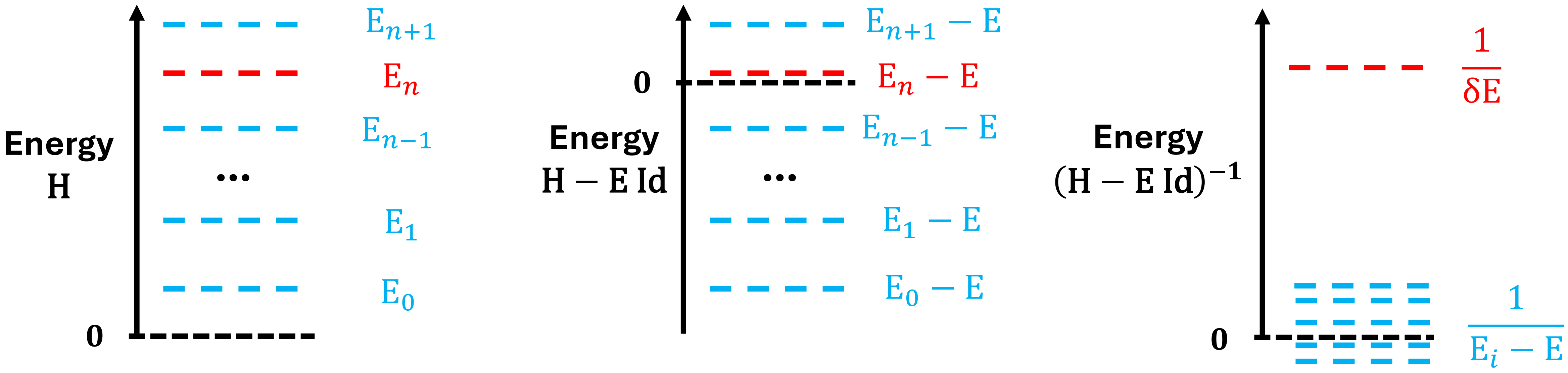
guess



Shift Invert : conceptually

$E_n \simeq E$: Mixed with other energies → propel it to the top of the spectrum

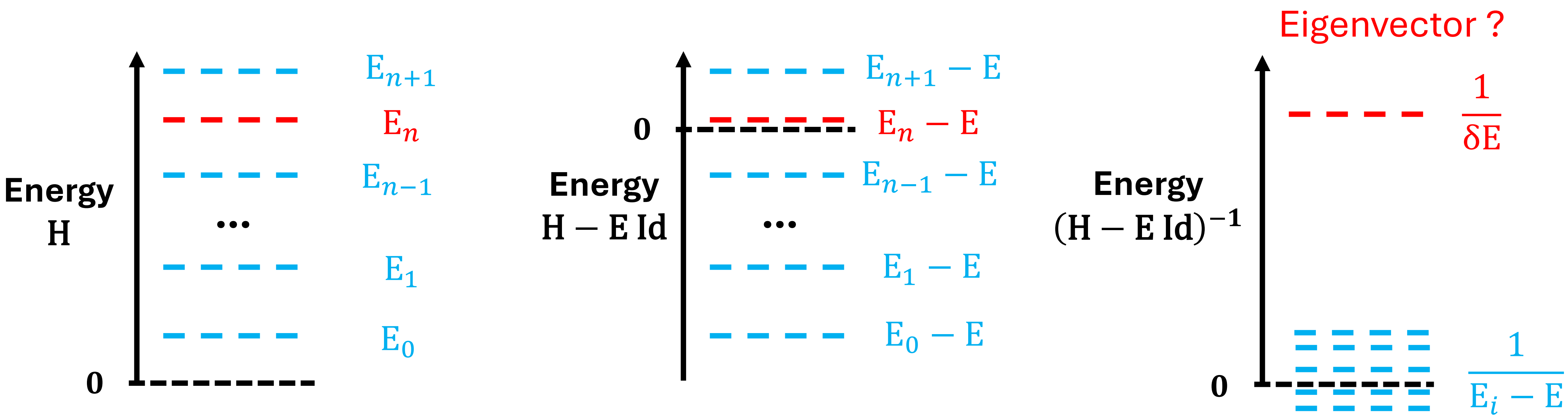
guess



Shift Invert : conceptually

$E_n \simeq E$: Mixed with other energies → propel it to the top of the spectrum

guess



$(\mathbf{H - E\,Id})^{-1}$ computationally hard

Minres algorithm

$$(\mathbf{H} - \mathbf{E}\,\mathbf{Id})^{-1}|\boldsymbol{\Psi}^{(n)}\rangle = |\boldsymbol{\Psi}^{(n+1)}\rangle \iff (\mathbf{H} - \mathbf{E}\,\mathbf{Id})|\boldsymbol{\Psi}^{(n+1)}\rangle = |\boldsymbol{\Psi}^{(n)}\rangle$$

Minres algorithm

$$(\mathbf{H}-\mathbf{E}\,\mathbf{Id})^{-1}|\Psi^{(n)}\rangle = |\Psi^{(n+1)}\rangle \iff \underbrace{(\mathbf{H}-\mathbf{E}\,\mathbf{Id})|\Psi^{(n+1)}\rangle = |\Psi^{(n)}\rangle}$$

Solvable with Minres

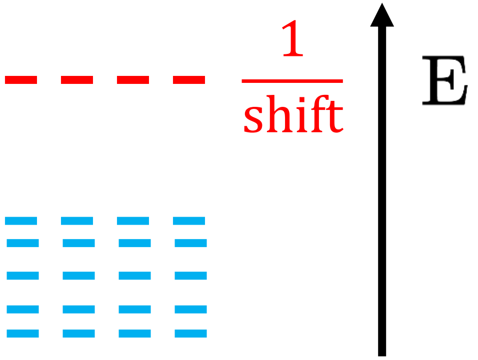
→ Krylov Solver $AX = Y$

→ A invertible

Minres algorithm

$$(\mathrm{H} - \mathrm{E\ Id})^{-1}|\Psi^{(n)}\rangle = |\Psi^{(n+1)}\rangle \iff \underbrace{(\mathrm{H} - \mathrm{E\ Id})|\Psi^{(n+1)}\rangle = |\Psi^{(n)}\rangle}_{\text{Solvable with Minres}}$$

guess + shift



Solvable with Minres

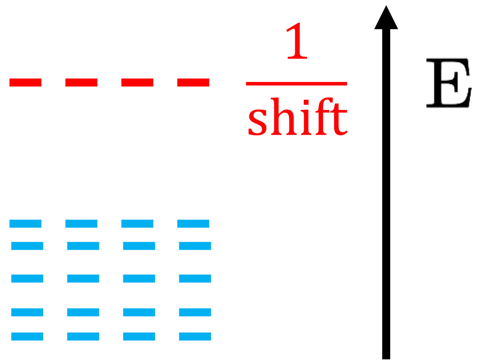
→ Krylov Solver $AX = Y$

→ A invertible

Minres algorithm

$$(\mathrm{H} - \mathrm{E}\ \mathrm{Id})^{-1}|\Psi^{(n)}\rangle = |\Psi^{(n+1)}\rangle \iff \underbrace{(\mathrm{H} - \mathrm{E}\ \mathrm{Id})|\Psi^{(n+1)}\rangle = |\Psi^{(n)}\rangle}$$

guess + shift



Solvable with Minres
→ Krylov Solver $AX = Y$
→ A invertible

H_n $\quad$ H_{n+1}

$(|\psi_n\rangle, \lambda_n)$ $\quad$ $(|\psi_{n+1}\rangle, \lambda_{n+1})$?

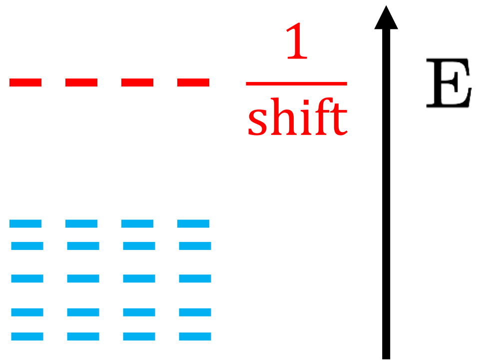
φ_{ext} $\quad$ $\varphi_{ext} + \delta\varphi$

$$(\mathrm{H}_{n+1} - [\langle\psi_n|\mathrm{H}_{n+1}|\psi_n\rangle + \mathrm{shift}]\ \mathrm{Id})X^{(0)} = |\psi_n\rangle$$

Minres algorithm

$$(\mathrm{H} - \mathrm{E}\ \mathrm{Id})^{-1}|\Psi^{(n)}\rangle = |\Psi^{(n+1)}\rangle \iff \underbrace{(\mathrm{H} - \mathrm{E}\ \mathrm{Id})|\Psi^{(n+1)}\rangle = |\Psi^{(n)}\rangle}$$

guess + shift



Solvable with Minres
→ Krylov Solver $AX = Y$
→ A invertible

H_n $\quad$ H_{n+1}

$(|\psi_n\rangle, \lambda_n)$ $\quad$ $(|\psi_{n+1}\rangle, \lambda_{n+1})$?

φ_{ext} $\quad$ $\varphi_{ext} + \delta\varphi$

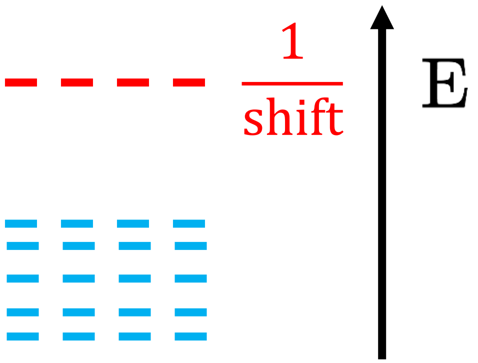
$$(\mathrm{H}_{n+1} - [\underbrace{\langle\psi_n|\mathrm{H}_{n+1}|\psi_n\rangle}_{\simeq \lambda_n + \langle\psi_n|\delta\mathrm{H}|\psi_n\rangle} + \text{shift}]\ \mathrm{Id})X^{(0)} = |\psi_n\rangle$$

First order approximation

Minres algorithm

$$(\mathrm{H}-\mathrm{E}\ \mathrm{Id})^{-1}|\Psi^{(n)}\rangle = |\Psi^{(n+1)}\rangle \iff \underbrace{(\mathrm{H}-\mathrm{E}\ \mathrm{Id})|\Psi^{(n+1)}\rangle = |\Psi^{(n)}\rangle}$$

guess + shift



Solvable with Minres

→ Krylov Solver $AX = Y$

→ A invertible

H_n H_{n+1}

$(|\psi_n\rangle, \lambda_n)$ $(|\psi_{n+1}\rangle, \lambda_{n+1})$?

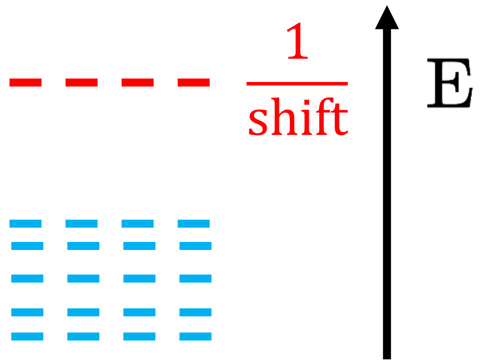
φ_{ext} $\varphi_{ext} + \delta\varphi$

$$(\mathrm{H}_{n+1} - [\langle\psi_n|\mathrm{H}_{n+1}|\psi_n\rangle + \mathrm{shift}]\ \mathrm{Id})X^{(1)} = X^{(0)}$$

Minres algorithm

$$(\mathrm{H} - \mathrm{E}\ \mathrm{Id})^{-1}|\Psi^{(n)}\rangle = |\Psi^{(n+1)}\rangle \iff \underbrace{(\mathrm{H} - \mathrm{E}\ \mathrm{Id})|\Psi^{(n+1)}\rangle = |\Psi^{(n)}\rangle}$$

guess + shift



Solvable with Minres

→ Krylov Solver $AX = Y$

→ A invertible

H_n $\qquad$ H_{n+1}

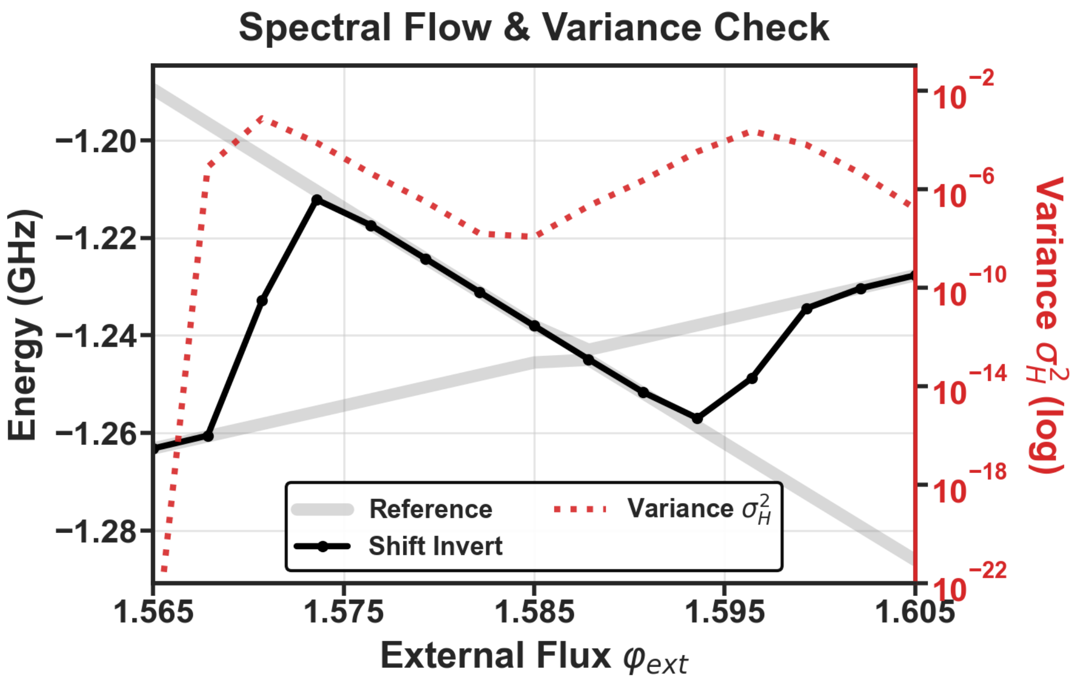
$(|\psi_n\rangle, \lambda_n)$ $\qquad$ $(|\psi_{n+1}\rangle, \lambda_{n+1})$?

φ_{ext} $\qquad$ $\varphi_{ext} + \delta\varphi$

$$(\mathrm{H}_{n+1} - [\langle\psi_n|\mathrm{H}_{n+1}|\psi_n\rangle + \mathbf{shift}]\ \mathrm{Id})X^{(k+1)} = X^{(k)}$$

Self consistency accuracy check

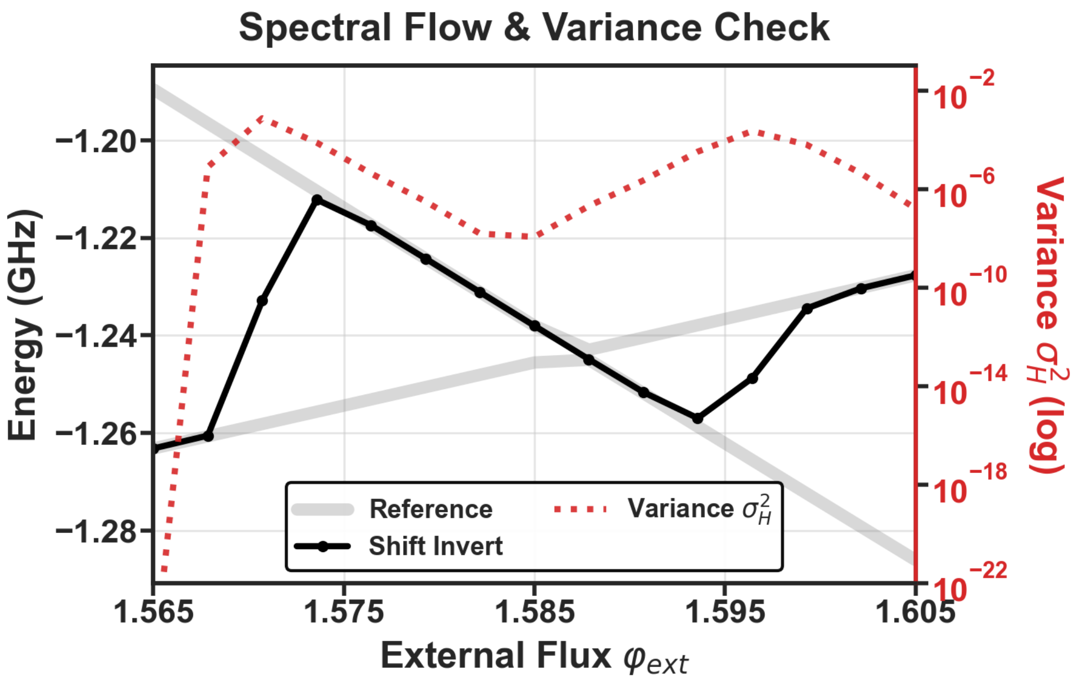
$$\sigma_H^2 = \langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2 \simeq 0$$



Self consistency accuracy check

$$\sigma_H^2 = \langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2 \simeq 0$$

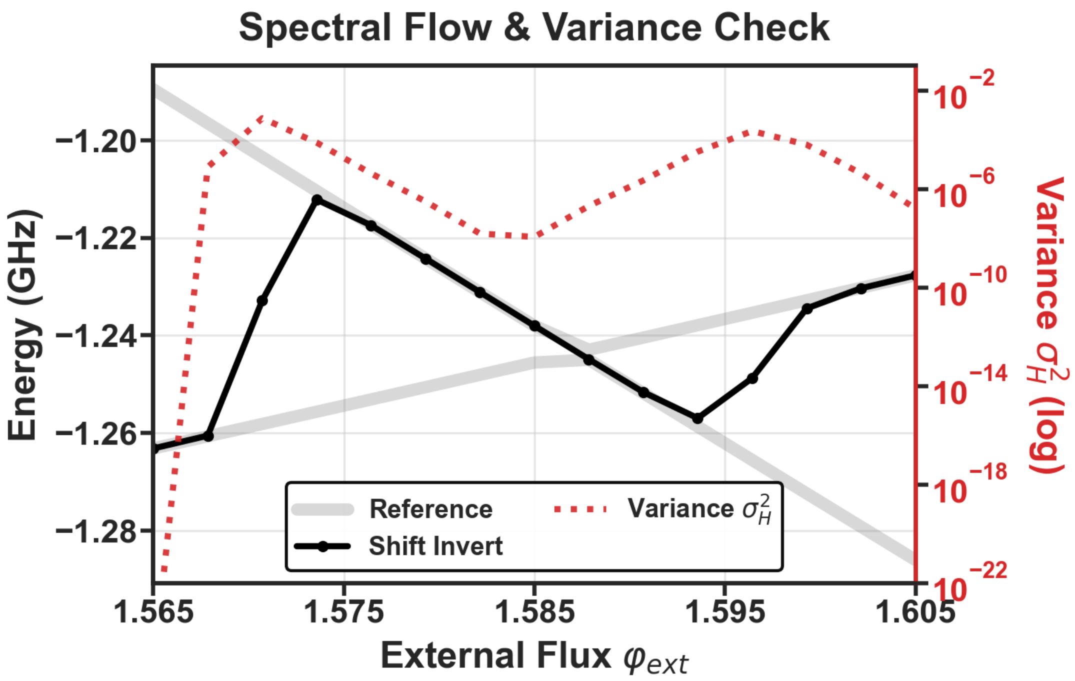
$$|\langle\psi_i|\psi_{i+1}\rangle| \simeq 1$$

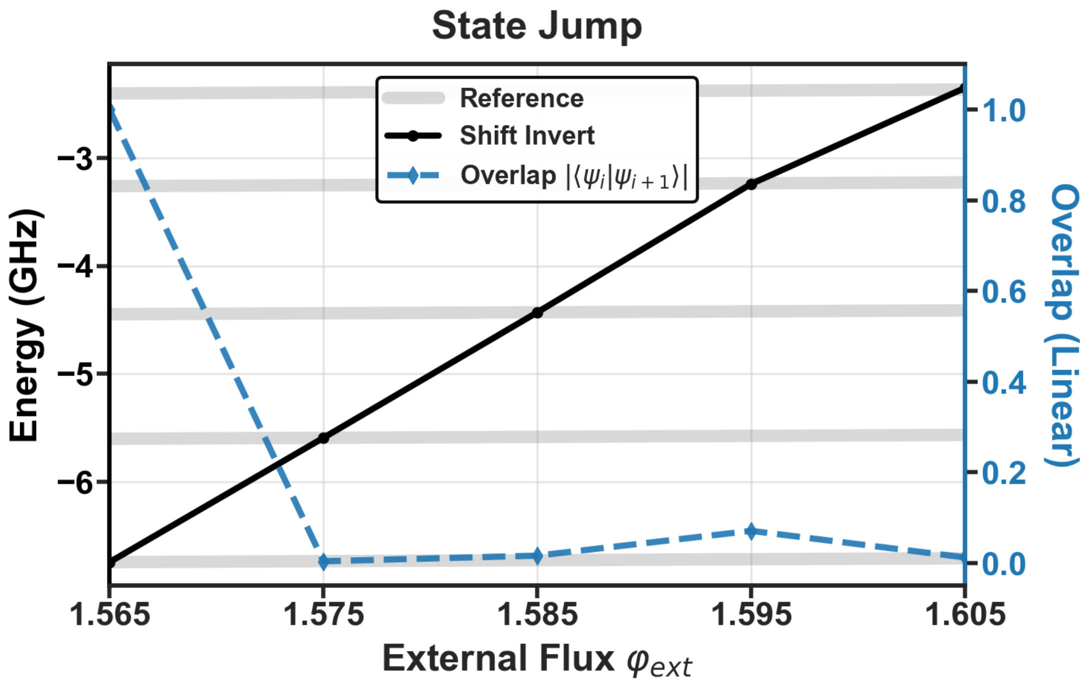


Self consistency accuracy check

$$\sigma_H^2 = \langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2 \simeq 0$$

$$|\langle\psi_i|\psi_{i+1}\rangle| \simeq 1$$

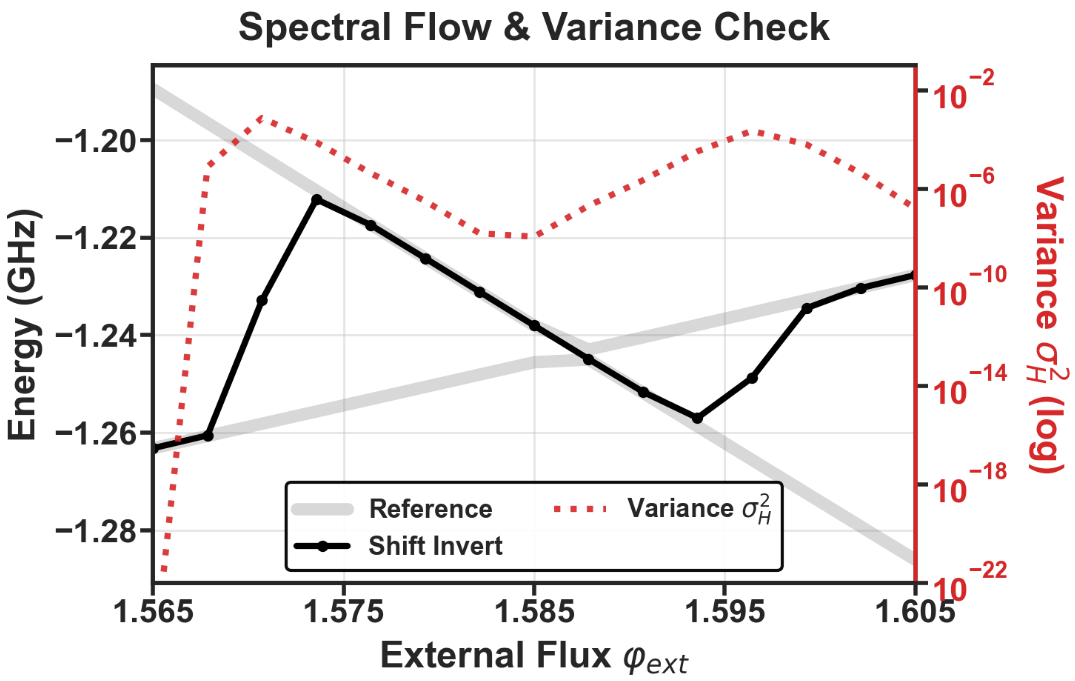


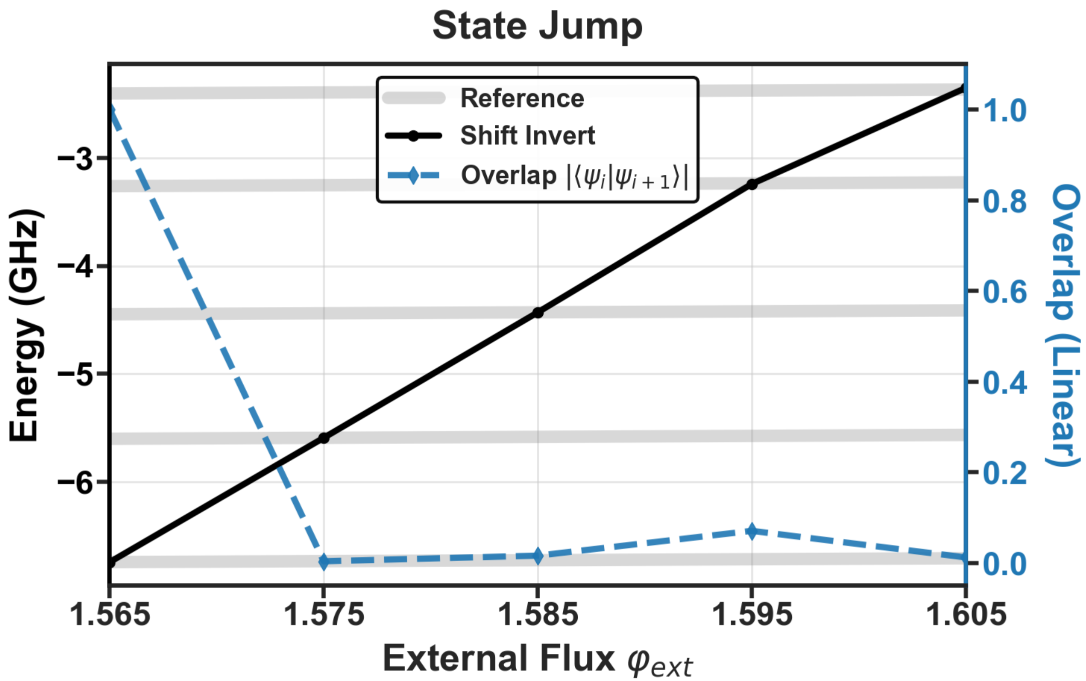


Self consistency accuracy check

$$\sigma_H^2 = \langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2 \simeq 0$$

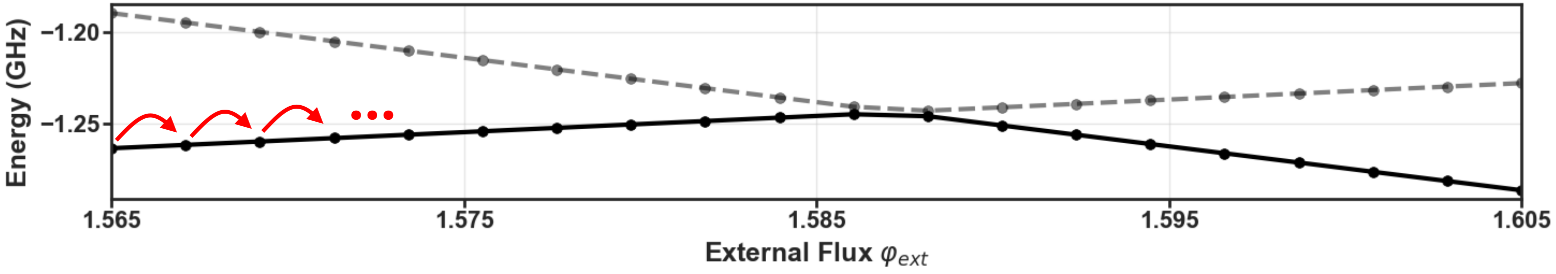
$$|\langle\psi_i|\psi_{i+1}\rangle| \simeq 1$$





⇨ Choose carefully shift value

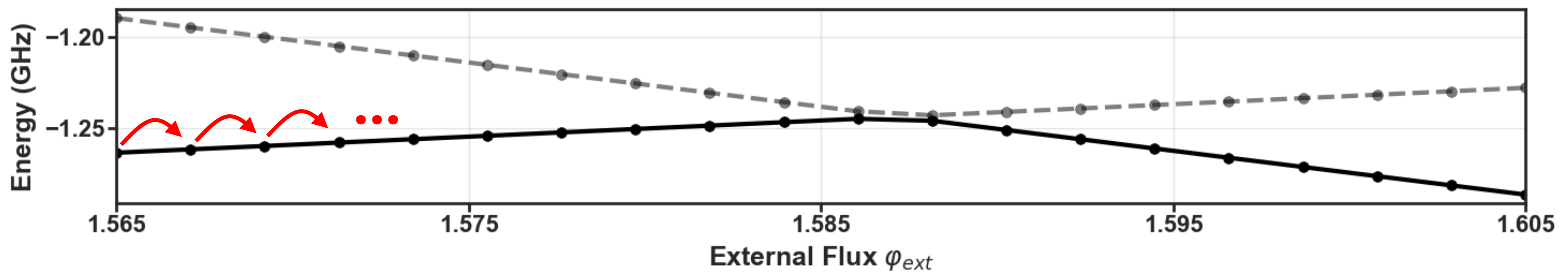
Shift Benchmark



Follow the lower branch for different shift values

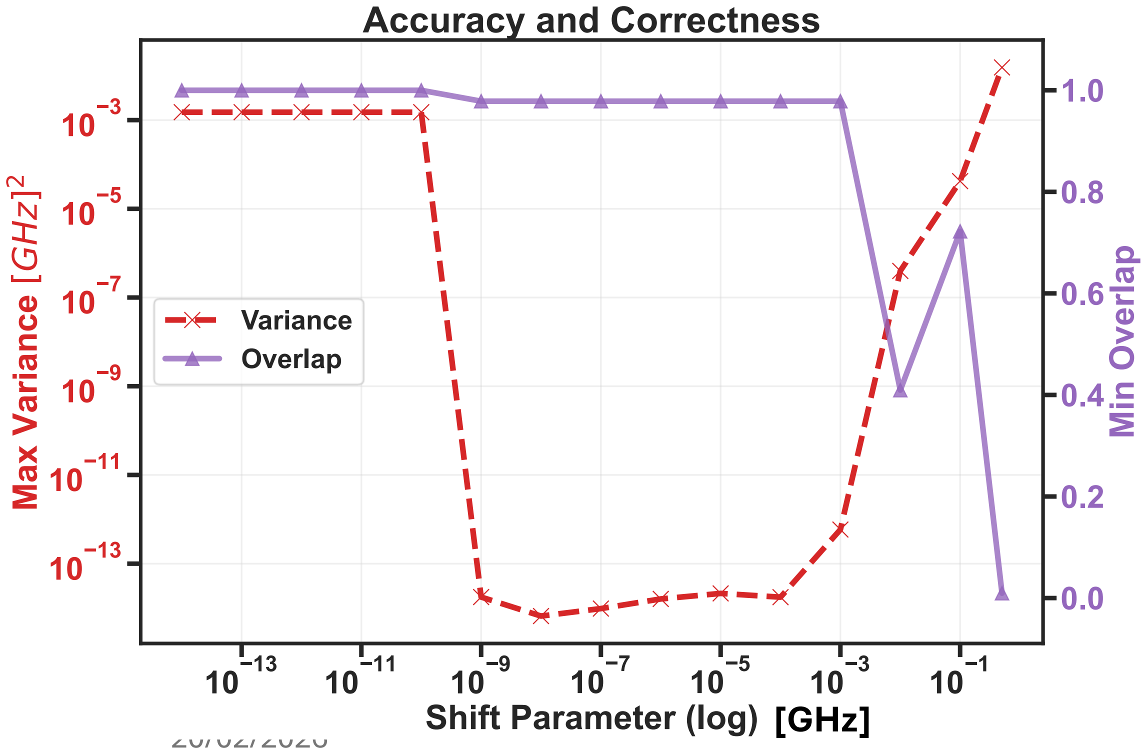
- Variance
- Overlap
- Computational time

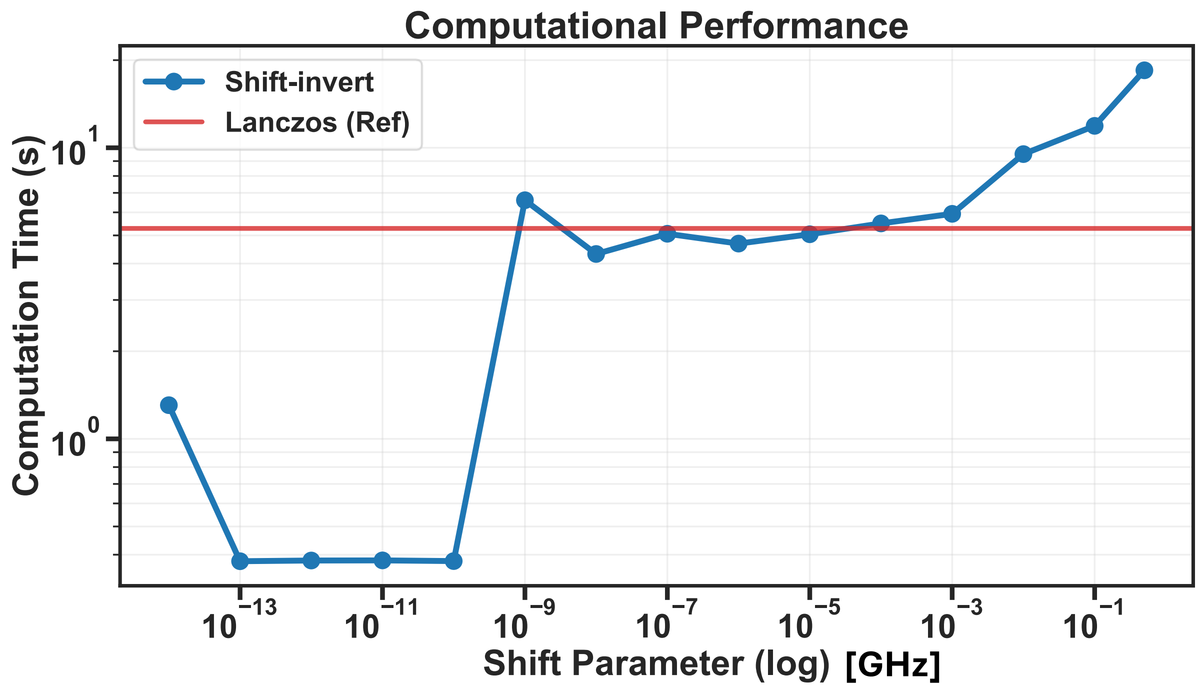
Shift Benchmark



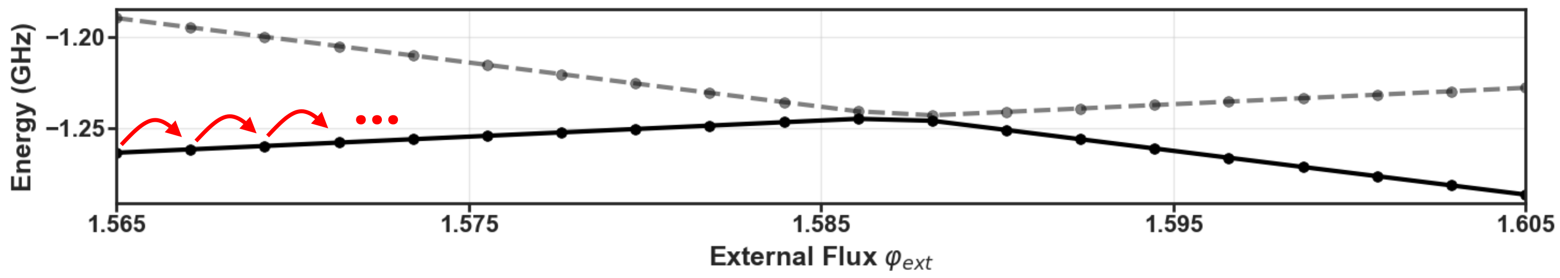
Follow the lower branch for different shift values

- Variance
- Overlap
- Computational time



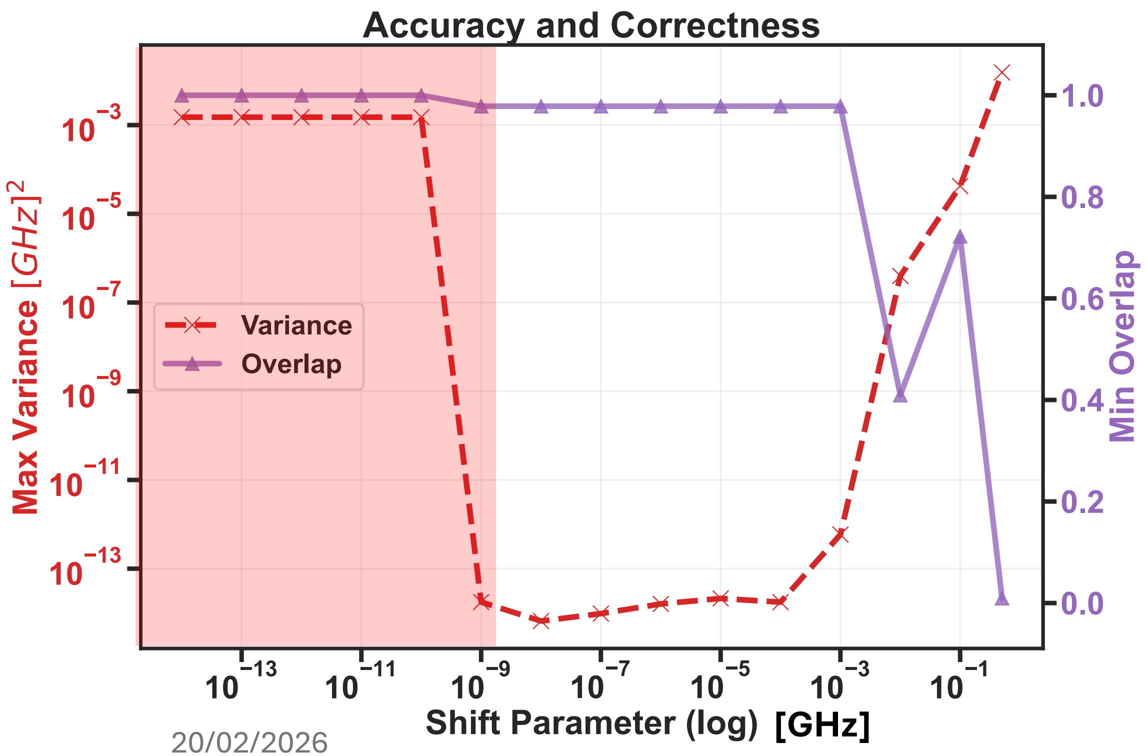


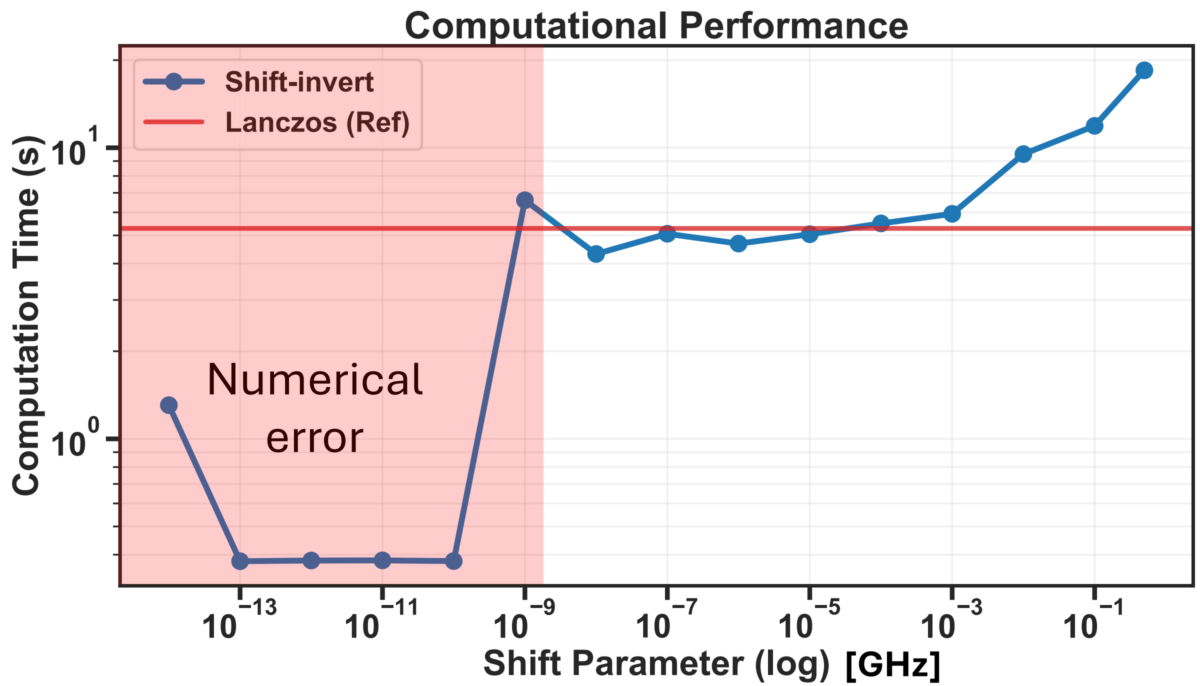
Shift Benchmark



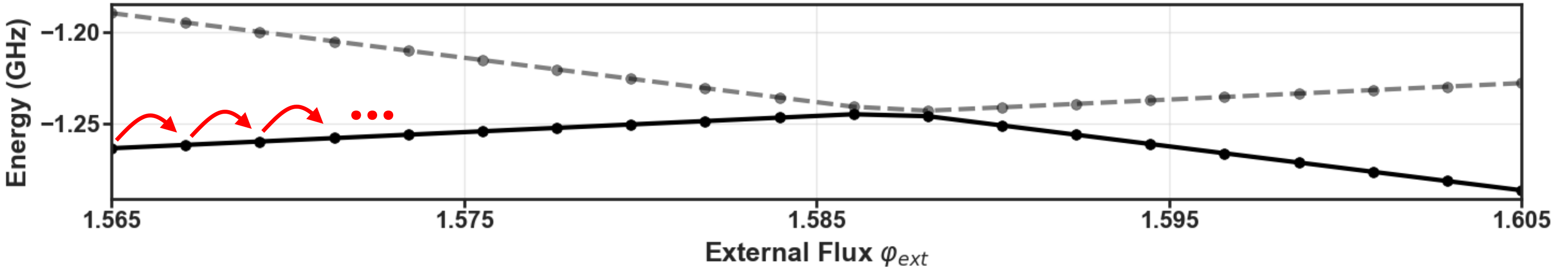
Follow the lower branch for different shift values

- Variance
- Overlap
- Computational time



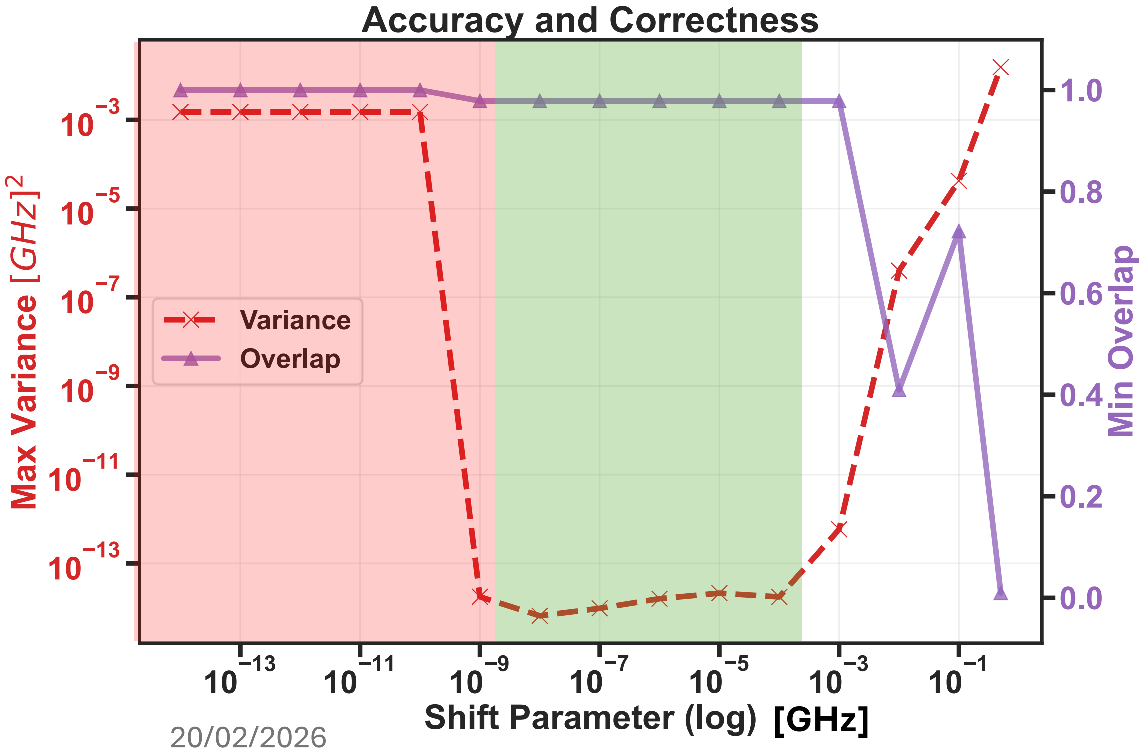


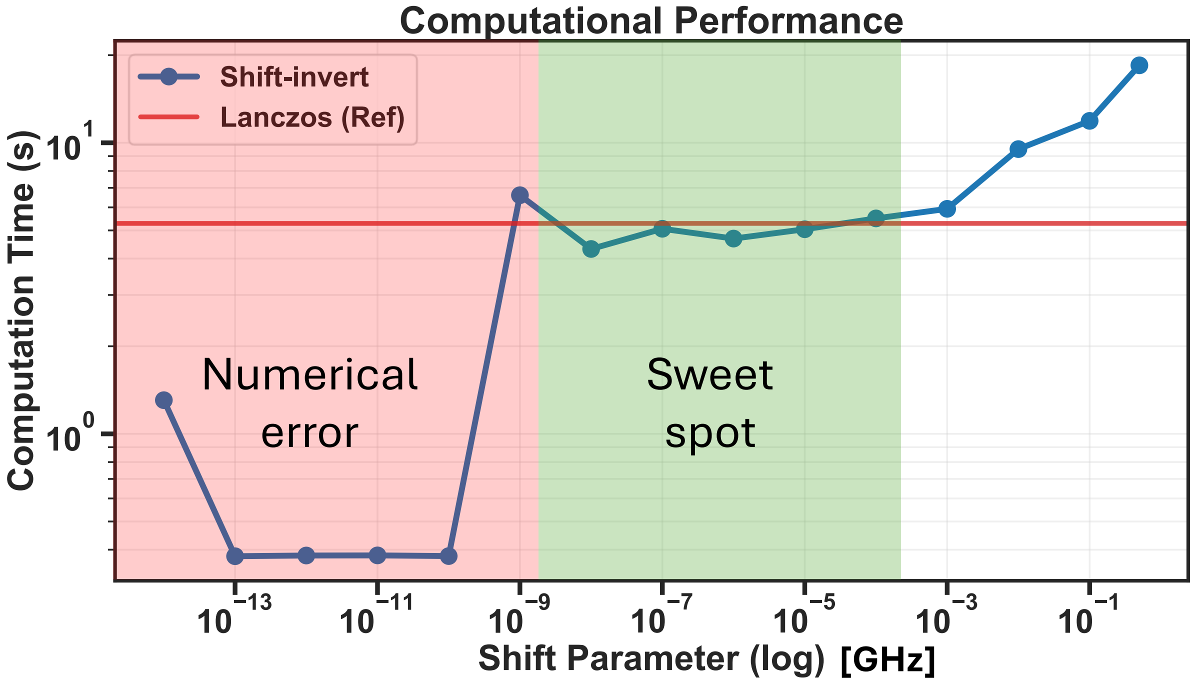
Shift Benchmark



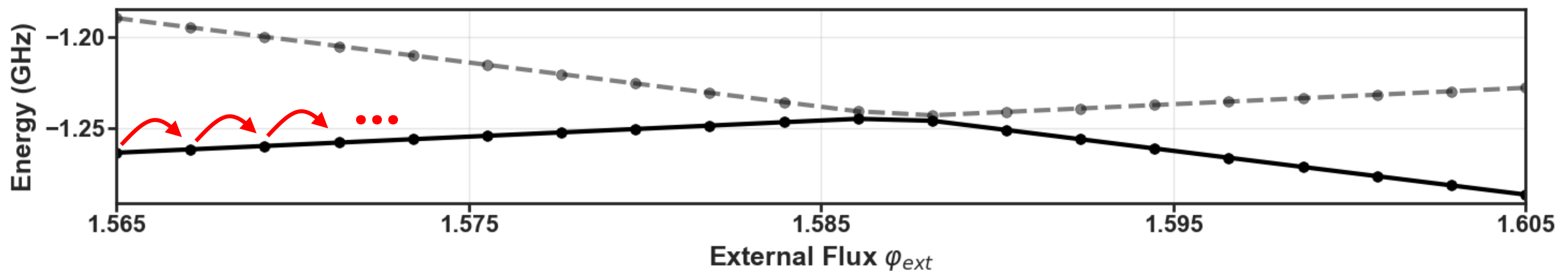
Follow the lower branch for different shift values

- Variance
- Overlap
- Computational time



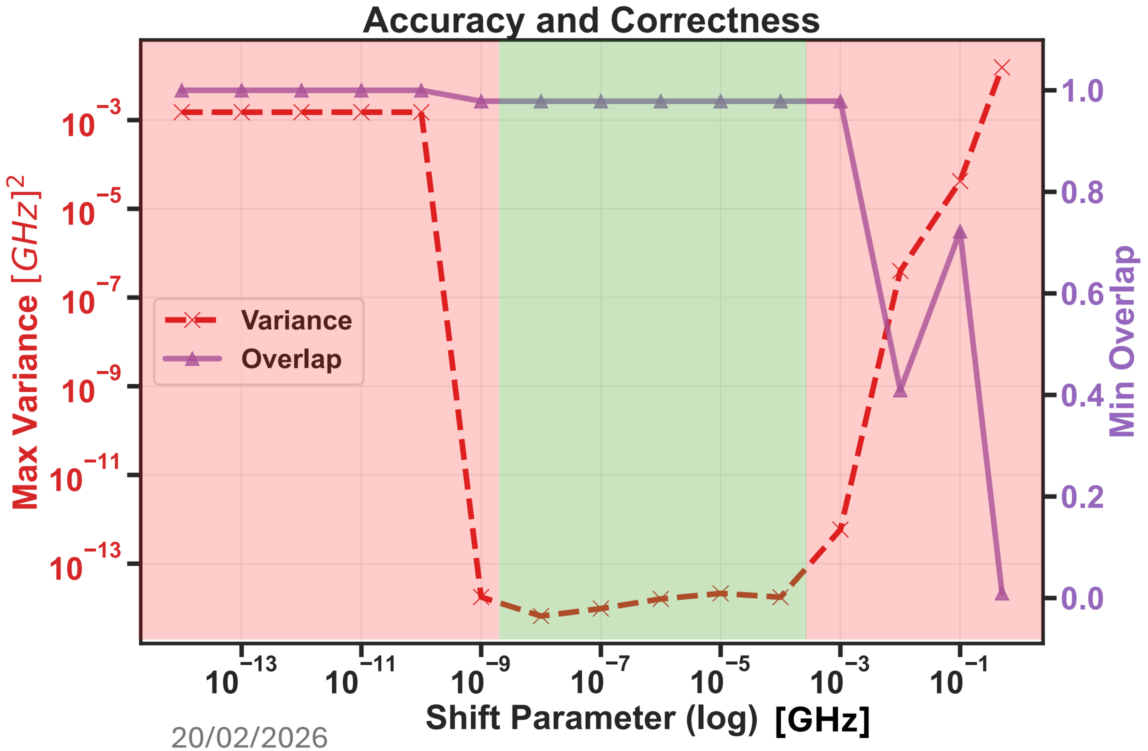


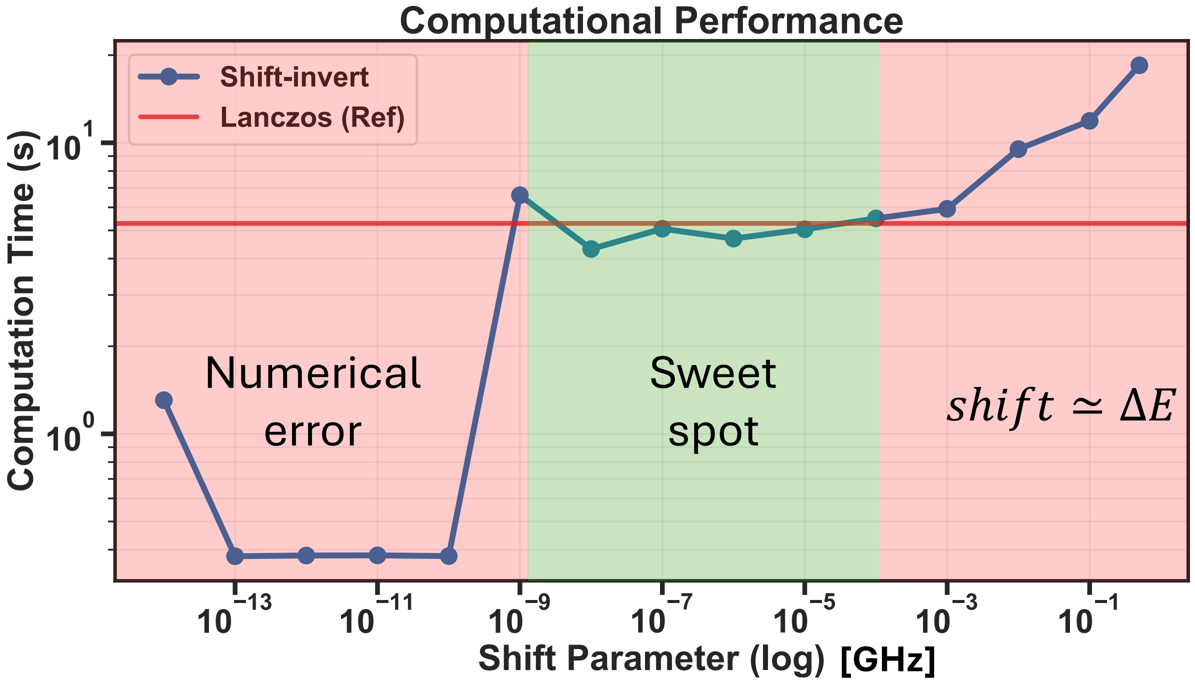
Shift Benchmark



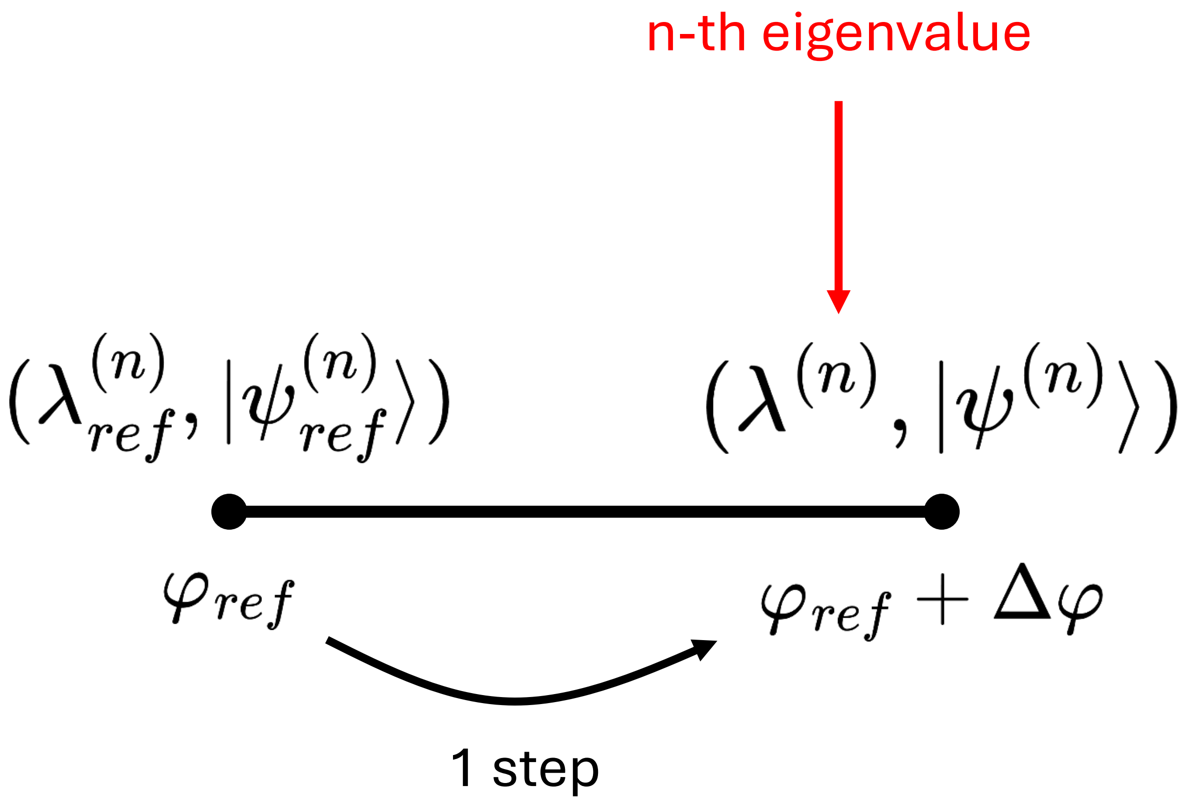
Follow the lower branch for different shift values

- Variance
- Overlap
- Computational time

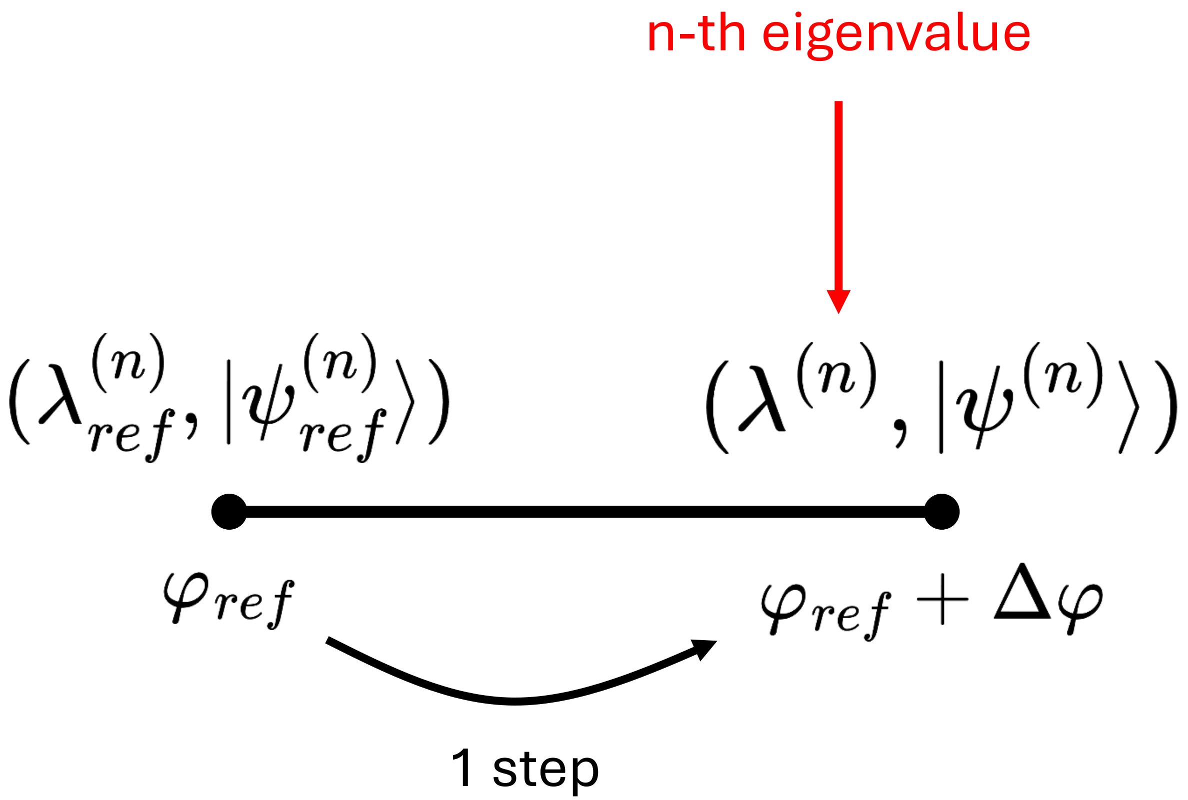




Final benchmark



Final benchmark



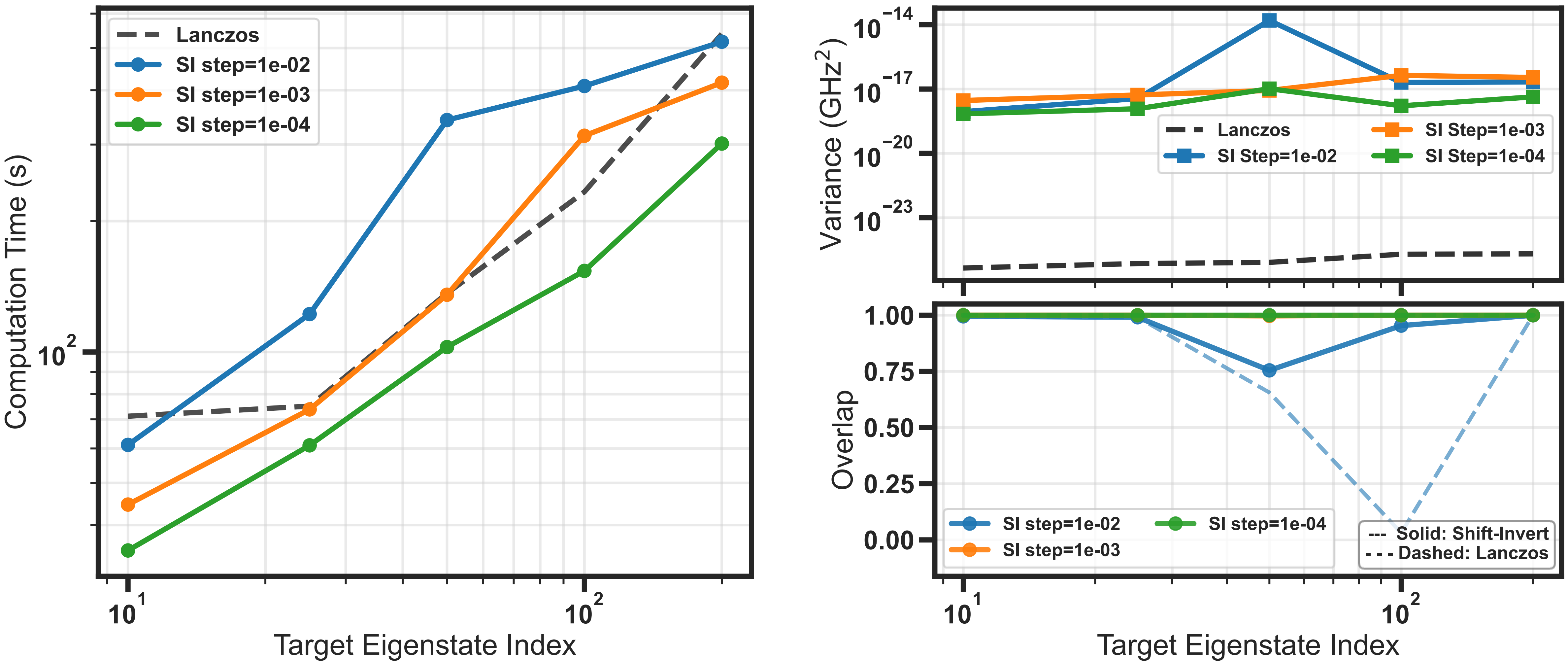
<u>Varying parameters :</u>

- n
- $\Delta\varphi$

<u>Benchmark metrics :</u>

- Computation time
- Variance
- Overlap

Shift invert versus Lanczos



Conclusion

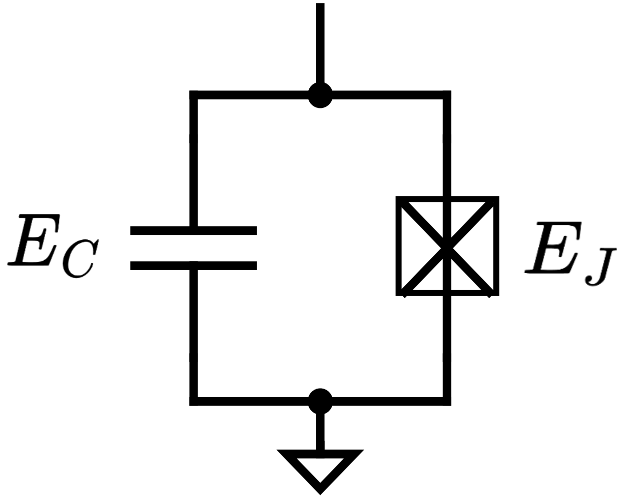
- Usefull in very specific case

- Could be optimized (Minres for complex Hamiltonian)

- Cannot beat Lanczos when we want several eigenvalues

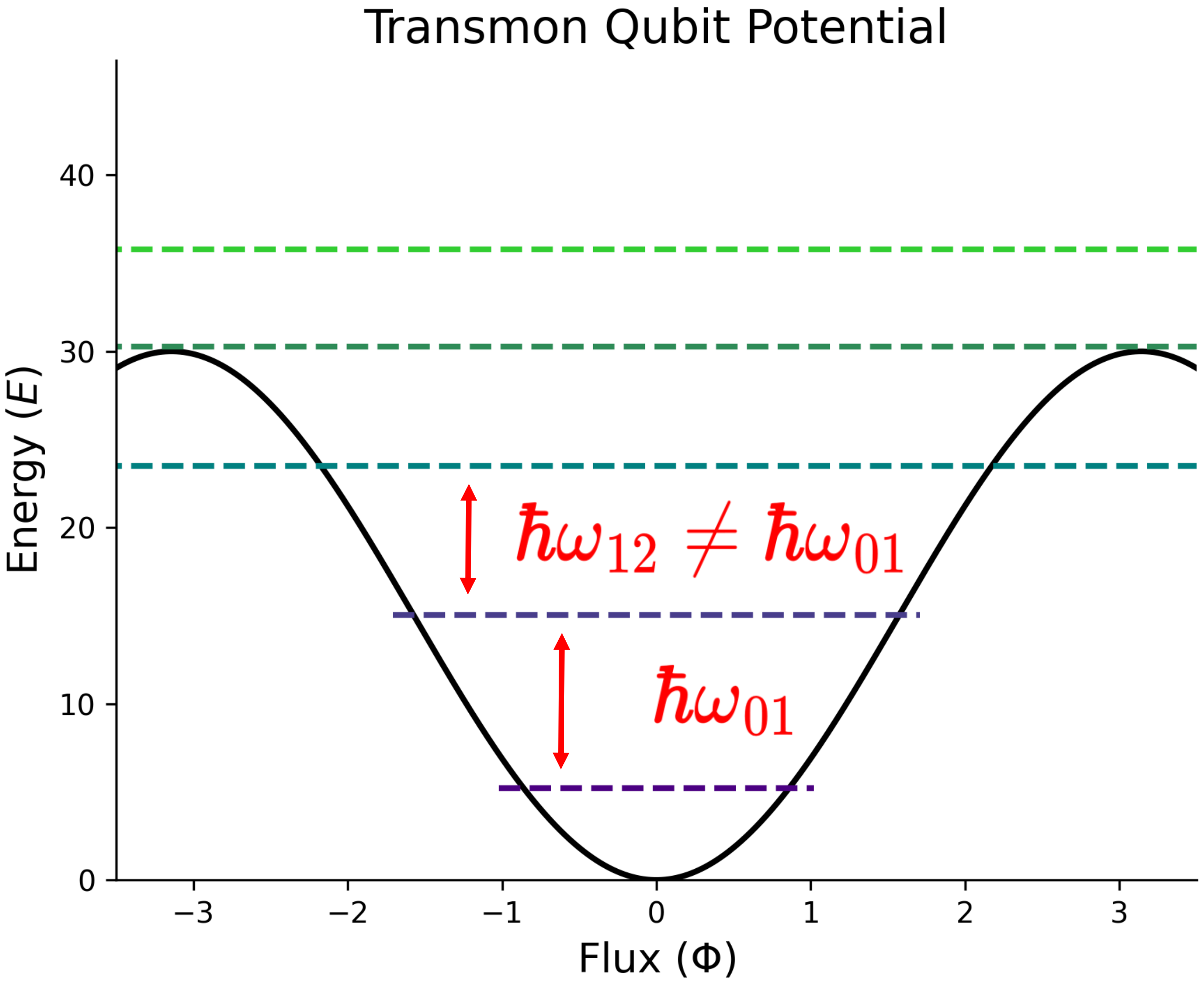
Annex Common Part

Transmon



Josephson with shunted capacitor

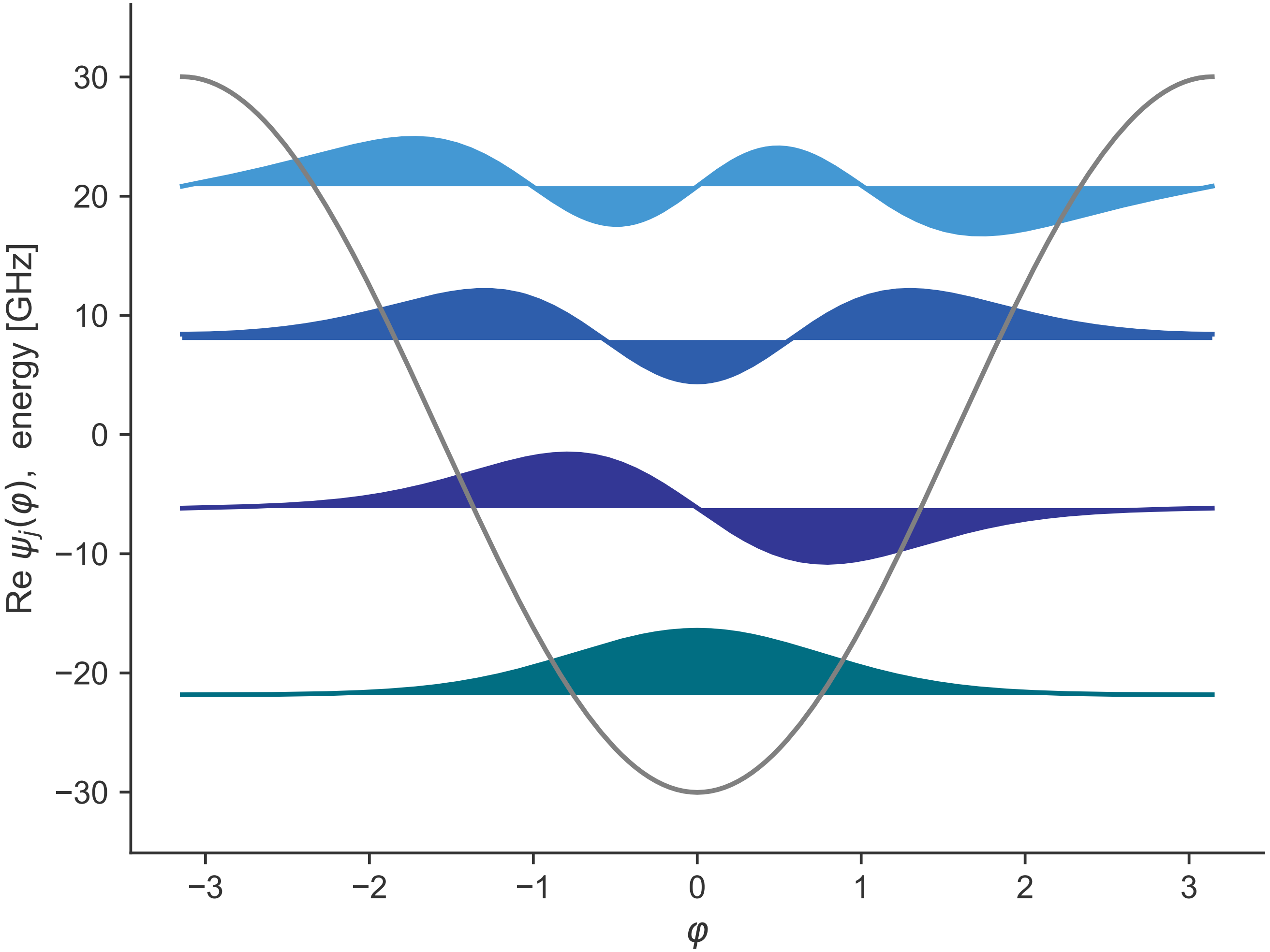
$$\hat{H} = 4E_{CJ}(\hat{n} - n_g)^2 - E_J \cos(\hat{\varphi})$$



Transmon : wavefunctions

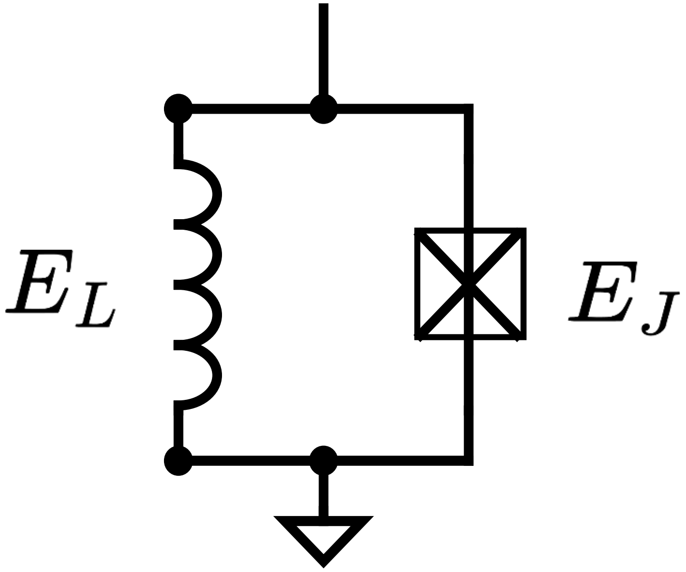
<u>Simulated with different packages</u>

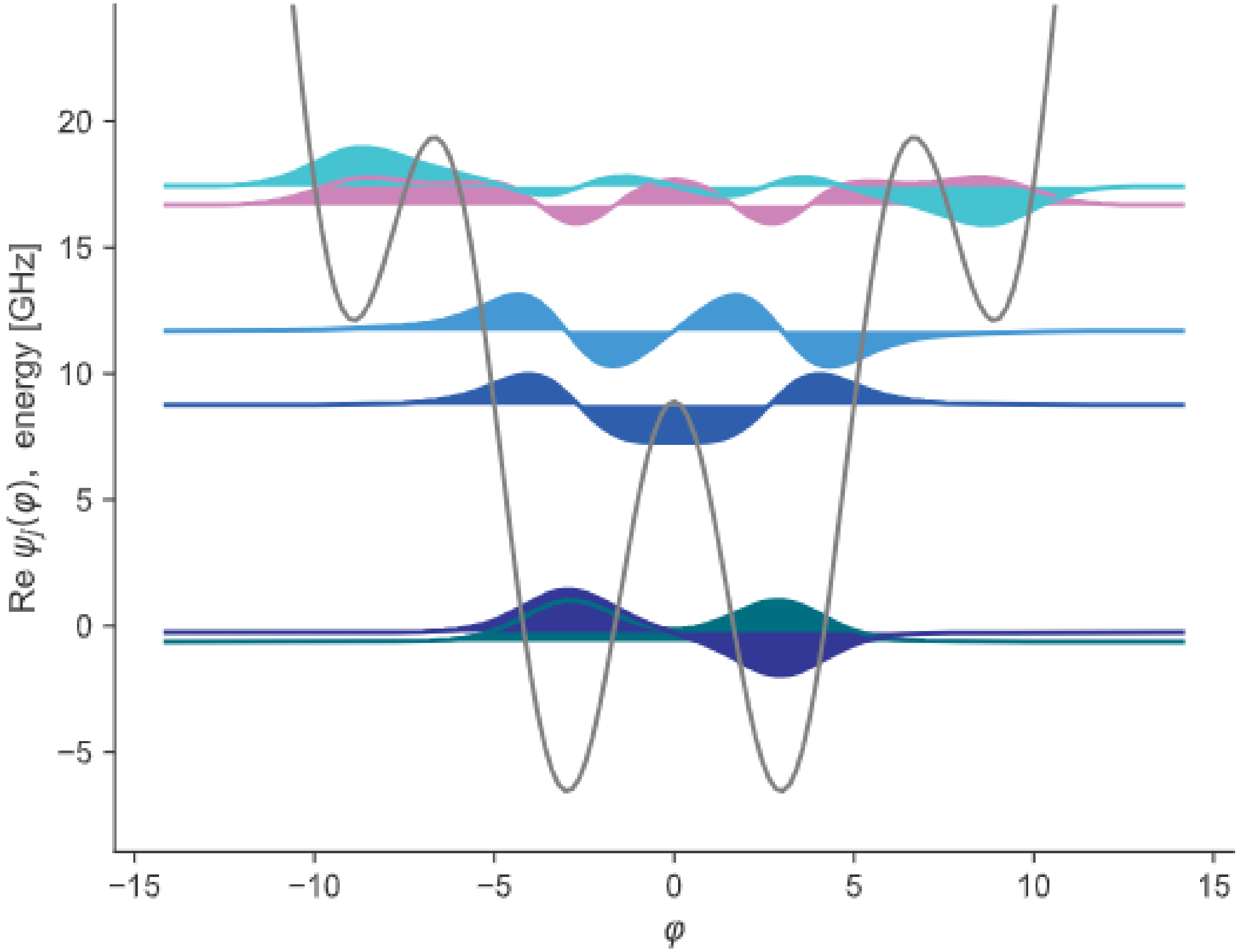
- Scqbits
- Qutip
- Numpy



$$\hat{H} = 4E_{CJ}(\hat{n} - n_g)^2 - E_J \cos(\hat{\varphi})$$

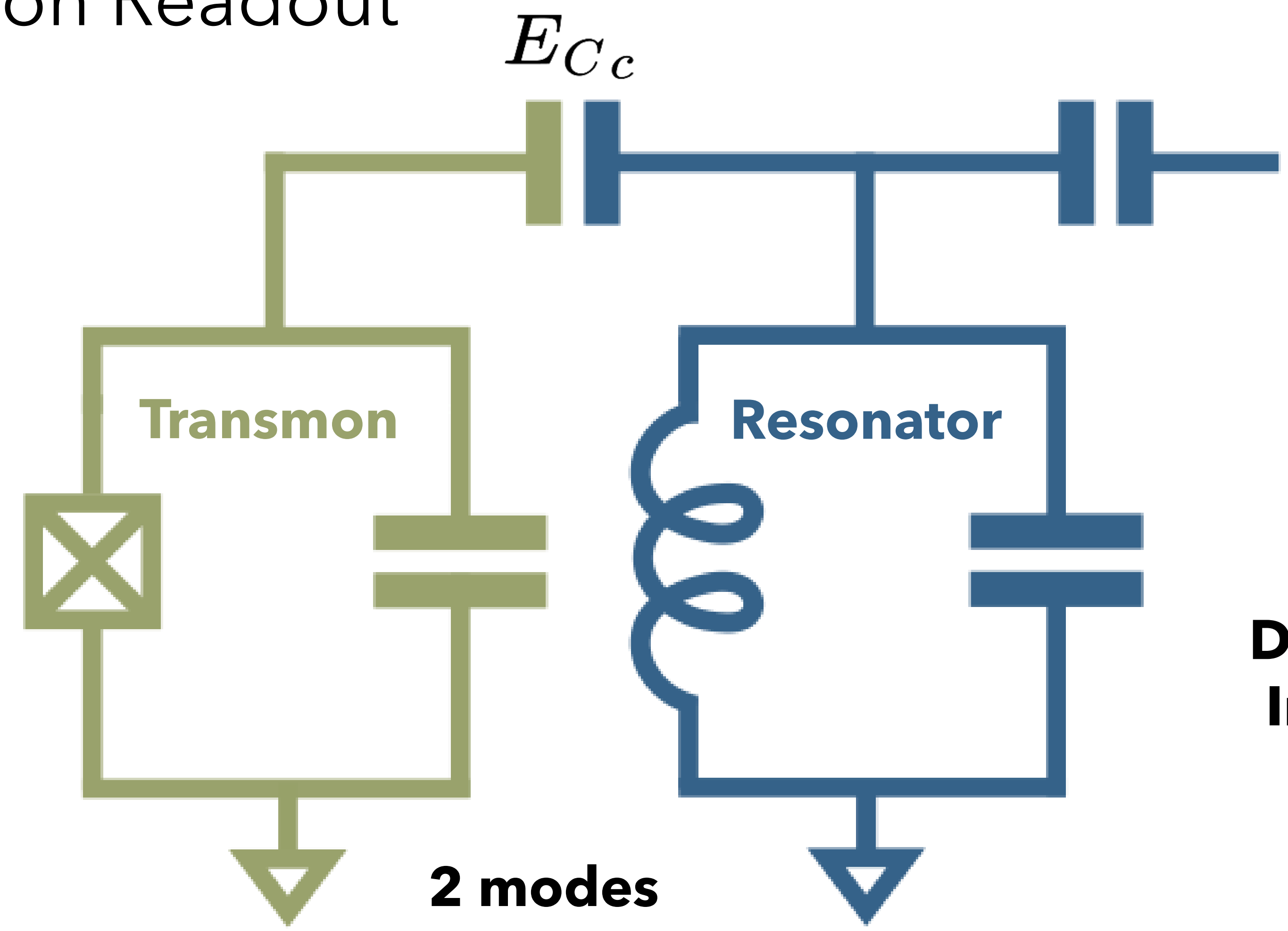
Fluxonium

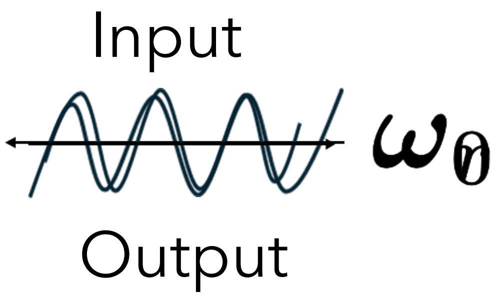




$$\hat{H} = 4E_C\hat{n}^2 + \frac{E_L}{2}(\hat{\phi} - \phi_{ext})^2 - E_J\cos\left(\hat{\phi}\right)$$

Transmon Readout





More photons

⇩

Decrease readout time (+)
Increase Hilbert space (-)

$$\hat{H} = \hat{H}_T + \hat{H}_R - 4E_{C_C} i n_{ZPF} \hat{n}_T (\hat{a}^\dagger - \hat{a})$$

Cross-Kerr : Measurement

Hamiltonian in the dispersive regime, i.e. $|g/\Delta| \ll 1$, truncated to the first two levels (Blais *et al., 2004)* :

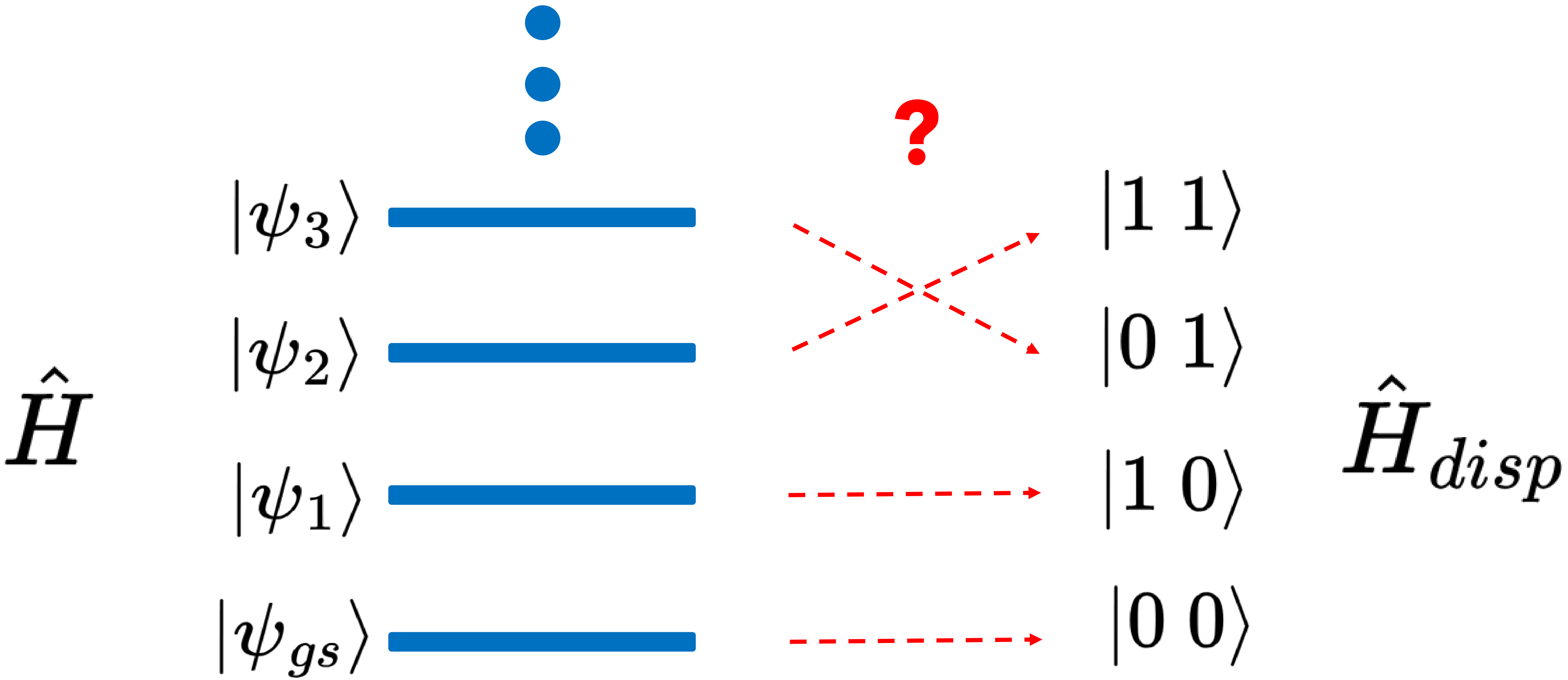
$$\hat{H}_{disp} \simeq \hbar\omega_r'\hat{a}^\dagger\hat{a} + \frac{\hbar\omega_q'}{2}\hat{\sigma}_z + \hbar\chi\hat{a}^\dagger\hat{a}\hat{\sigma}_z$$

Dispersive shift

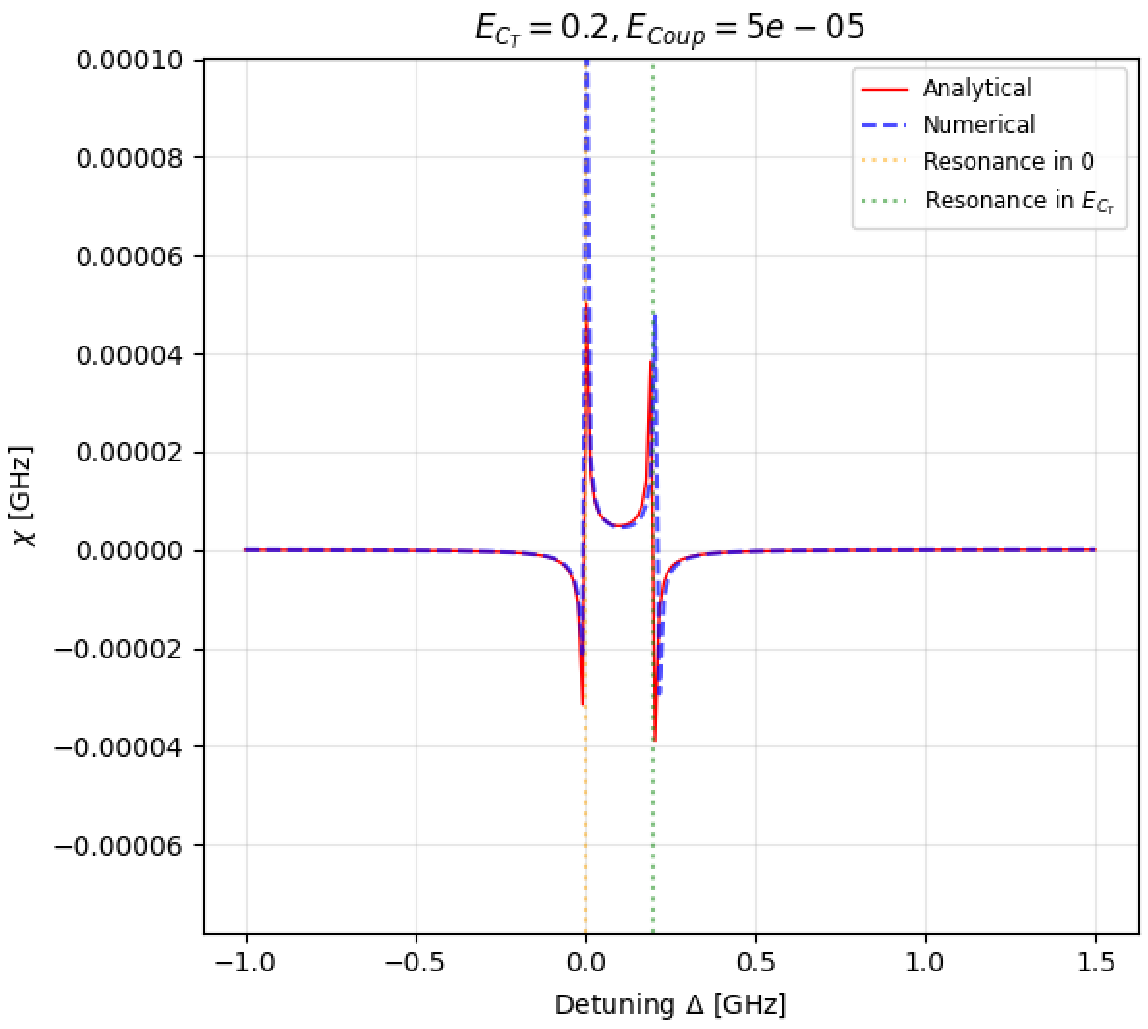
Eigenstates : $|0\,0\rangle,\ |1\,0\rangle,\ |0\,1\rangle,\ |1\,1\rangle,\ \ldots$

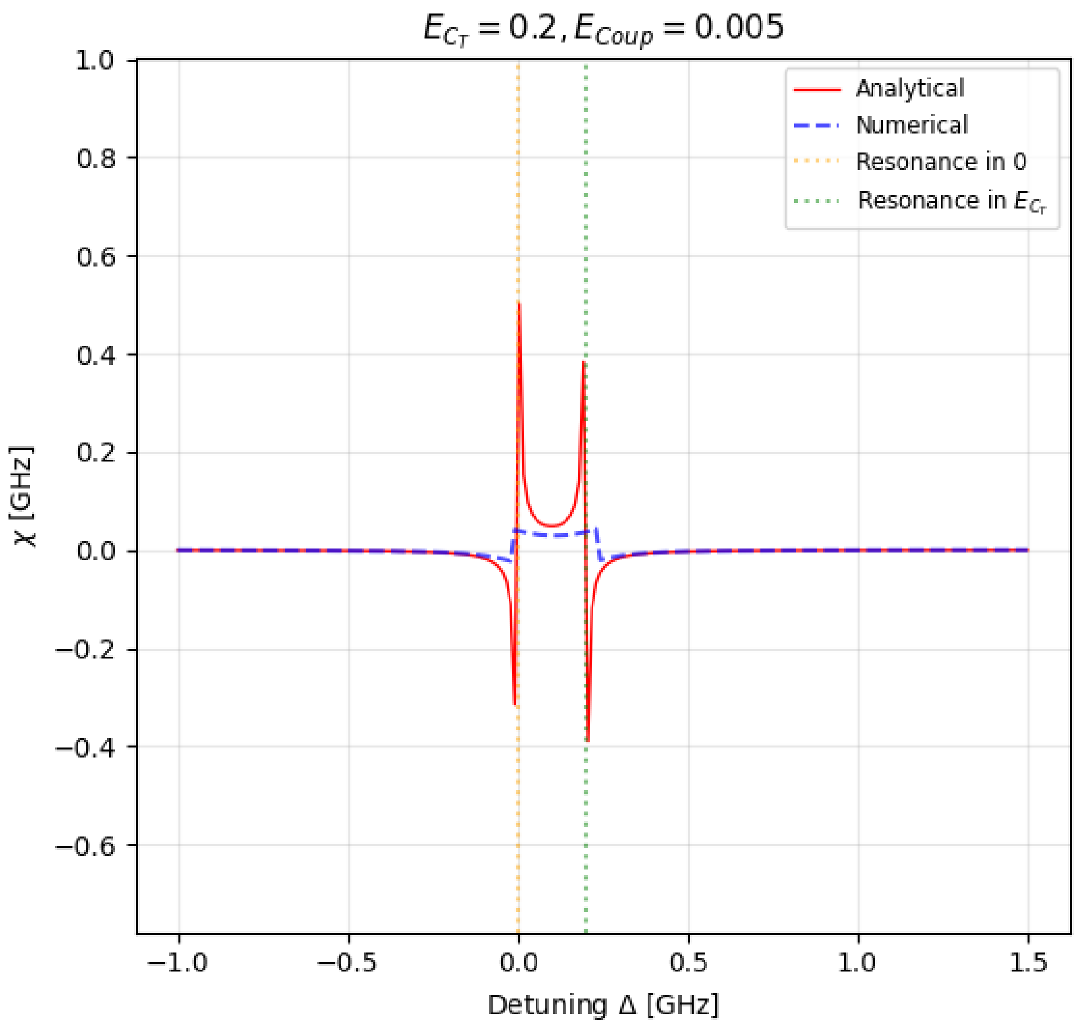
Eigenvalues : $\pm\frac{\omega_q'}{2},\ \omega_r' \pm \left(\frac{\omega_q'}{2} + \chi\right),\ \ldots$

Maximizing overlap



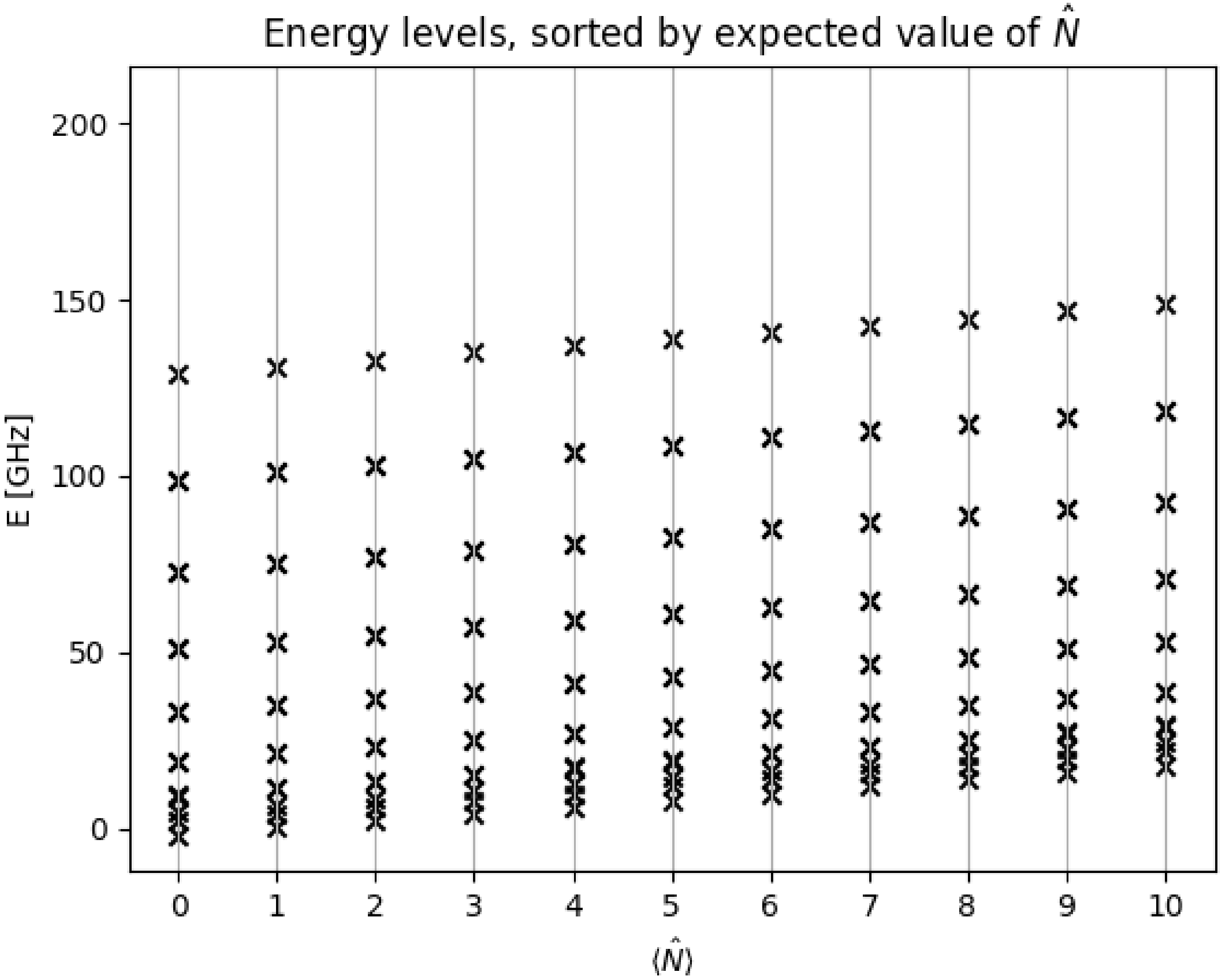
Dispersive shift χ as function of detuning Δ





Rm : Numerical Method uses QuTiP package and Exact Diagonalisation

Another Method



Kite Qubit Hamiltonian (no assymetry)

$$
\begin{aligned}
H = {} & 4E_C(n + n_\Sigma + n_g)^2 + 2E_{C_J}(n_\Sigma^2 + n_\Delta^2) \\
& + E_L(\varphi_\Sigma^2 + \varphi_\Delta^2) \\
& - 2E_J \cos(\varphi - \varphi_\Sigma) \cos\left(\varphi_\Delta + \frac{\varphi_{\text{ext}}}{2}\right) \\
& + \hbar\omega(N_R + \frac{1}{2}) \\
& + E_{C_C}(n + n_\Sigma + n_g)n_R
\end{aligned}
$$

Annex Eliot

The power algorithm : Find the dominant eigenspace

1. Spectral Decomposition (Operator View)

$A = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i| \quad \text{with} \quad |\lambda_0| \leq \cdots < |\lambda_{\mathbf{max}}|$

2. Initial State Expansion

$|\Psi^{(0)}\rangle = c_{max}|\psi_{max}\rangle + \sum_{i\neq max} c_i|\psi_i\rangle$

3. Applying A^n (Power Iteration)

$A^n|\Psi^{(0)}\rangle = c_{max}\lambda^n_{max}|\psi_{max}\rangle + \sum_{i\neq max} c_i\lambda^n_i|\psi_i\rangle$

$\implies$ Even faster when $|\Psi^{(0)}\rangle \simeq |\psi_{max}\rangle$

4. Factorization \& Convergence

$$= \lambda^n_{max}\left[c_{max}|\psi_{max}\rangle + \sum_{i\neq max} c_i \underbrace{\left(\frac{\lambda_i}{\lambda_{max}}\right)^n}_{\to 0 \text{ as } n\to\infty} |\psi_i\rangle\right]$$

$\implies \lim_{\mathbf{n}\to\infty} \mathbf{A}^{\mathbf{n}}|\mathbf{\Psi}^{(\mathbf{0})}\rangle \propto |\psi_{\mathbf{max}}\rangle$

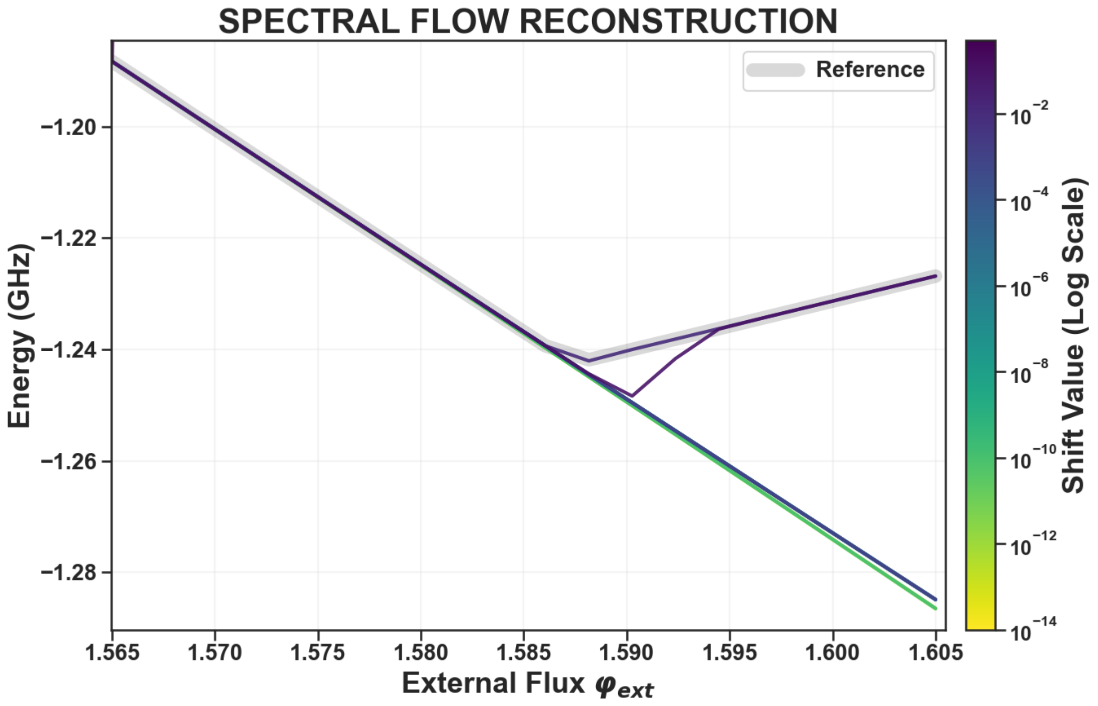
Shift Invert

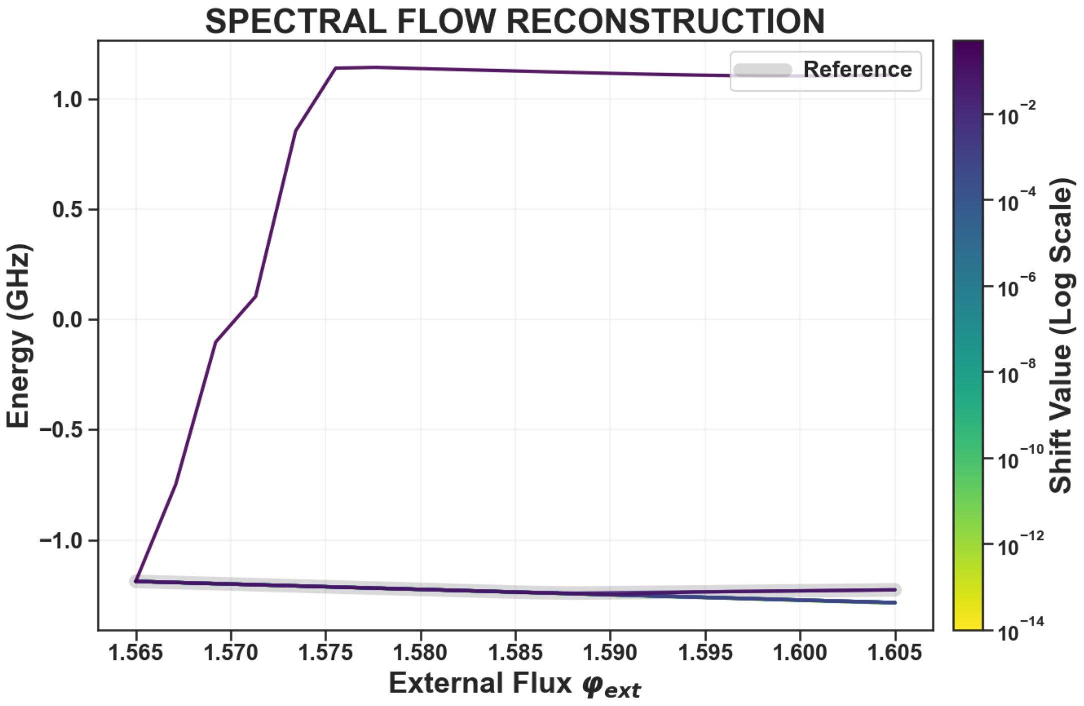
- Starting point $\begin{cases} \lambda \\ \psi \end{cases}$ $s.t.$ $H(\varphi_{ext})|\psi\rangle = \lambda|\psi\rangle$ and we want $\begin{cases} \tilde{\lambda} \\ \tilde{\psi} \end{cases}$ $s.t.$ $H(\varphi_{ext} + \delta\varphi)|\tilde{\psi}\rangle = \tilde{\lambda}|\tilde{\psi}\rangle$
- As we are doing small variations, $\begin{cases} |\tilde{\psi}\rangle = |\psi\rangle + \delta\psi \\ \tilde{\lambda} = \lambda + \delta\lambda \end{cases}$
- so $(H(\varphi_{ext} + \delta\varphi) - \lambda\,\mathrm{Id})$ has $\delta\lambda$ as eigenvalue $\implies (H(\varphi_{ext} + \delta\varphi) - \lambda\,\mathrm{Id})^{-1}$ has $\dfrac{1}{\delta\lambda} \gg 1$ as eigenvalue
- Power method on $(H(\varphi_{ext} + \delta\varphi) - \lambda\mathrm{Id})^{-1} \implies (H(\varphi_{ext} + \delta\varphi) - \lambda\mathrm{Id})^{-1}|\tilde{\psi}\rangle = \dfrac{1}{\delta\lambda}|\tilde{\psi}\rangle$

$$\implies H(\varphi_{ext} + \delta\varphi)|\tilde{\psi}\rangle = \underbrace{(\lambda + \delta\lambda)}_{\tilde{\lambda}}|\tilde{\psi}\rangle$$

- $A^{-1}|\Psi^{(n)}\rangle = |\Psi^{(n+1)}\rangle \Leftrightarrow A|\Psi^{(n+1)}\rangle = |\Psi^{(n)}\rangle$ We will use minres from scipy to solve it

Follow trajectory, shift benchmark





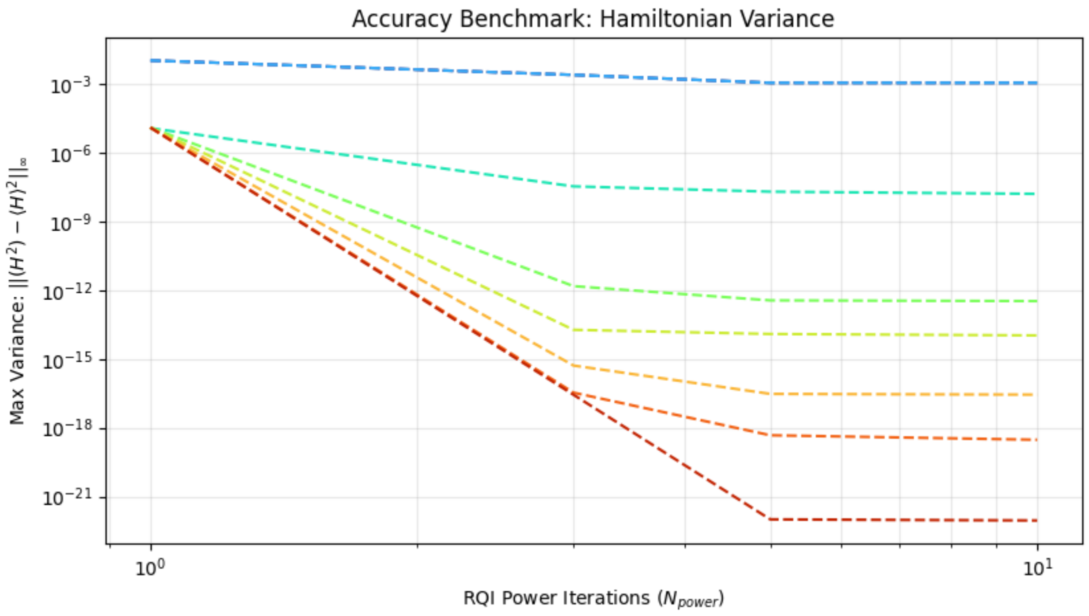
N_{power} and ϵ benchmark

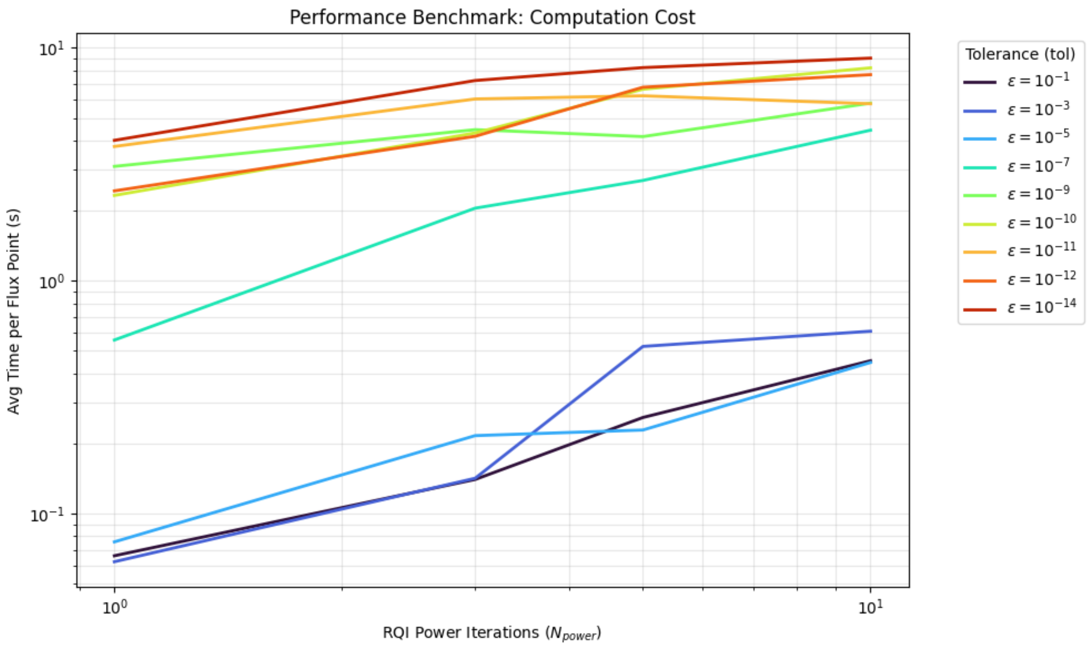
$$(H(\varphi_{ext} + \delta\varphi) - (\lambda + shift)\ \mathrm{Id})|\Psi^{(1)}\rangle = |\Psi^{(0)}\rangle$$

$$\cdots$$

$$(H(\varphi_{ext} + \delta\varphi) - (\lambda + shift)\ \mathrm{Id})|\Psi^{(N_{power})}\rangle = |\Psi^{(N_{power}-1)}\rangle$$

Solved N_{power} times with precision ϵ





Shift invert versus Lanczos different dim