Variational algorithms and quantum computer Co-Design

Frank Wilhelm
Saarland University

UNIVERSITÄT
DES
SAARLANDES

Team and current projects

- EU Flagship project „An Open Superconducting Quantum Computer“ (OpenSuperQ)
- IARPA project „Flux-based quantum speedup“ (FluQS) in the quantum-enhanced optimization program
- EU ITN „Quantum sensing with optimal control“ (Qusco)
- BMBF project Verticons
- BSI study „status of quantum computers“
- Industry graduate students: Daimler, DLR, IBM, HQS

OpenSuperQ

Bundesamt für Sicherheit in der Informationstechnik

QuSCo

August 2019

Contents

- Why co-Design? Why a not-quite-universal quantum computer?
- Example: A crossing-free architecture for variational self-energy calculations
- Example: QAOA with only single-qubit controls
- Excursion: A route to extremely high gate fidelities
- Conclusion and speculation: Programming a variational quantum computer

Why co-design?

Noisy Intermediate-scale quantum computer (NSQ)

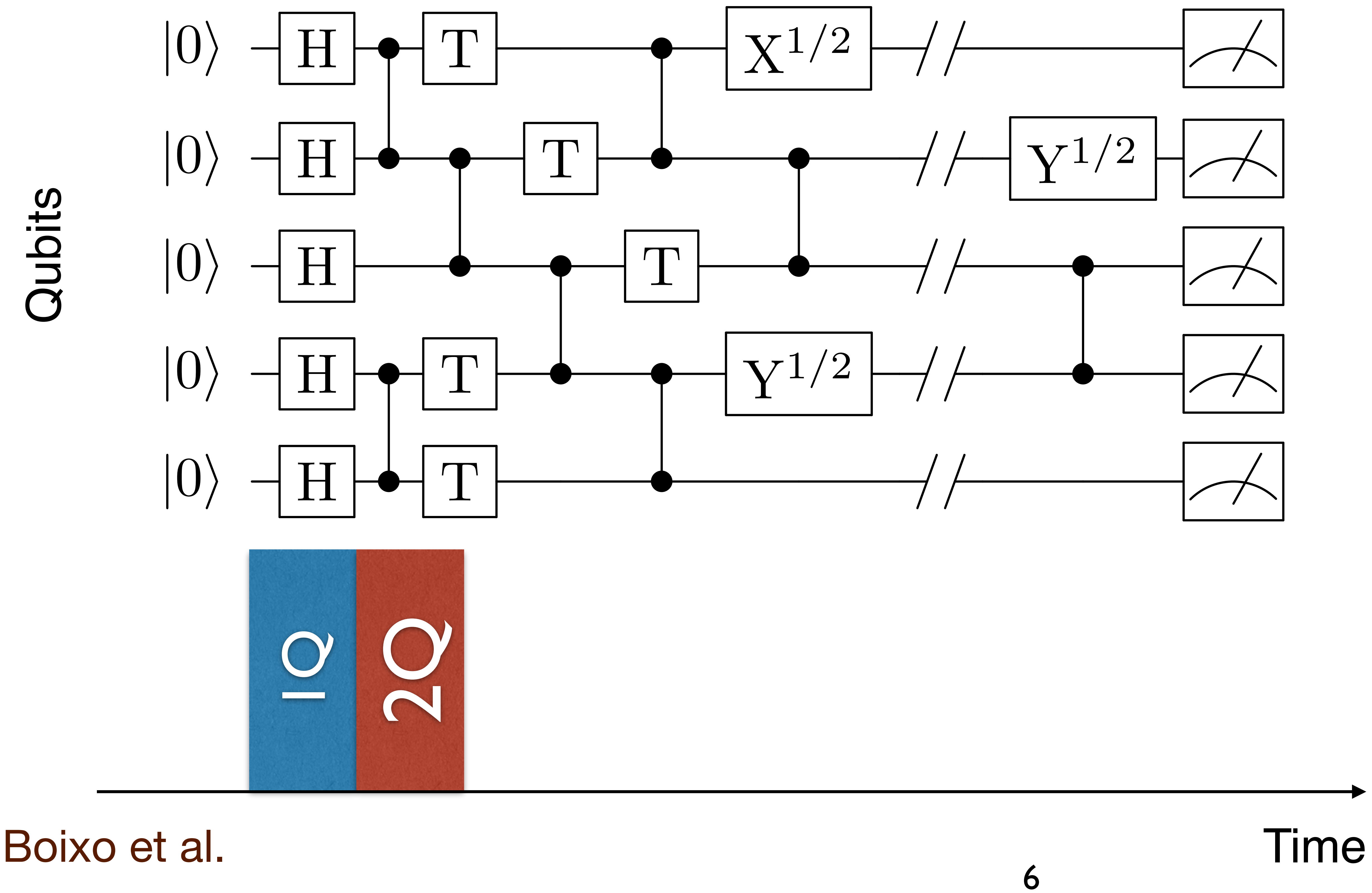
Clive Sinclair

Simple, primitive, error-prone hardware: Coding needs to follow architecture

Gates and physical interactions

$$\hat{H} = \hat{H}_0 + \sum_i F_i(t)\hat{H}_i$$

$$\hat{H} = \sum_i \hat{H}_i(t) + \sum_{i<j} \hat{H}_{ij}(t)$$



$$\hat{U}_{\text{gate}} = \exp(-i\hat{H}t_g)$$

$$\hat{U}(t_f) = \mathbb{T}\exp\left(-\frac{i}{\hbar}\int_0^{t_f} d\tau\ \hat{H}(\tau)\right)$$

Physical connectivity / interaction range
Puts price to two-qubit gates

Boixo et al.

Quantum annealing as co-design

$$H(s) = (1 - A(s))H_d + A(s)H_p$$

Driver: $$H_d = -D\sum_i \hat{X}_i$$

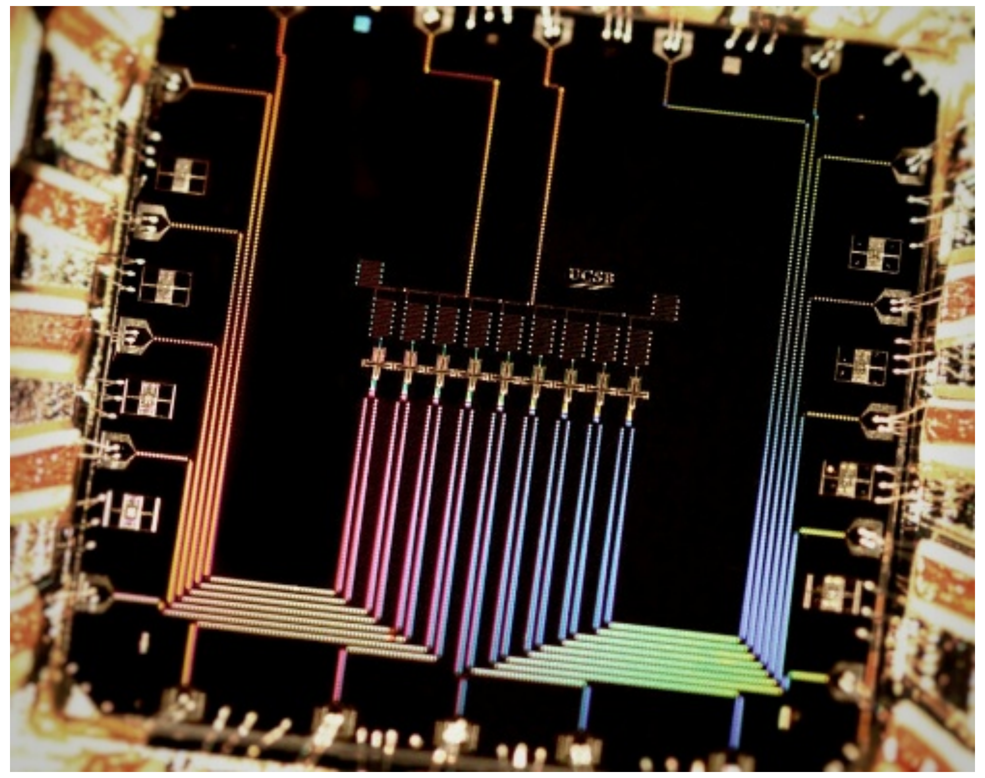
Problem Hamiltonian:

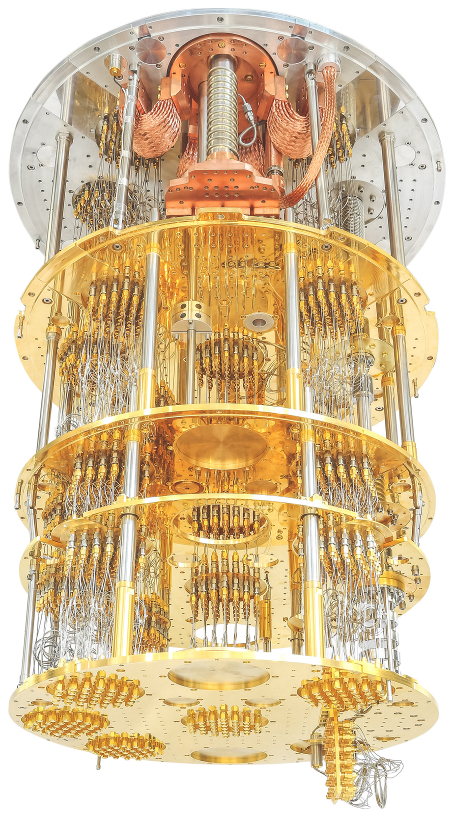
$$H_p = \sum_i h_i Z_i + \sum_{i<j} J_{ij} Z_i Z_j + \sum_{i<j<k} K_{ijk} Z_i Z_j Z_k + \ldots$$

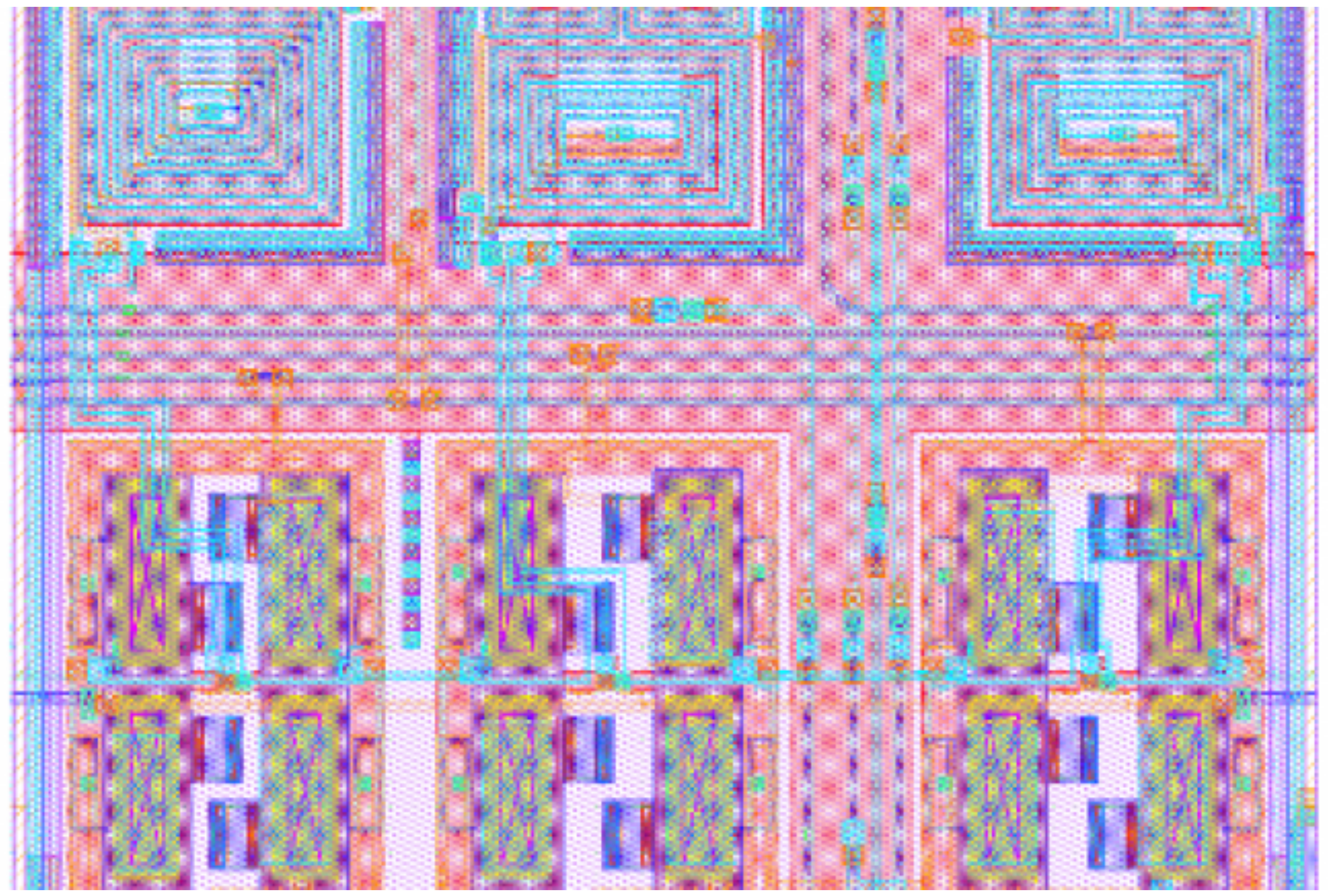
Annealing schedule:

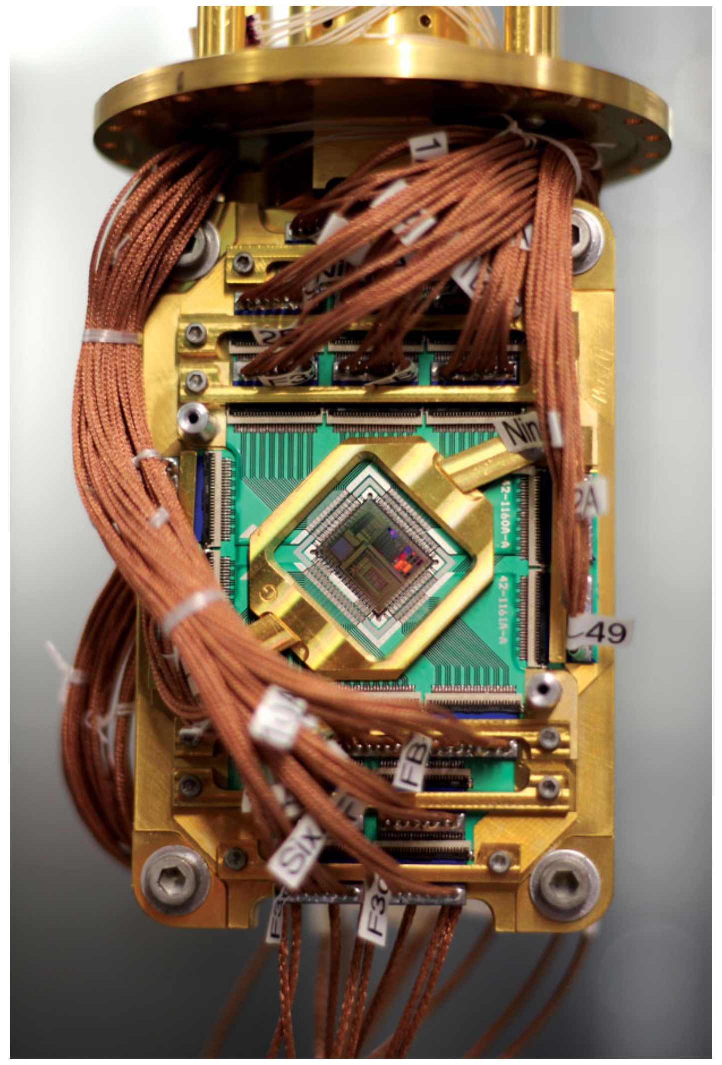
$$A\left(\frac{t}{T}\right) \qquad A(0) = 0 \qquad A(1) = 1$$

Gate model hardware





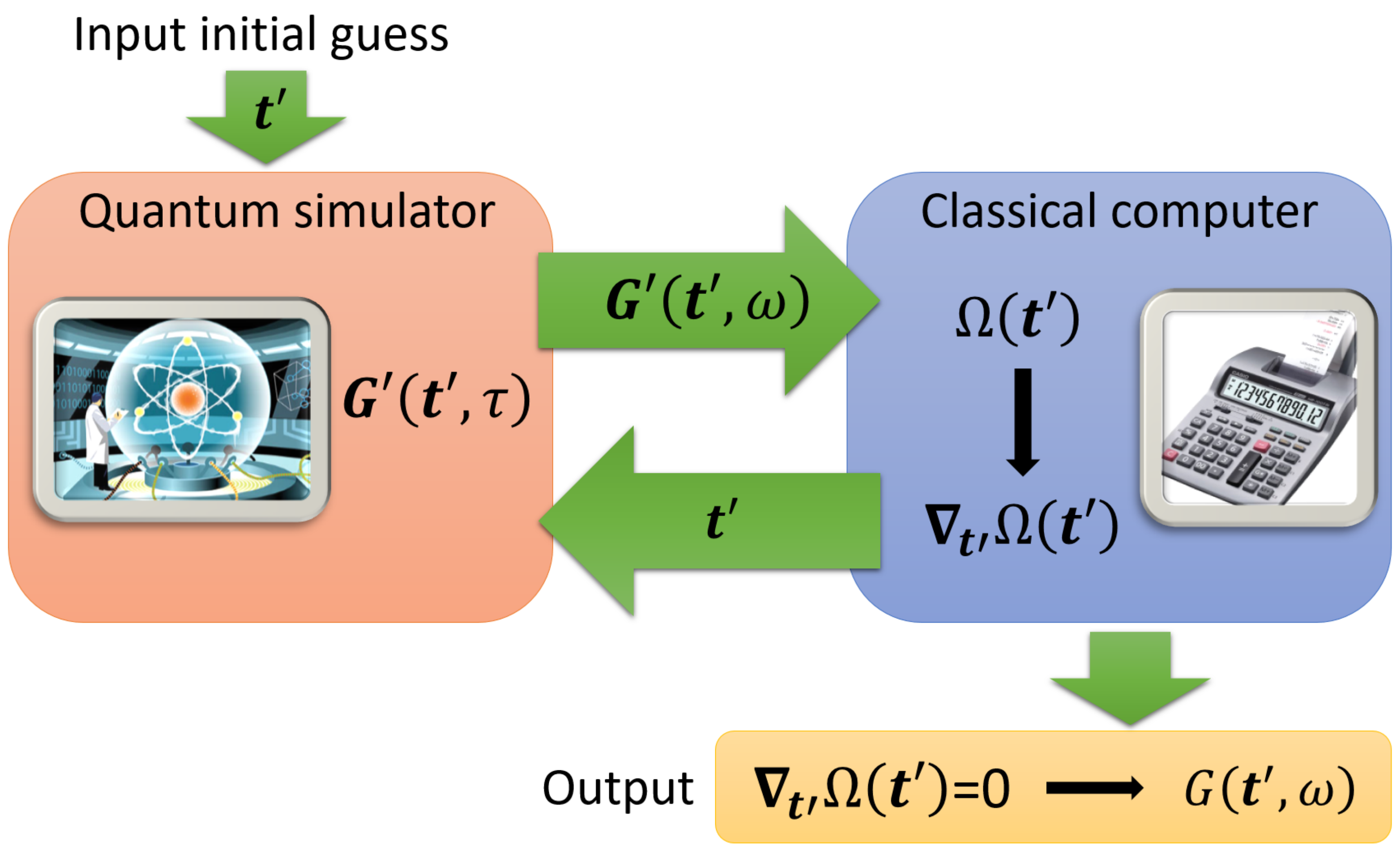




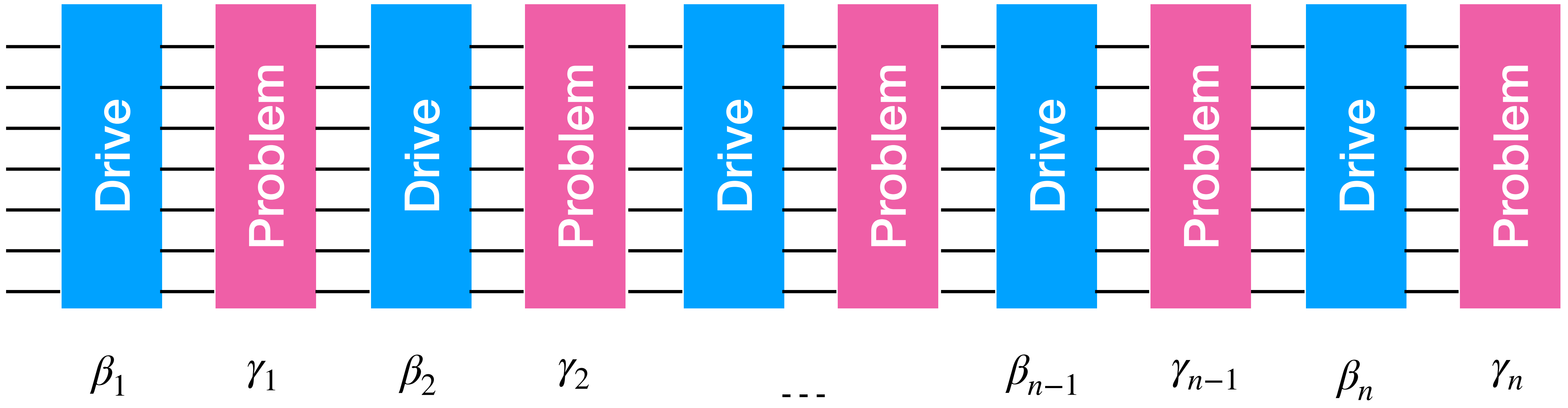
D-Wave

Hybrid algorithms

- let the (cheap) classical computer do what it is best at
- enhance its performance with the (expensive) quantum computer



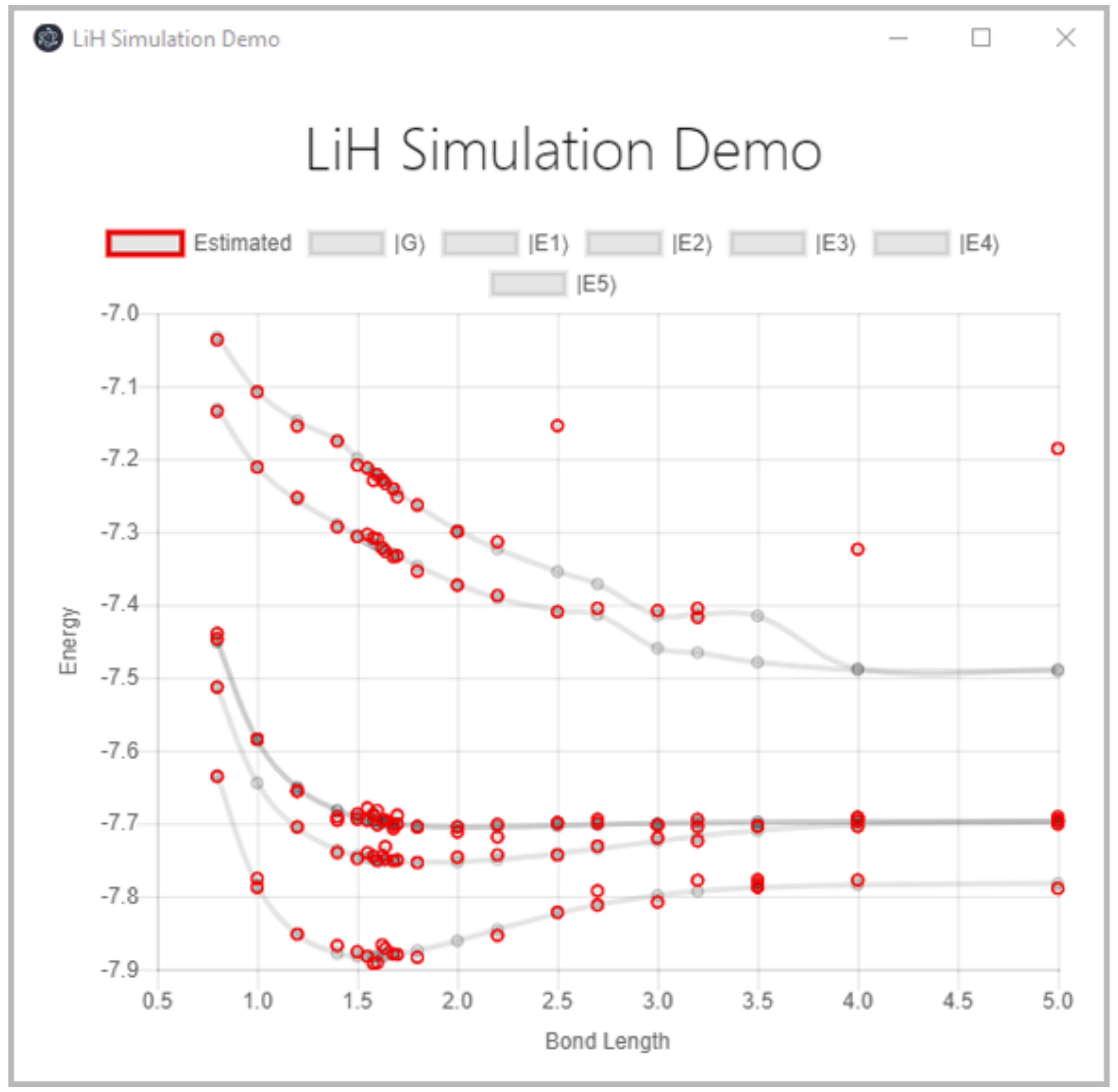
Is there a Co-design for this?



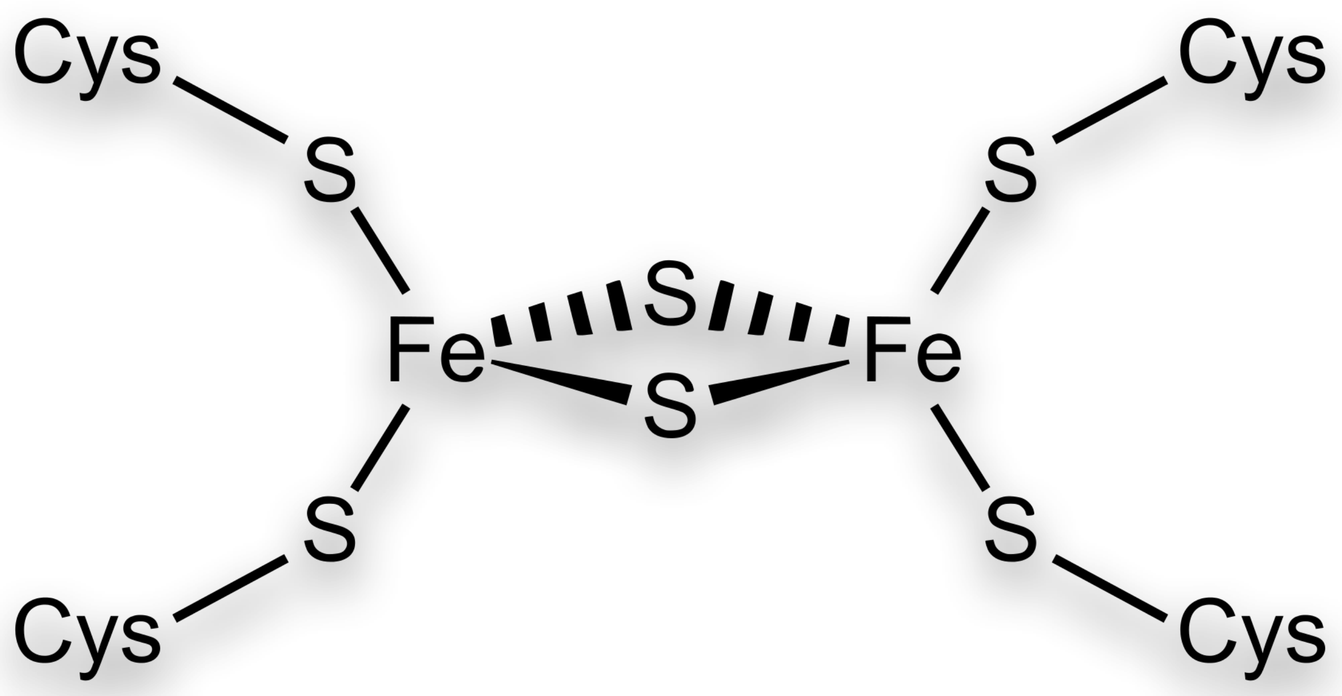
“Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.”
Richard P. Feynman, „Simulating physics with computers“, 1981

Co-Design for variational self-energy techniques

From molecules to materials!



Moonshot of quantum computer chemistry



YBCO

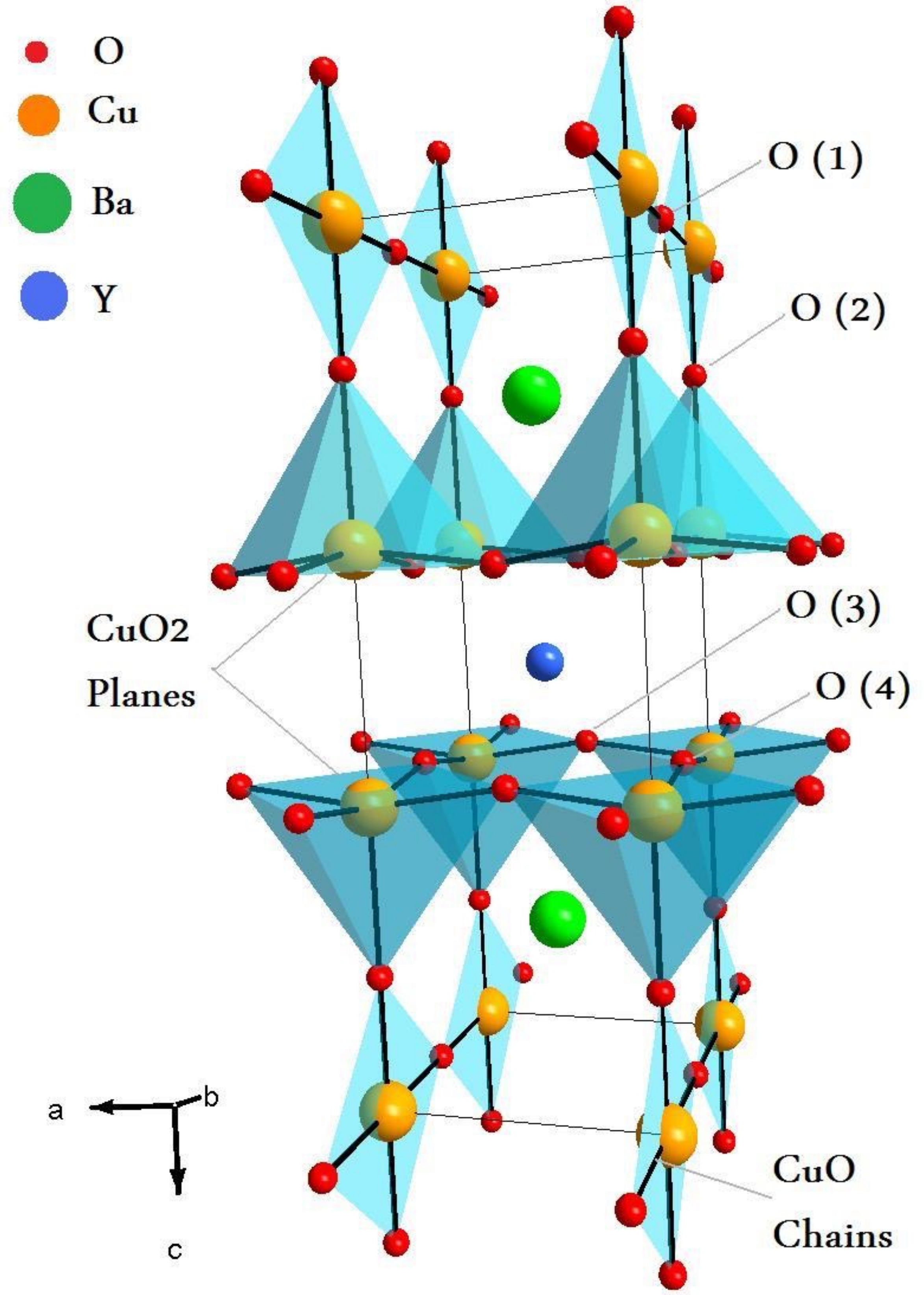
More is different

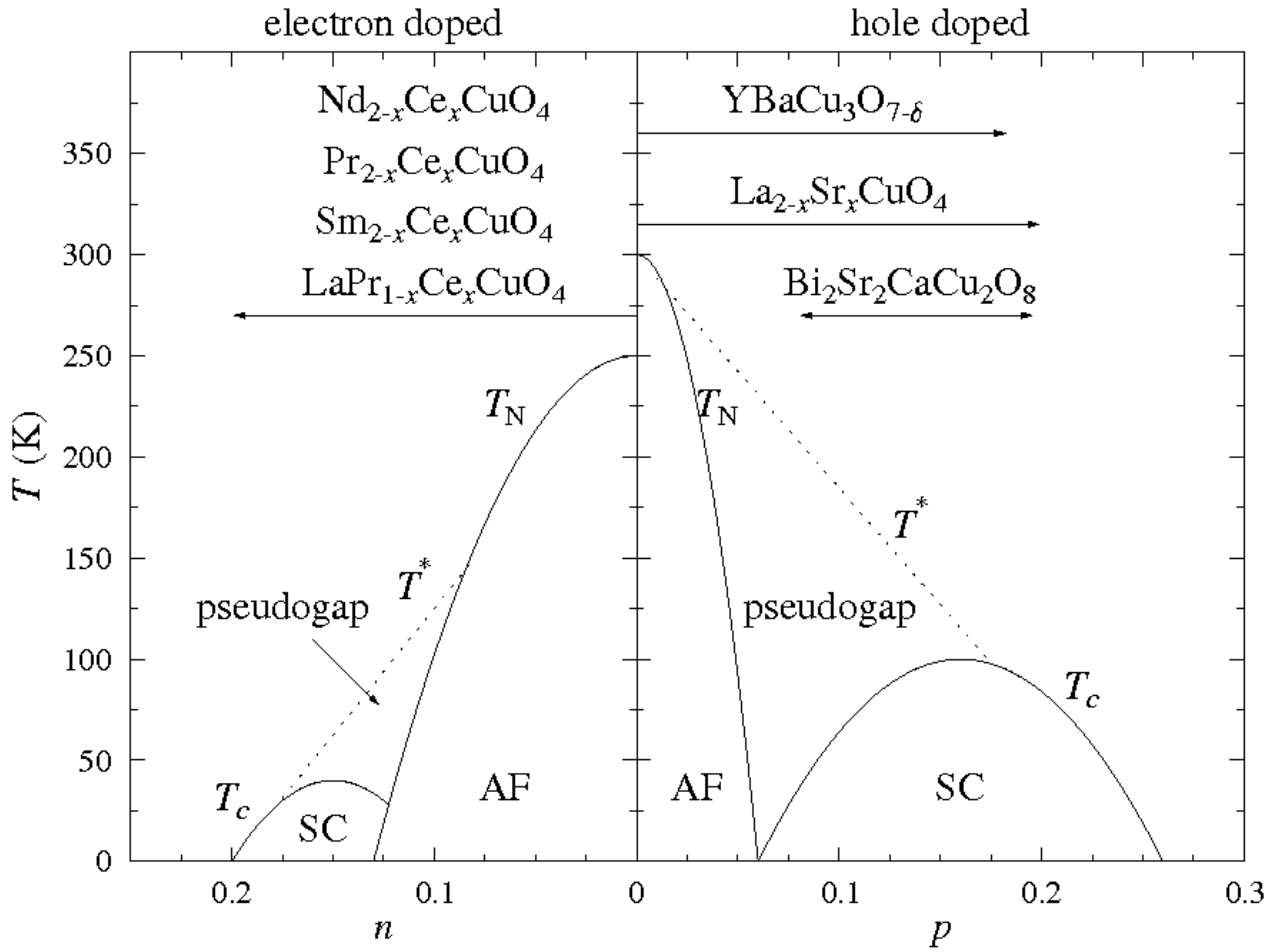
Do we need poly(N_A) qubits?

High-Tc and Hubbard model

Low (<1 eV) physics of electrons on lattices

$$H = -t \sum_{\langle i,j \rangle,\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + c^{\dagger}_{j,\sigma} c_{i,\sigma}) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow},$$





- non-integrable
- QMC: Fermionic sign problem
- reproduces d-wave superconductivity

Manybody dynamics

Goal: Characterize phases and find phase transtions

Describe physical properties through the time-ordered two-point Green's function

$$G^{(j)}\left(\vec{r},t|\vec{r}',t'\right) = -i\left\langle \mathbf{T}^{(j)}\Psi(\vec{r},t)\Psi^{\dagger}(\vec{r}',t')\right\rangle$$

Superconductivity: Nambu spinors: makes G a 2x2 matrix

$$\Psi = \begin{pmatrix} \Psi_{\uparrow} \\ \Psi^{\dagger}_{\downarrow} \end{pmatrix} \quad G = \begin{pmatrix} G & F \\ F^{*} & -G \end{pmatrix}$$

Off-diagonal component detects superconducting order: Pair amplitude

$$F(\vec{r},t|\vec{r}',t') = -i\left\langle \mathbf{T}\Psi(\vec{r},t)\Psi(\vec{r}',t')\right\rangle$$

Green's function allows to compute observables

Self-energy:
Effect of the manybody system on the single propagating particle:
Dyson equation

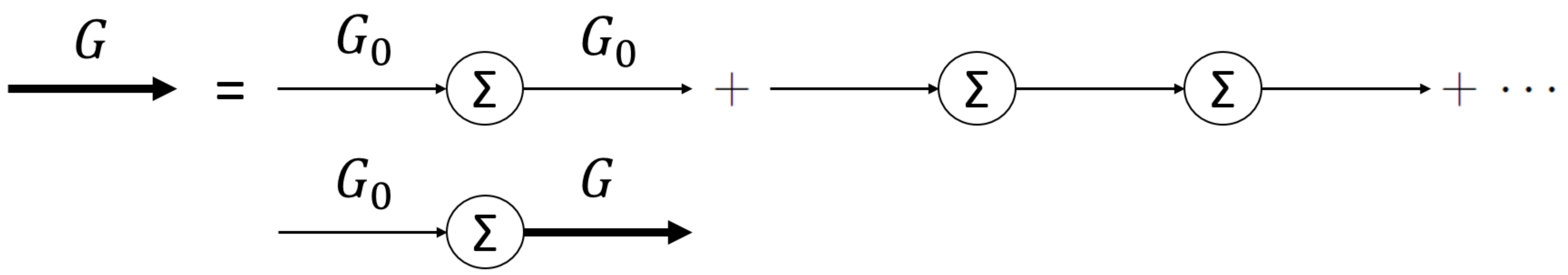
Useful manybody algorithms should give the Green's function

Variational eigensolver for solids

Describe physical properties through the time-ordered two-point Green's function

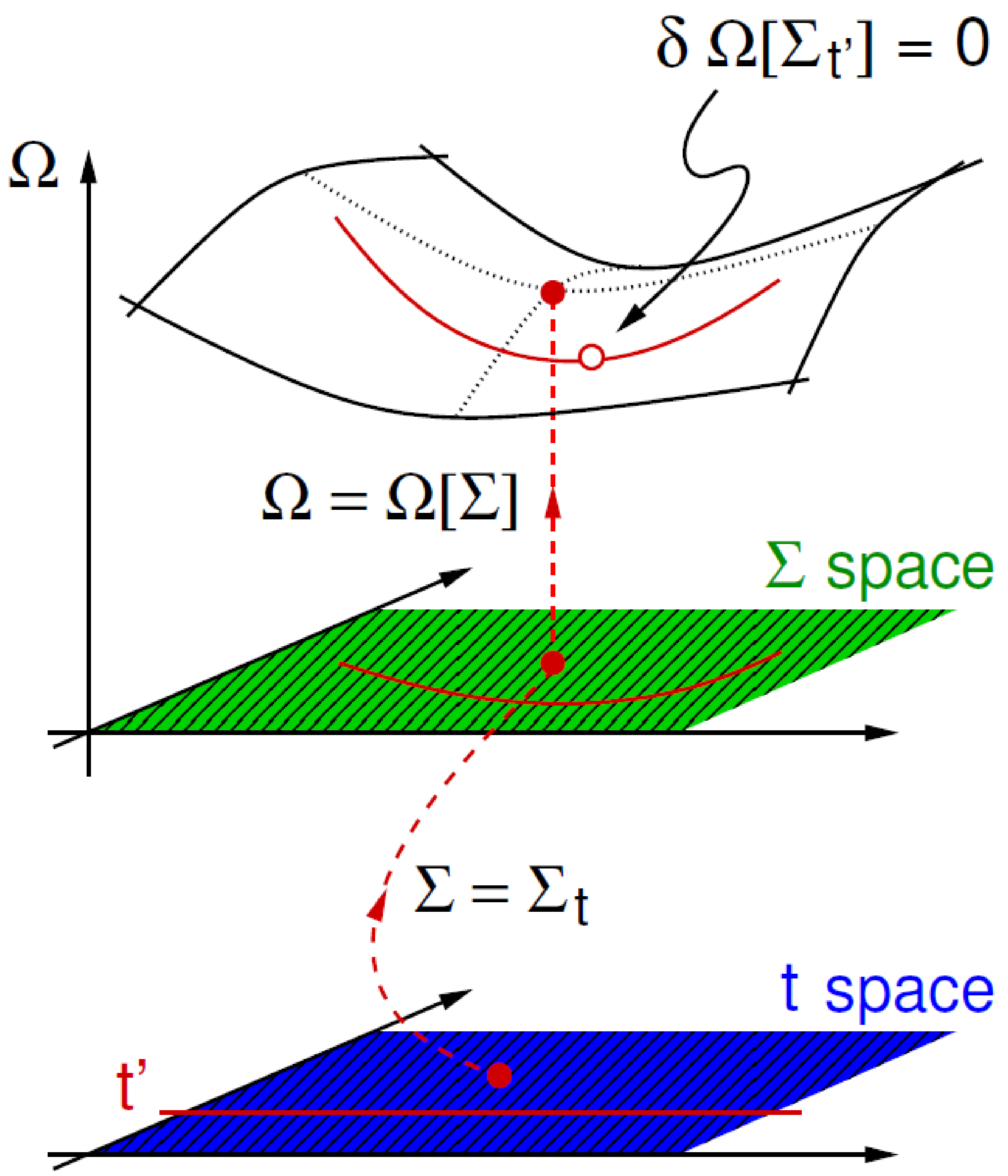
$$G^{(j)}\left(\vec{r}, t|\vec{r}', t'\right) = -i\left\langle \mathbf{T}^{(j)}\Psi(\vec{r}, t)\Psi^{\dagger}(\vec{r}', t')\right\rangle$$

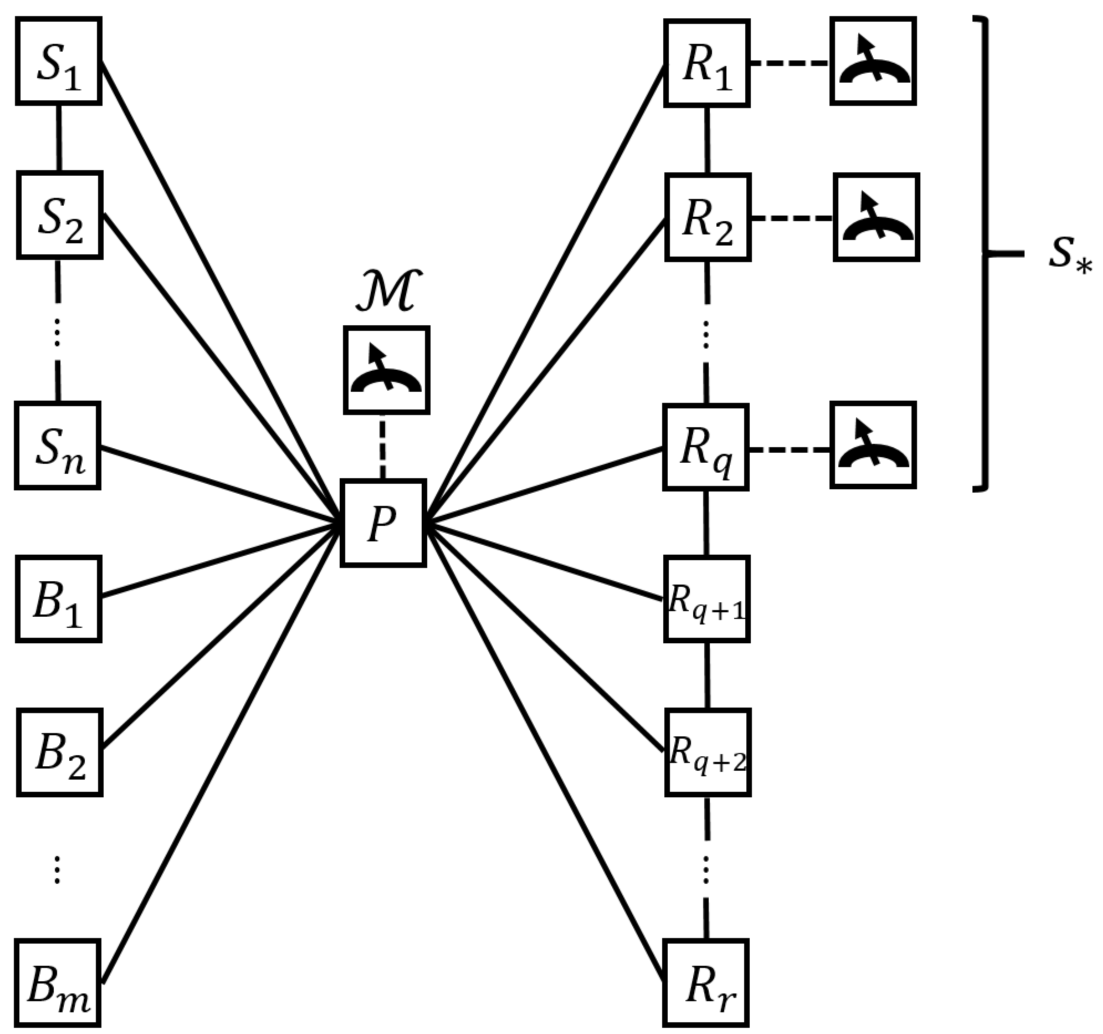
Self-energy: Effect of the manybody system on the single propagating particle:
Dyson equation



Variational principle

$$\frac{\delta\Omega_t\left[\Sigma\right]}{\delta\Sigma} = \left(\mathbf{G}_{0t}^{-1} - \Sigma\right)^{-1} - \mathbf{G} = 0.$$





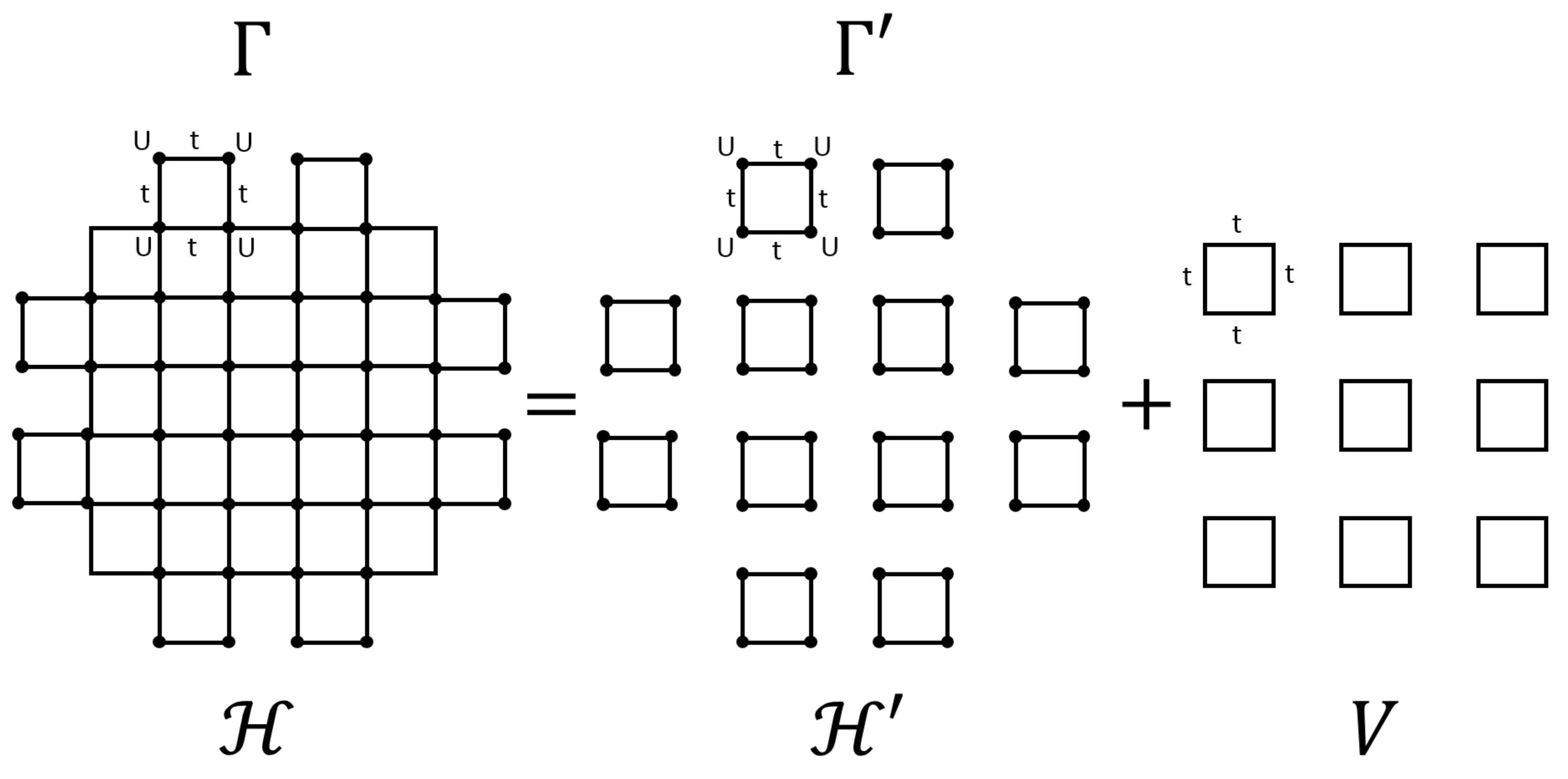
Varational principle for the self-energy:
Variational cluster method (Pothoff, Senechal)

P.-L. Dallaire-Demers and FKW, 2016 (2 papers)

 FQHE: M.P. Kaicher, S.B. Jäger, P.-L. Dallaire-Demers, and FKW, 2020

Variational cluster

Exact cluster Green's function $\mathbf{G}'^{-1}(\omega) = \omega - \mathbf{t}' - \Sigma'(\omega)$



- split lattice into exact clusters
- couple clusters perturbatively: Closed form

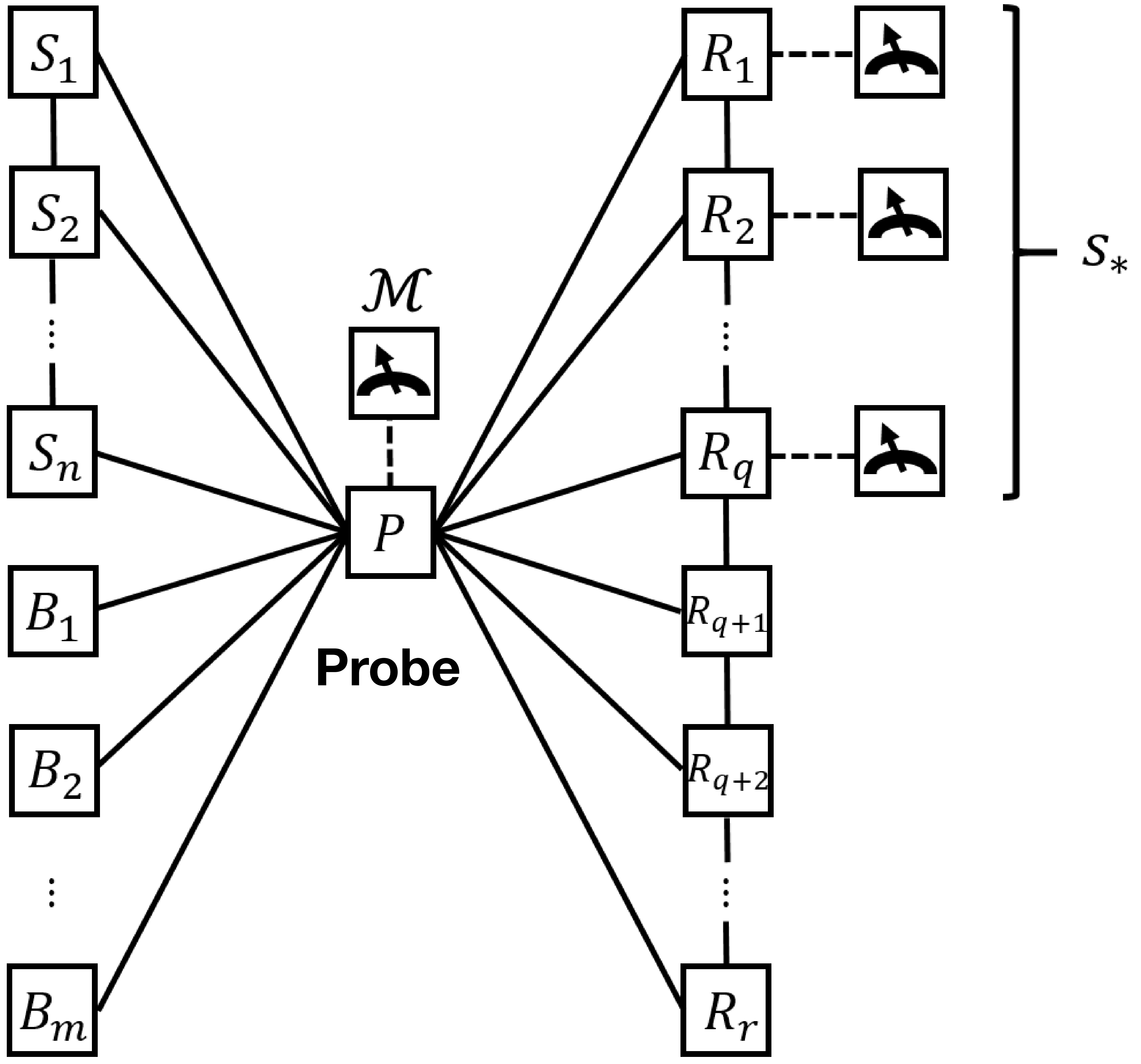
$$\mathbf{G}[\mathbf{\Sigma}'] = \mathbf{G}_{\text{cpt}} = \left(\mathbf{G}'^{-1} - \mathbf{V}\right)^{-1}.$$

Classical variational calculus for $\Omega_t[\mathbf{\Sigma}'] = \Omega' - \operatorname{Tr}\ln[\mathbf{1} - \mathbf{V}\mathbf{G}']\,.$

Potthoff, Senechal …

Architecture and performance

Look ma, no crossings!



Hubbard register
(acceptable SWAP-OH)

Thermalization
(acceptable SWAP-OH)

Dimension(s)	Size	Orbitals (singlets) $[n]$	Dim. of Hilbert space $[2^n]$	Qubits required $[n+1]$	Measured correl. functions $[< 4n^2]$	$c-$SQGs to tune $[7n]$	$c-\pm$iSWAPs to tune $[2n-2]$	Gates / Trotter-Suzuki step (hopping terms)
1D	2	4	16	5	64	28	6	24
1D	3	6	64	7	144	42	10	48
1D	4	8	256	9	256	56	14	72
2D	2×2	8	256	9	256	56	14	96
2D	3×3	18	262,144	19	1,296	126	34	336
2D	4×4	32	4,294,967,296	33	4,096	224	62	768
3D	$2 \times 2 \times 2$	16	65,536	17	1,024	112	30	416
3D	$3 \times 3 \times 3$	54	1.8×10^{16}	55	11,664	378	106	2,736
3D	$4 \times 4 \times 4$	128	3.4×10^{38}	129	65,536	896	254	10,368

P.-L. Dallaire-Demers and FKW, PRA 2017

QAOA with only single qubit controls

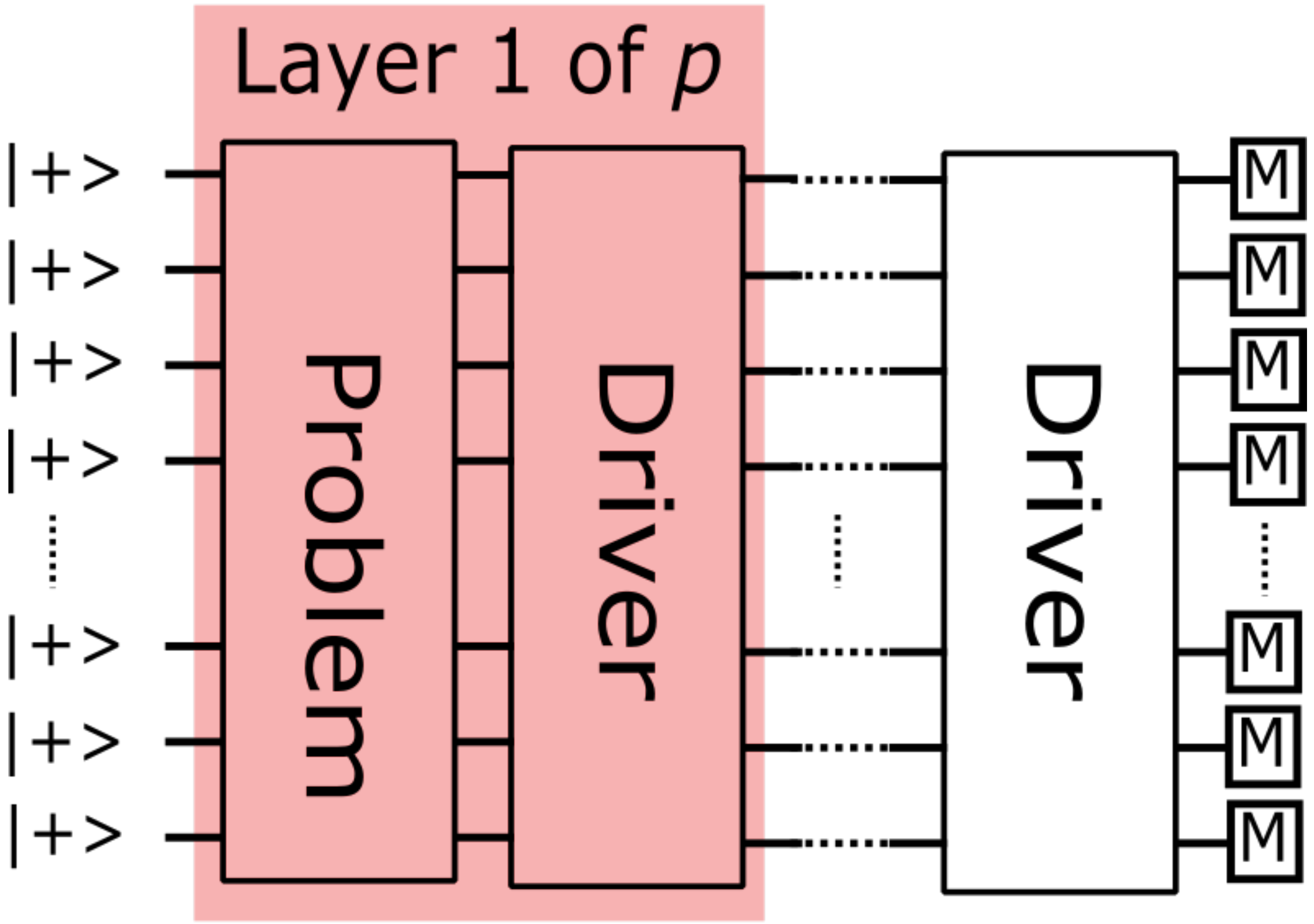
Approximating the quantum approximate optimization algorithm

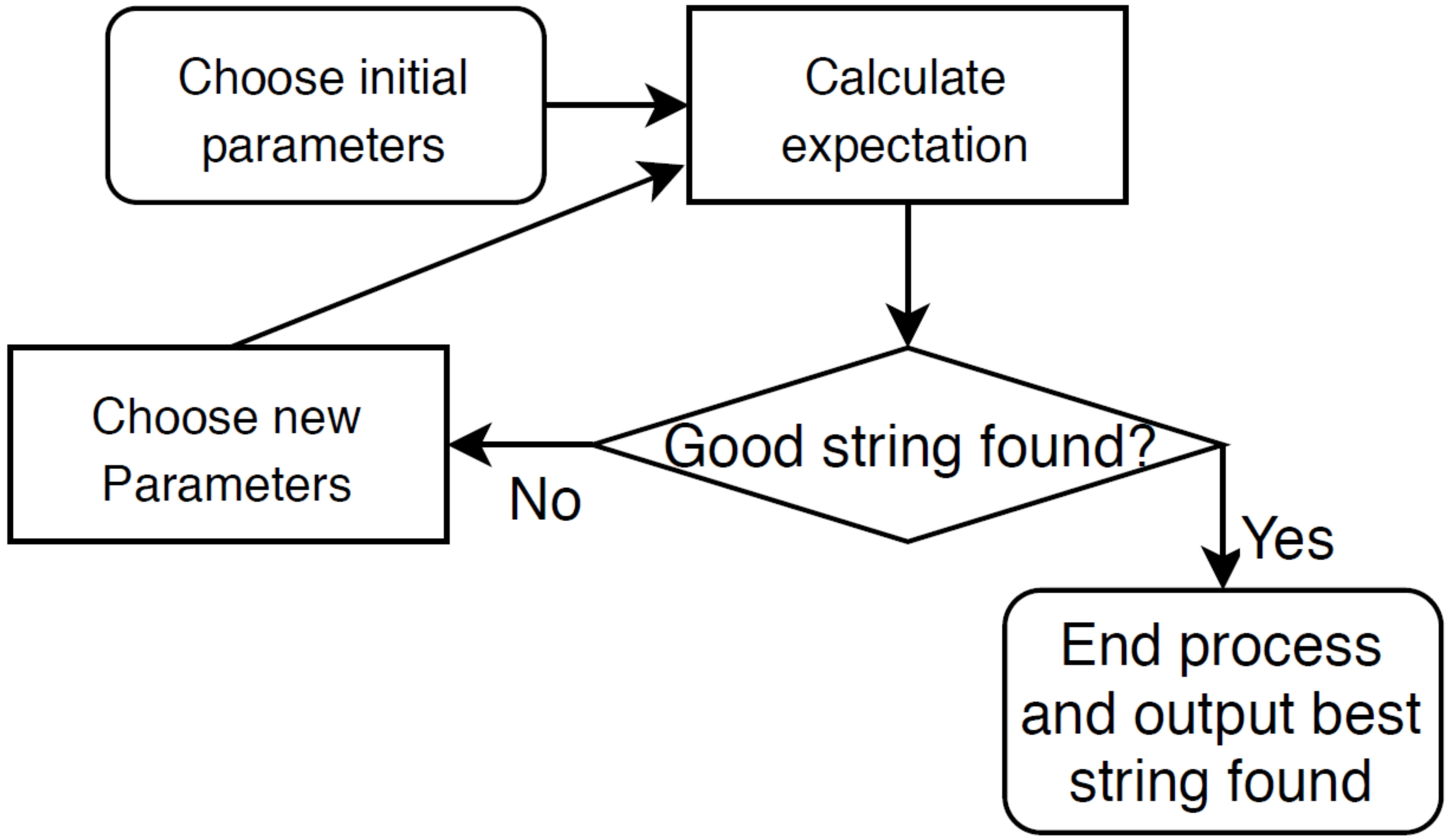
D. Headley, T. Müller, A. Martin, E. Solano, M. Sanz, FKW, arXiv:20002.12215

QAOA

$$\left|\vec{\beta},\vec{\gamma}\right\rangle = \prod_{p'=0}^{p} e^{i\beta_{p'} H_{\mathrm{D}}} e^{i\gamma_{p'} H_{\mathrm{P}}} \left|+\right\rangle^{\otimes n}$$

- A hybrid quantum classical variational algorithm
- Apply driver and problem Hamiltonian for time set by variational parameter
- Classical optimiser finds best parameters using expectation of problem
- Trotterized adiabatic quantum computing





Avoiding controls

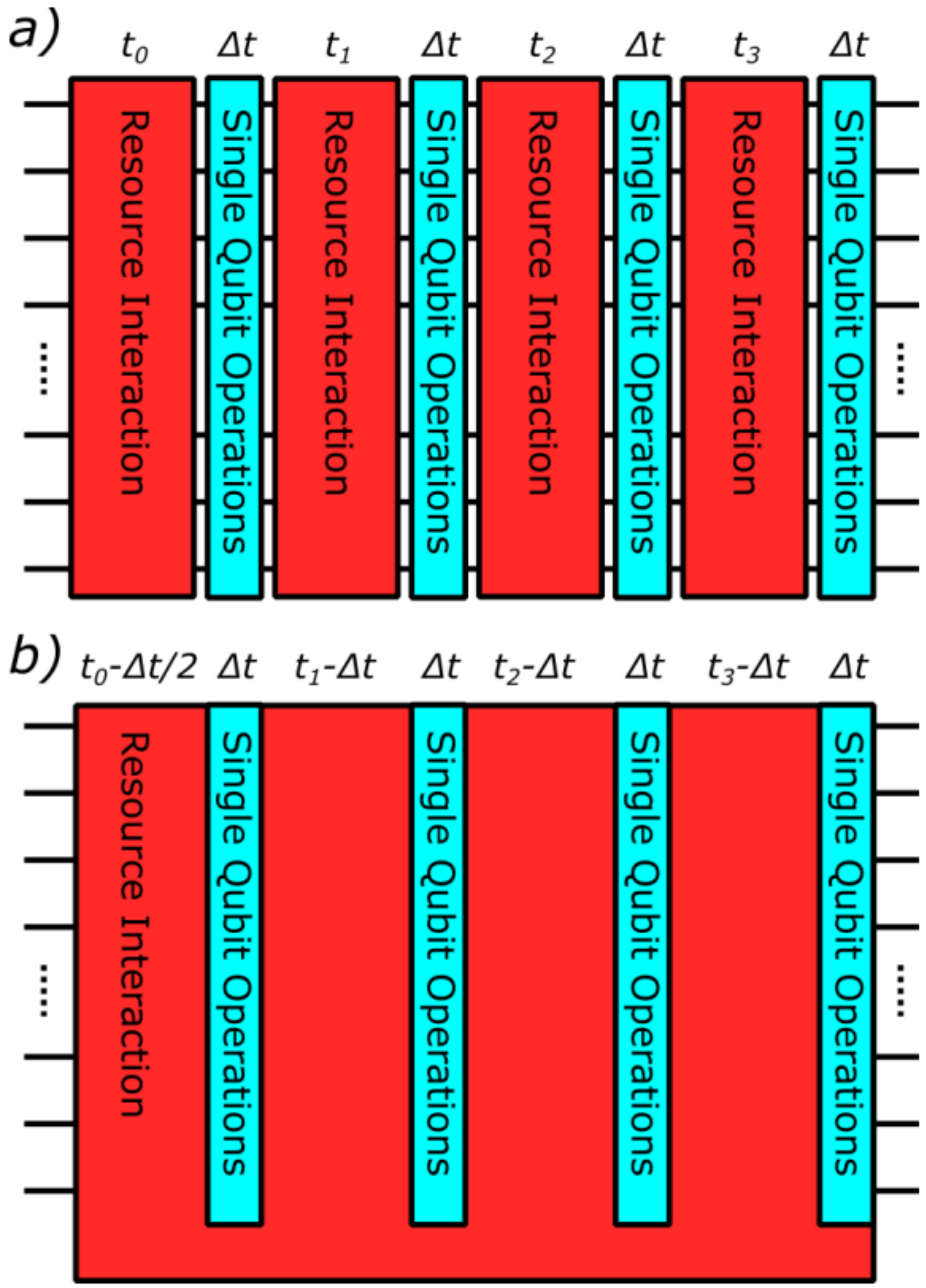
First step: Keep problem Hamiltonian static

- Time application of H_p through waiting times

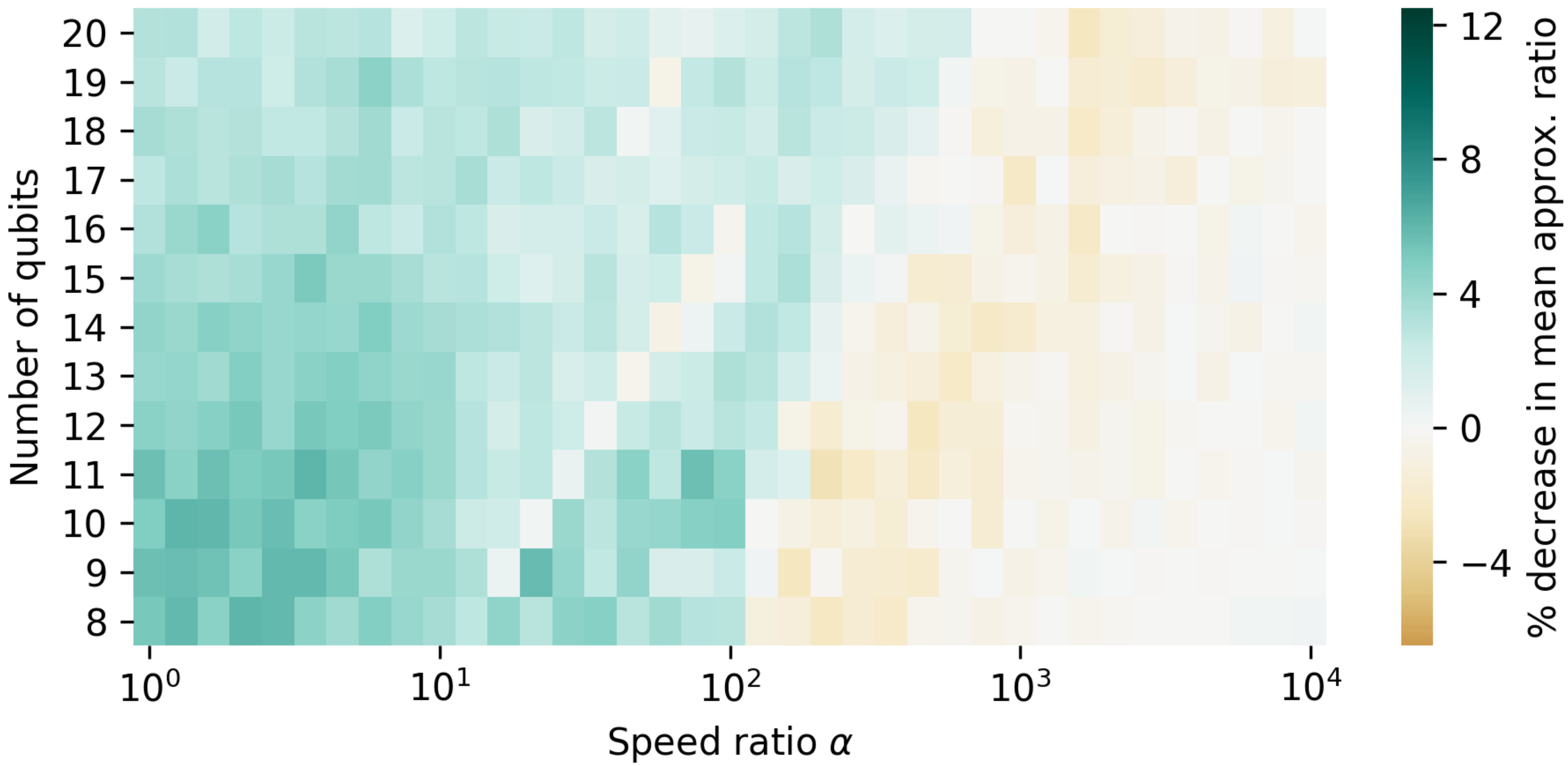
- Error during single-qubit application depends on speed ratio $\alpha = \frac{J}{\omega_r}$

- Error of simultaneous application $\simeq N^2\alpha^2$

- Too pessimistic

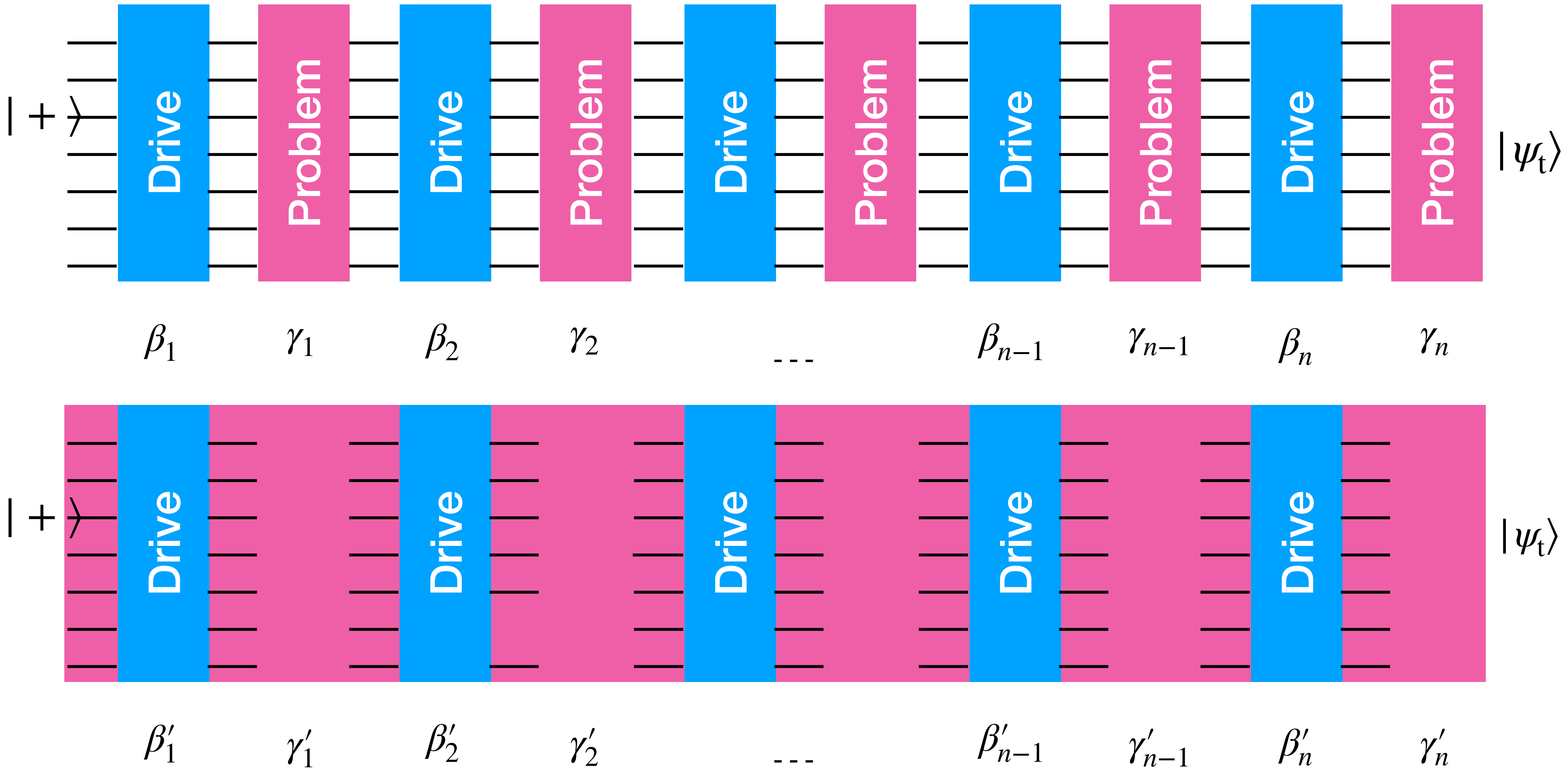


Numerical simulation



Extensive numerical simulation: Really good performance up to critical speed ratio

Variation to the rescue



- We do not need to get the same state based on the same β_i, γ_i
- We need to sample the state of possible solutions the same way
- Variational algorithm can adjust parameters to correct erors

Avoiding even more controls

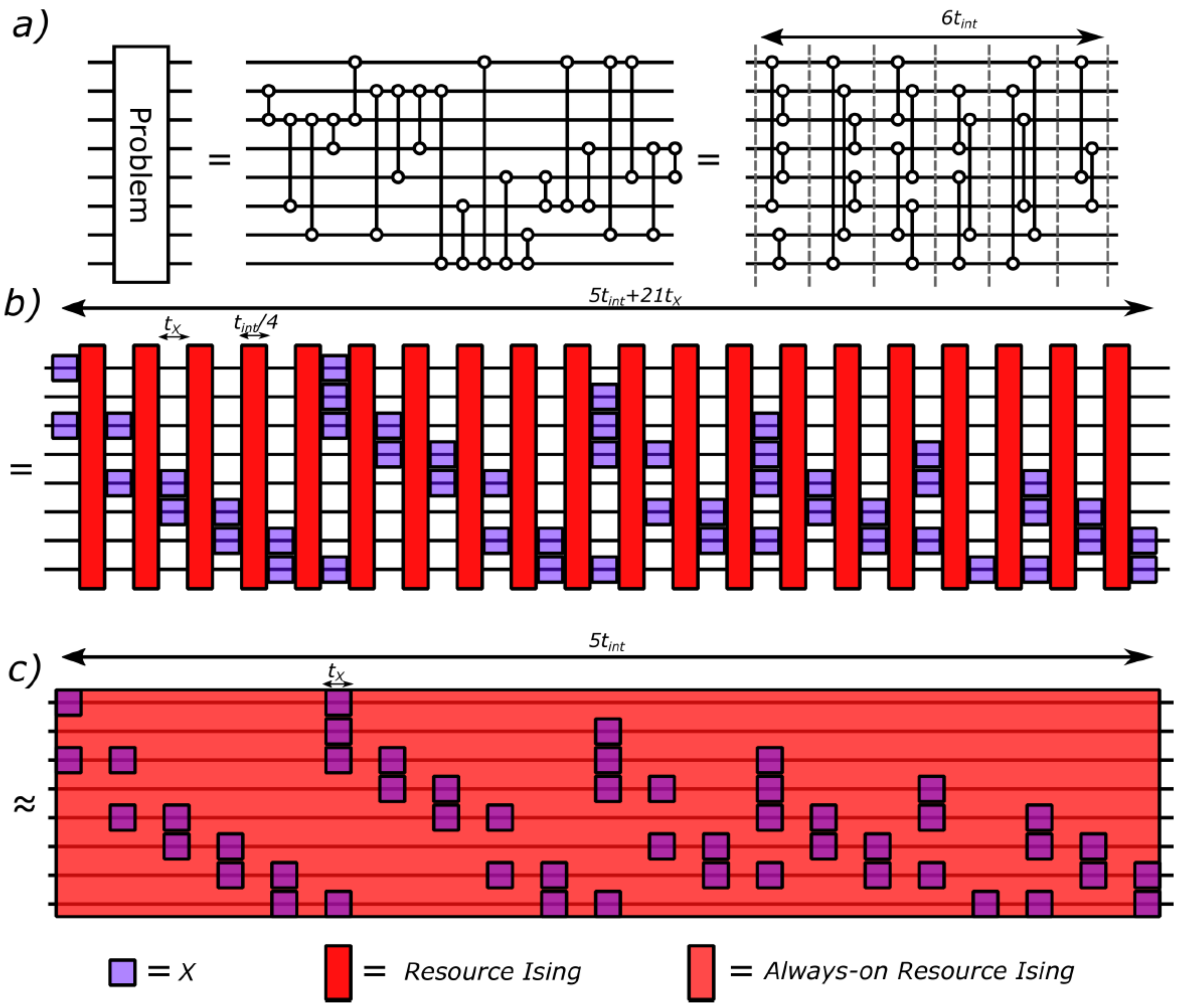
- So far: Needed to preset problem Hamiltonian, but avoid dynamic control — Hardware can work with d-wave style static preset
- Now: work with a single resource Hamiltonian
- All-to-all connectivity
- Use conjugation with X-gates to switch off unwanted interactions
- Finding the right pattern of X-gates is a polynomial matrix inversion problem

$$H_{\text{Resource}} = \sum_{j<k}^{n} r_{jk} Z_j Z_k$$

$$H_p = \left(\sum_{i,j} a_i a_j X_i X_j \right) H_{\text{Resource}} \left(\sum_{i,j} a_i a_j X_i X_j \right)$$

Compiling DA-QAOA

- Can take a QAOA problem Hamiltonian and express in DA-scheme
- Here is a 5-regular random MAX-CUT problem on 8 qubits



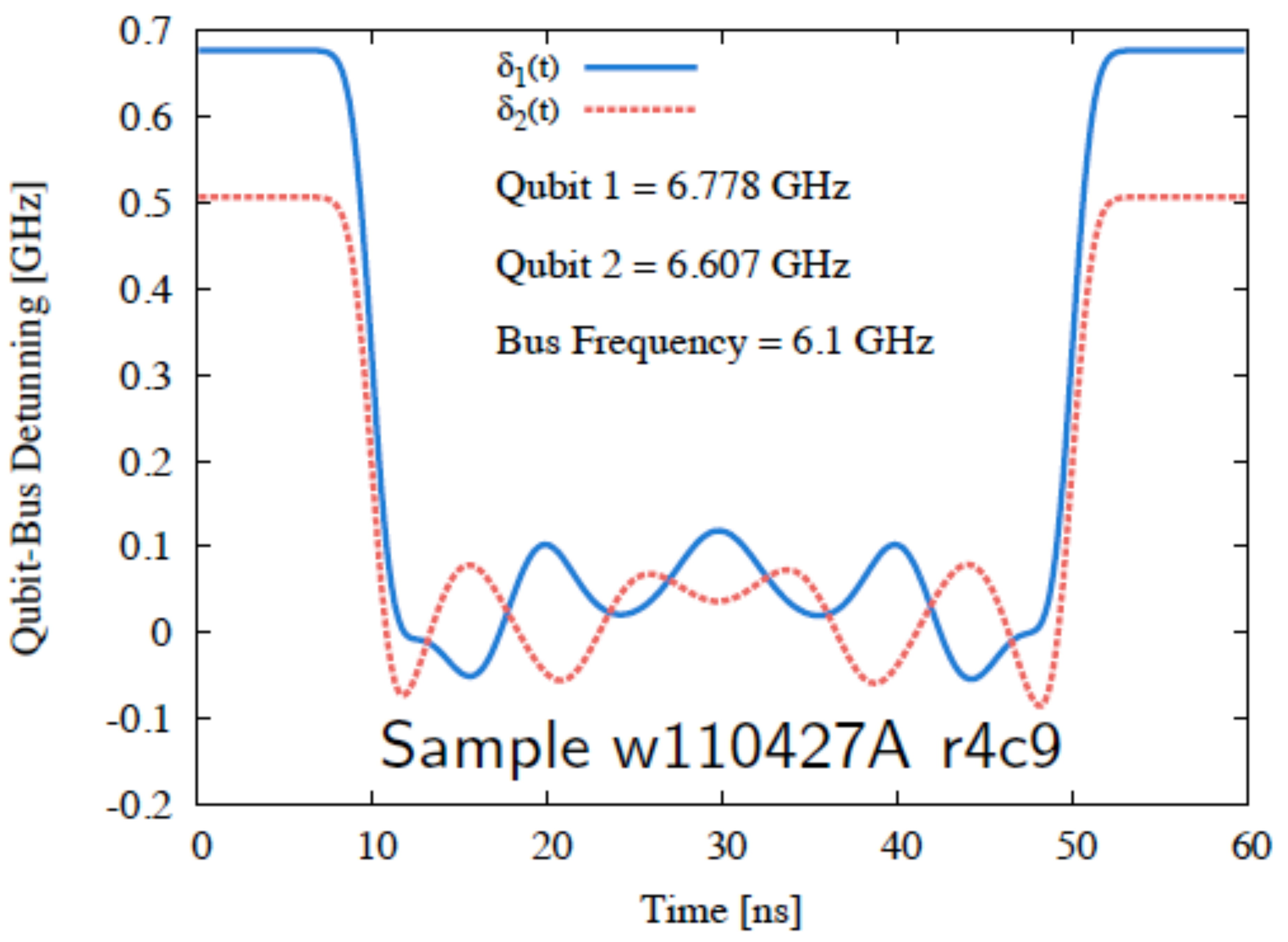
Lower error rates
And variational aspects

Pulse shaping control

Find out how to make a gate on given hardware

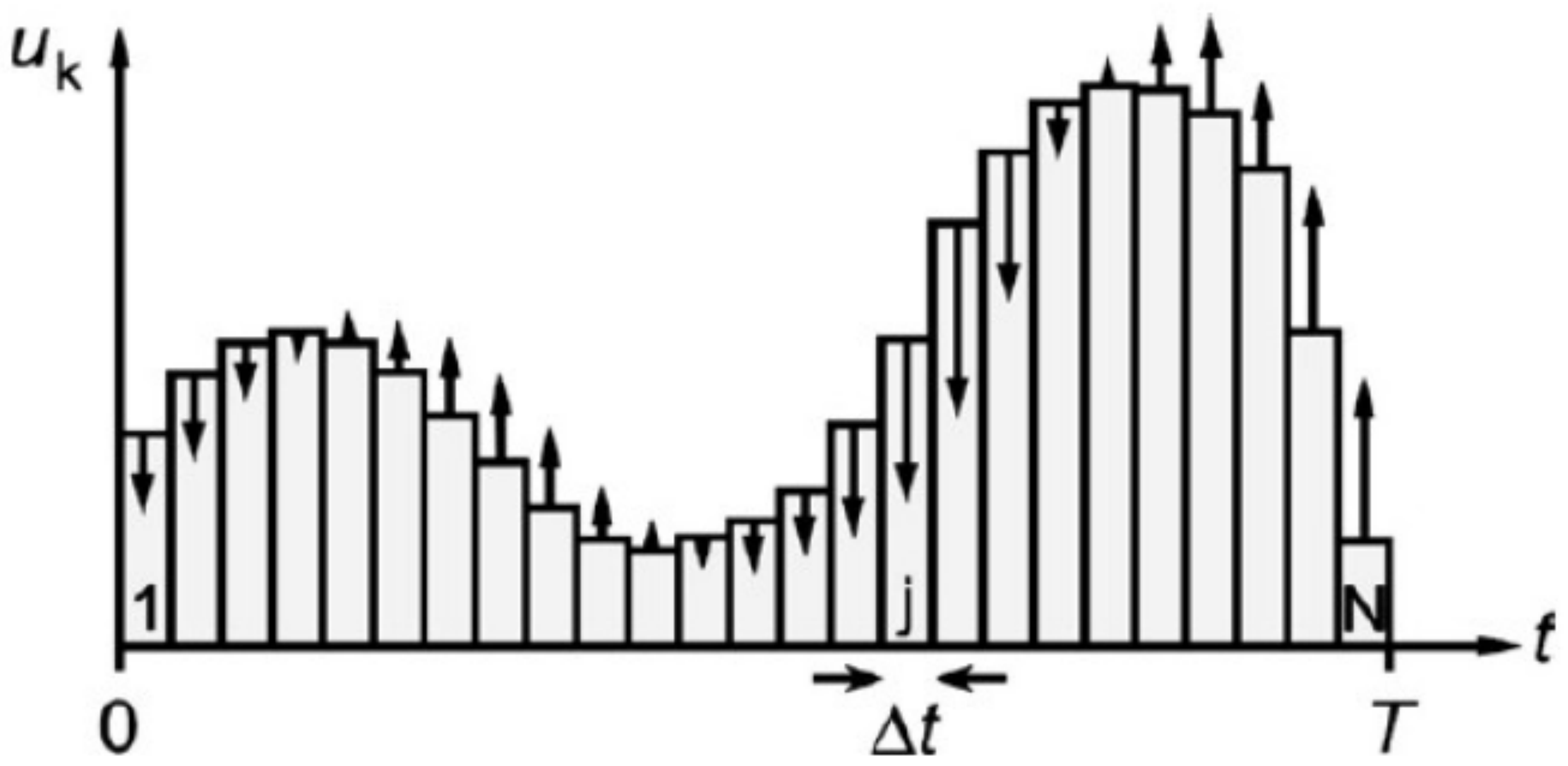
$$\hat{H} = \hat{H}_0 + \sum_i u_i(t)\hat{H}_i$$

H_0: Drift, u_i: Control fields,
H_i: Control Hamiltonians



Find $u_i(t)$ to reach

$$\hat{U}(t_f) = \mathbb{T}\exp\left(-\frac{i}{\hbar}\int_0^{t_f} d\tau\ \hat{H}(\tau)\right)$$



with search based on analytical gradients

How to debug something complex, non-intuitive?

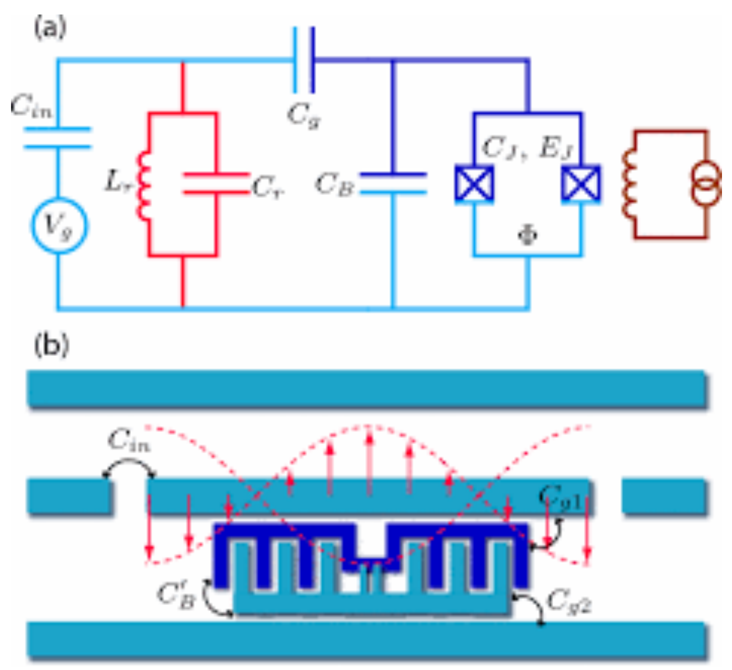
S.J. Glaser et al., EPJ D 2015

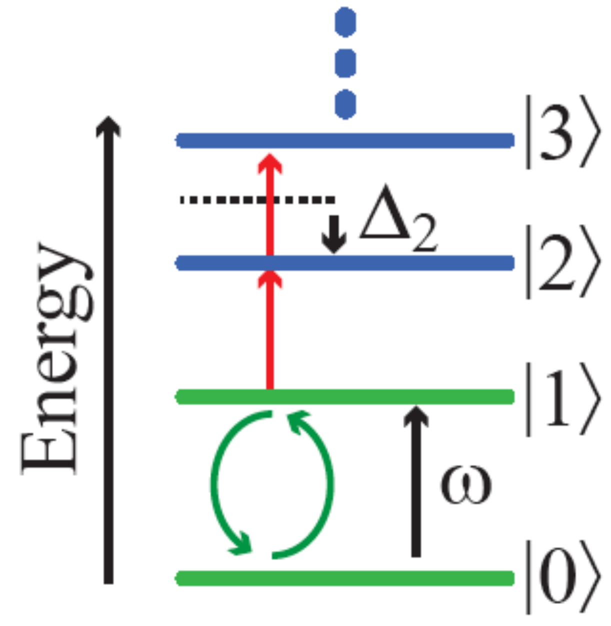
D.J. Egger and FKW, SUST 2014

Find controls that maximize fidelity

DRAG - pulse-shaping

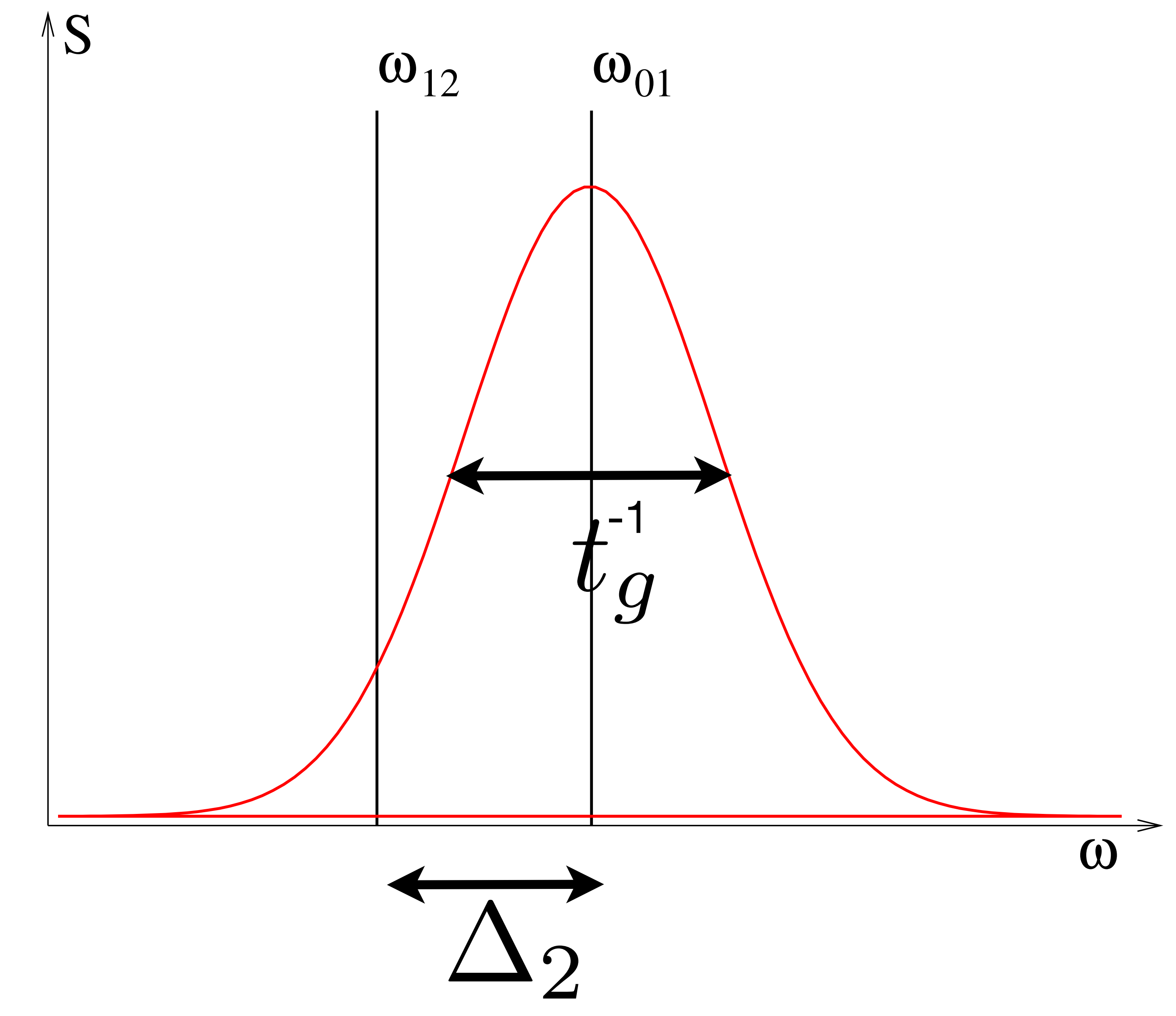
Bandwidth limitations from higher levels





Drive between 0 and 1

Spectral limitation:
Duration/bandwith uncertainty



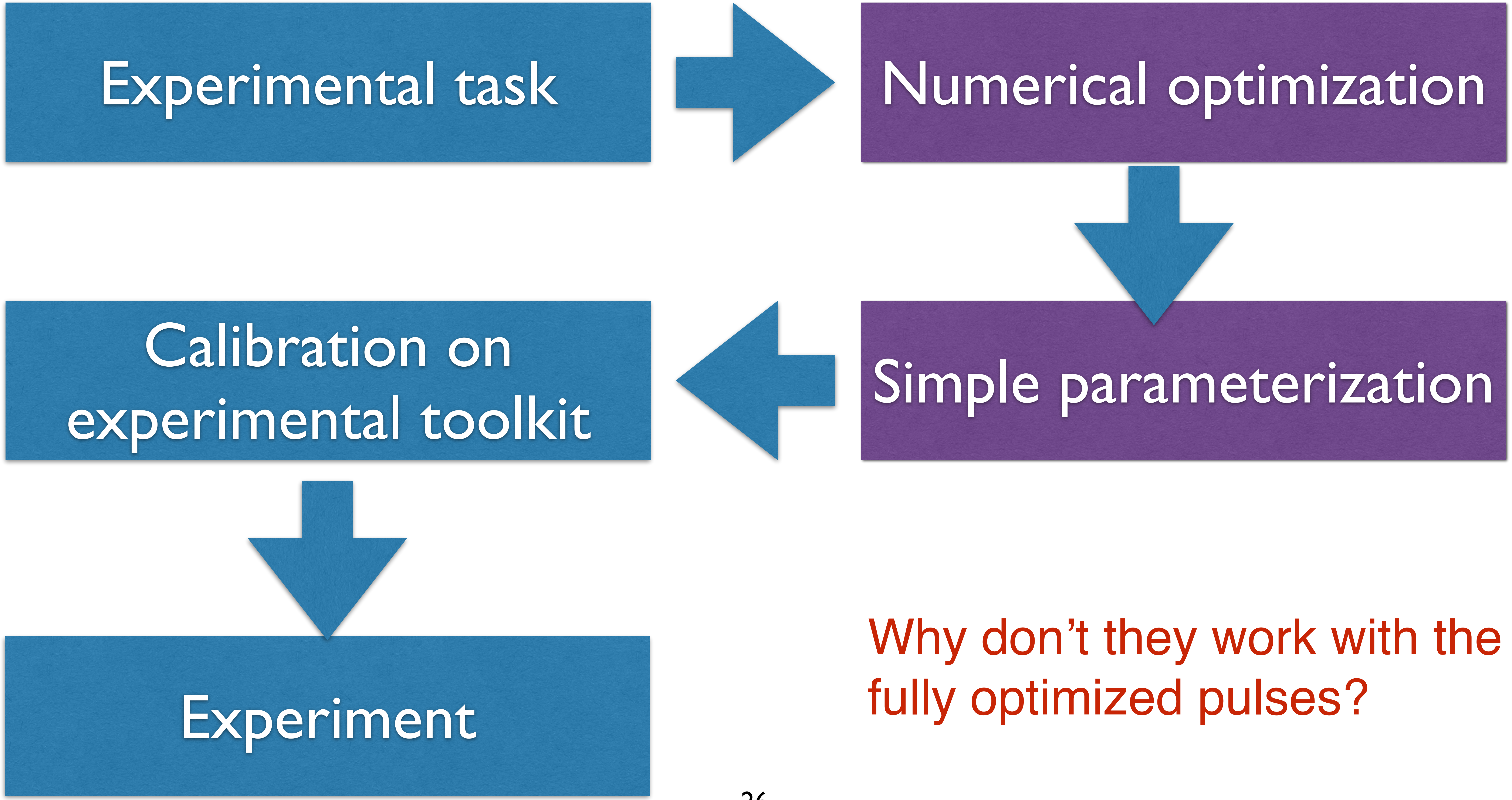
$$u_1(t)\cos\omega t + u_2(t)\sin\omega t$$

$$u_2 = \frac{\dot{u}_1}{\Delta_2}$$

Simple parameterization of numerical result:
Implementable pulse

DRAG: Motzoi et al., PRL 2009

Few-Parameter Workflow



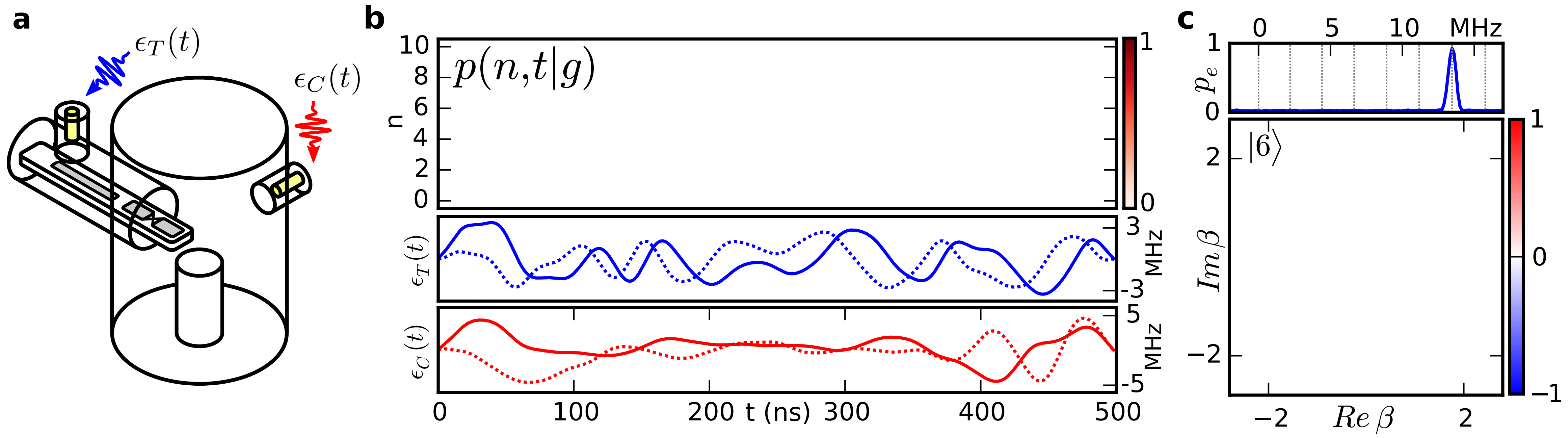
Why don’t they work with the fully optimized pulses?

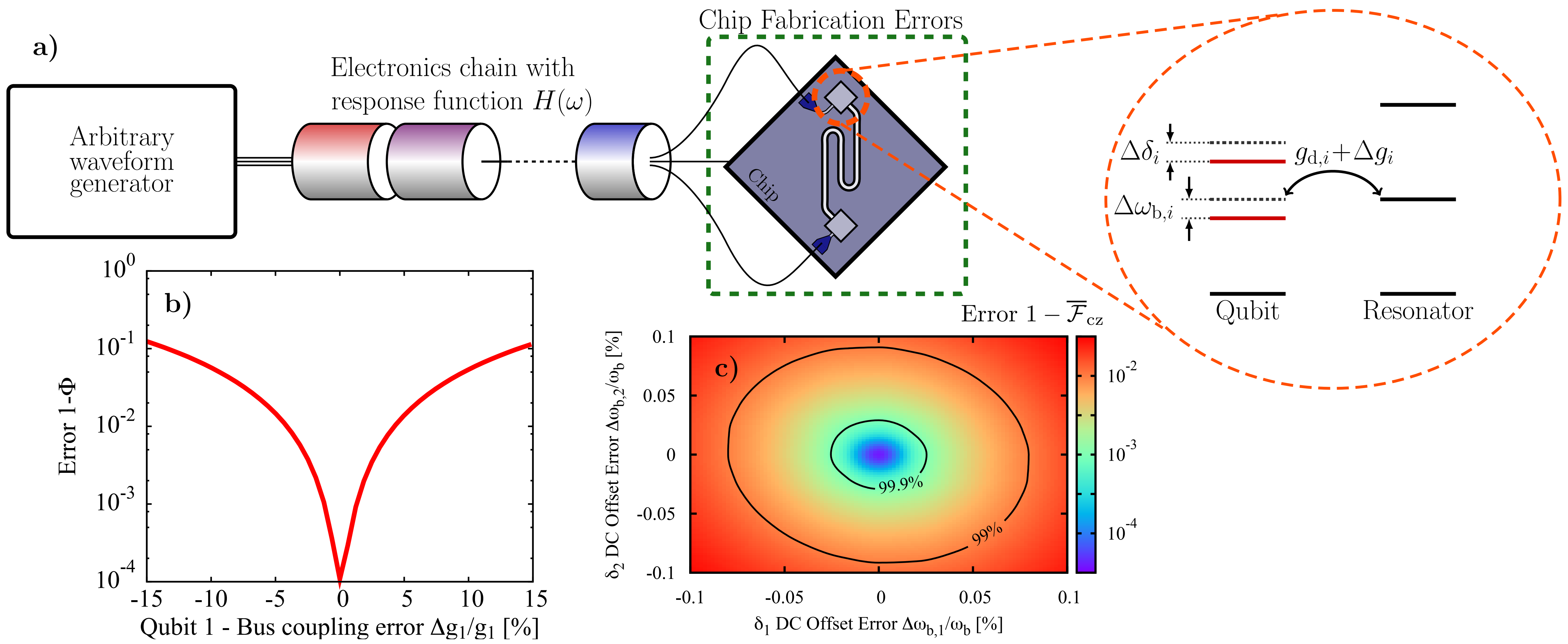
Tuneup challenge

- Fabrication uncertainty
- Transfer function uncertainty
- Best detector: The qubit itself
- One solution: Be like the other fields (Heeres et al., 2016): Extreme precision at limited bandwidth (not exploring all of OC potential)

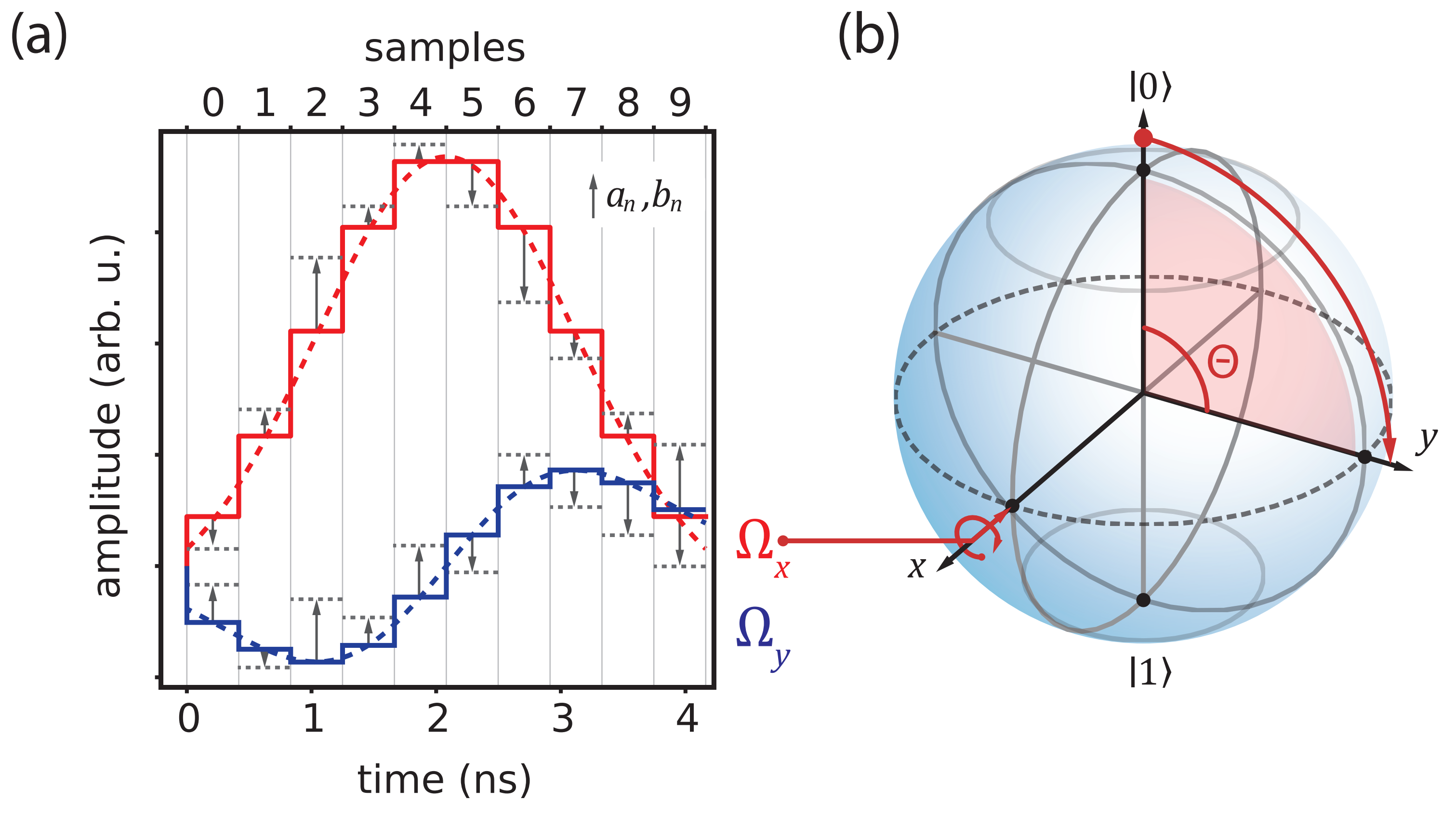
$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{junk}} + \sum_i u_i(t)\left(\hat{H}_i + \hat{H}_{i,\text{junk}}\right)$$

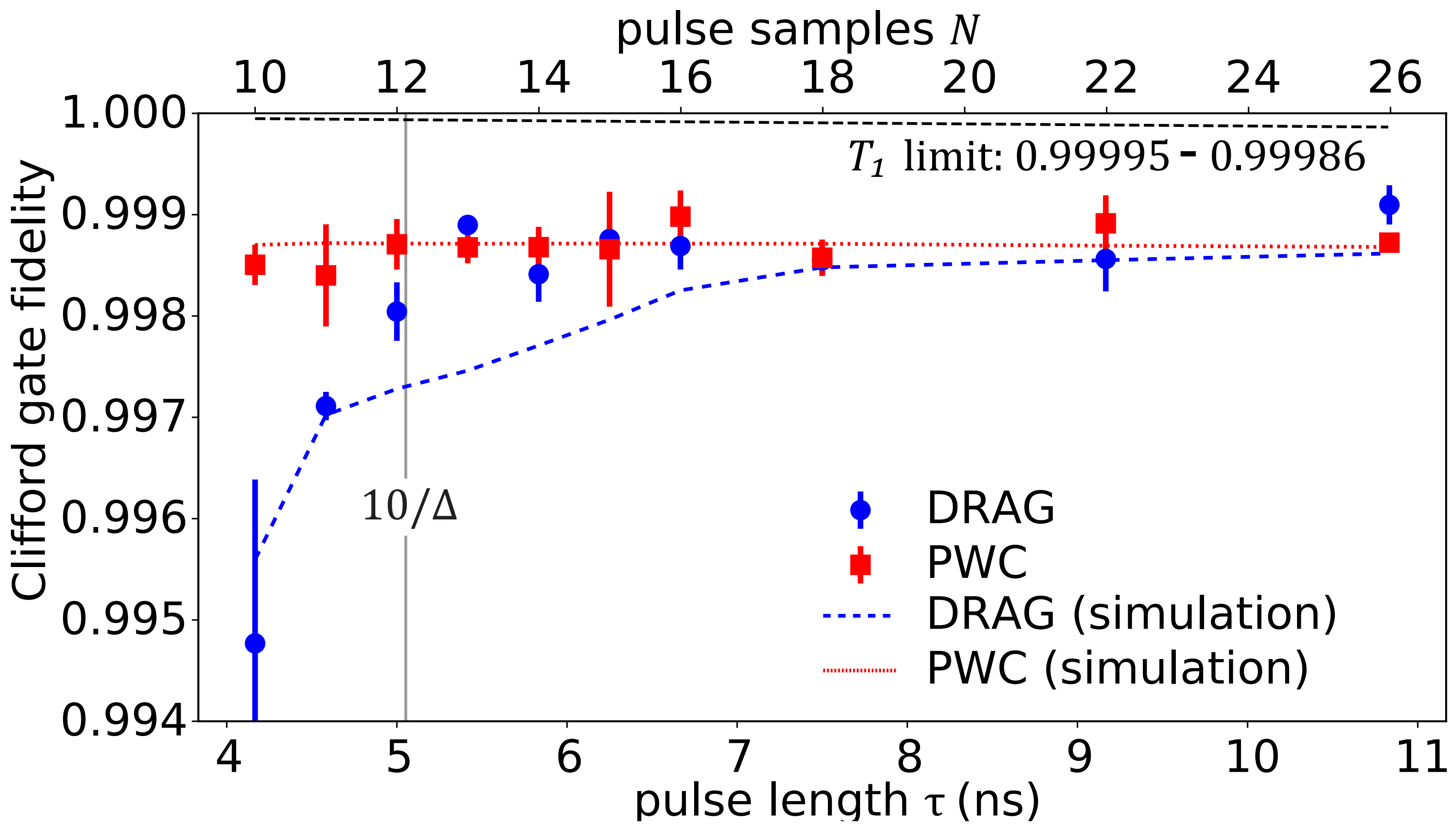
Unwanted degrees of freedom: i) non-computational energy levels ii) spurious DOFs [Markovian decoherence usually beaten by speed]

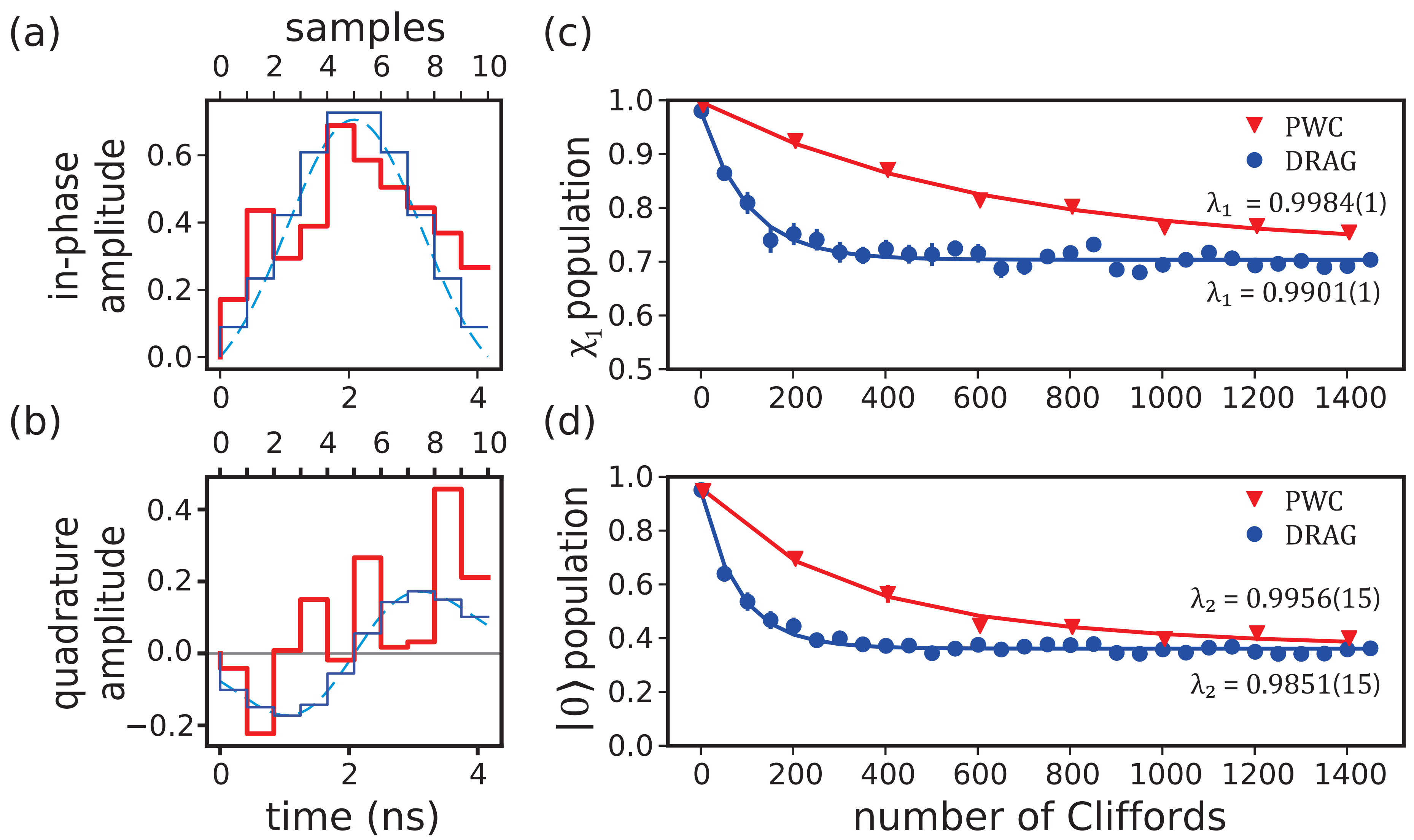




The breakthrough





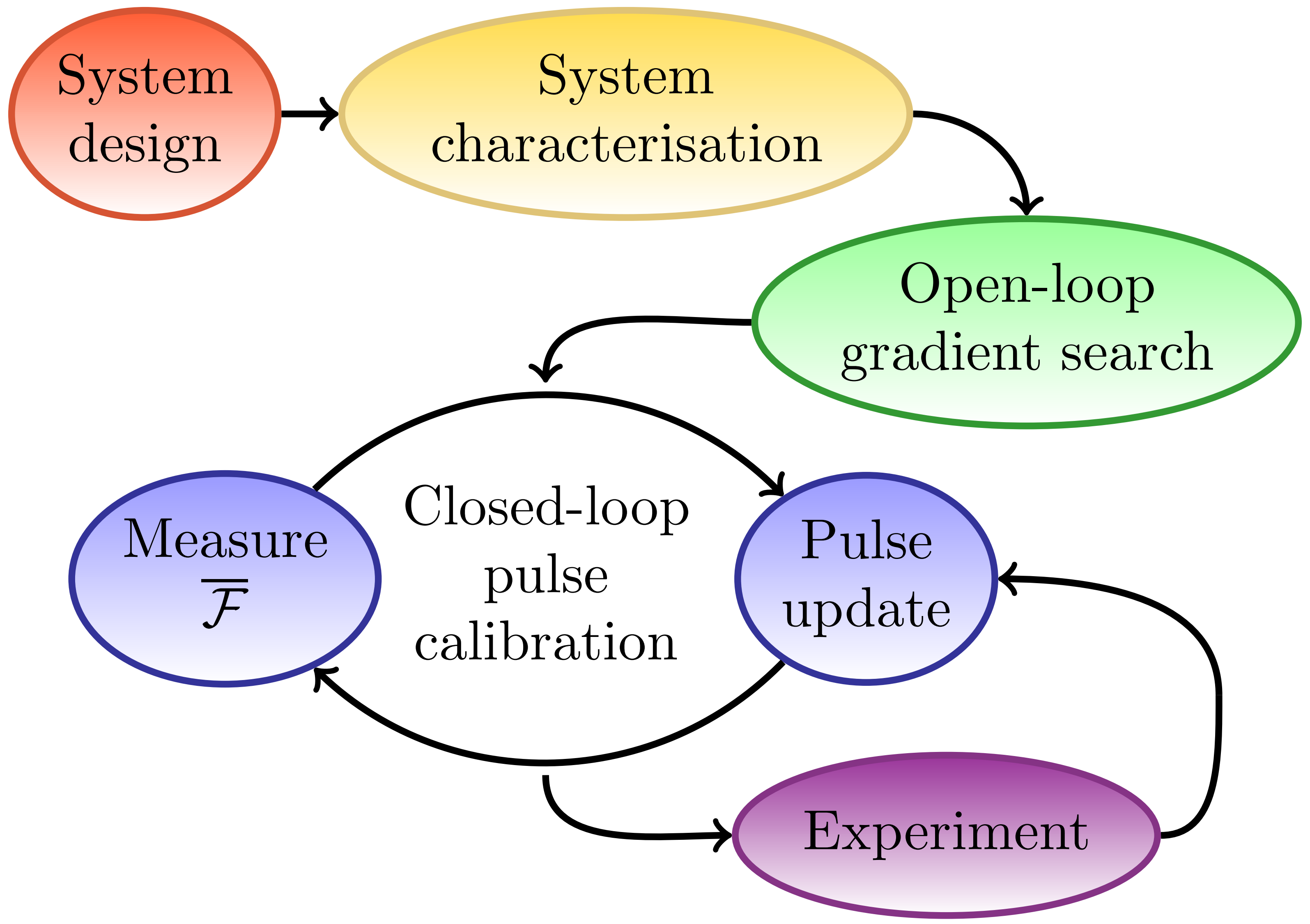


- trace out quantum speed limit
- 7-fold reduction of error
- strong deviation from DRAG

M. Werninghaus, D.J. Egger, F. Roy, S. Machnes, FKW, and S. Fillip 2020

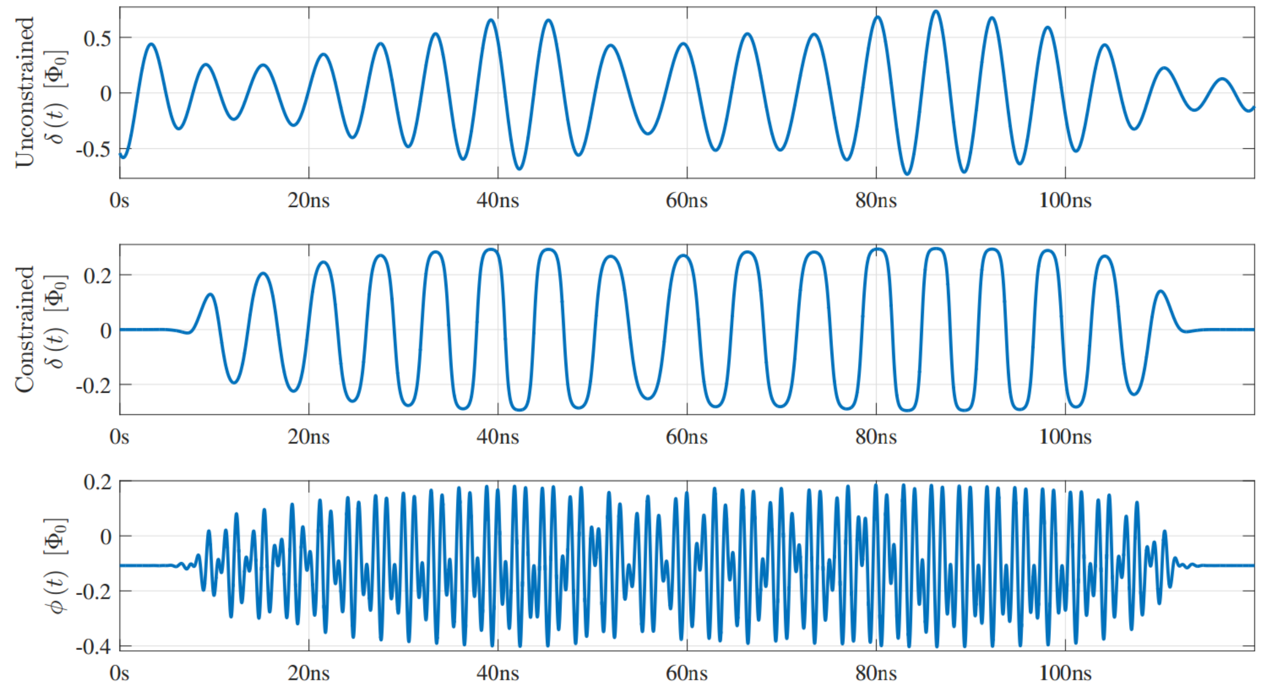
Ingredients

Closing the loop



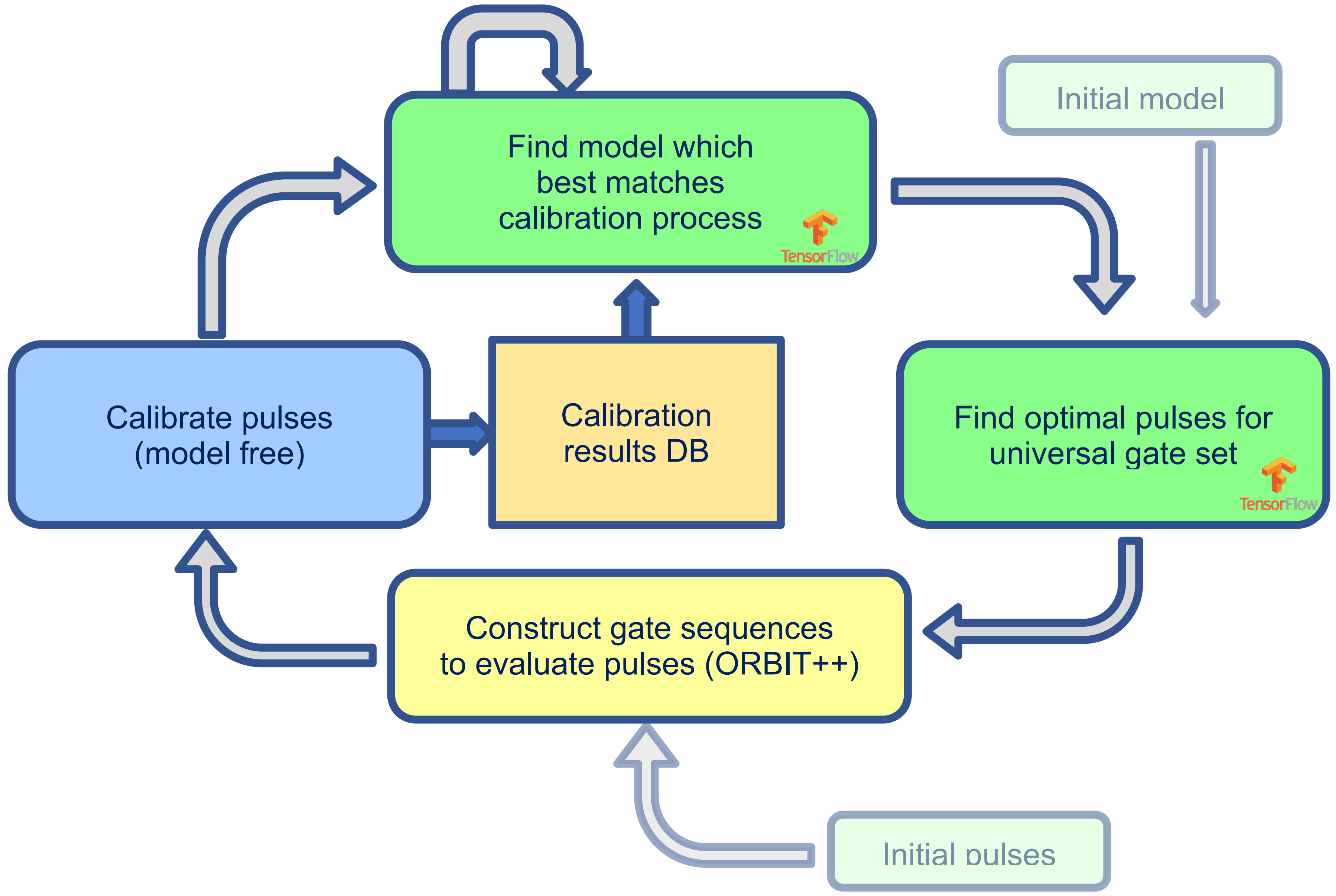
D.J. Egger and FKW, PRL 2014

Gradient search on simple Ansatz



S. Machnes, E. Assemat, D. Tannor, FKW, 2018
S.Kirchhoff, T. Keßler, P.J. Liebermann, E. Assémat, S. Machnes, F. Motzoi, FKW, 2018

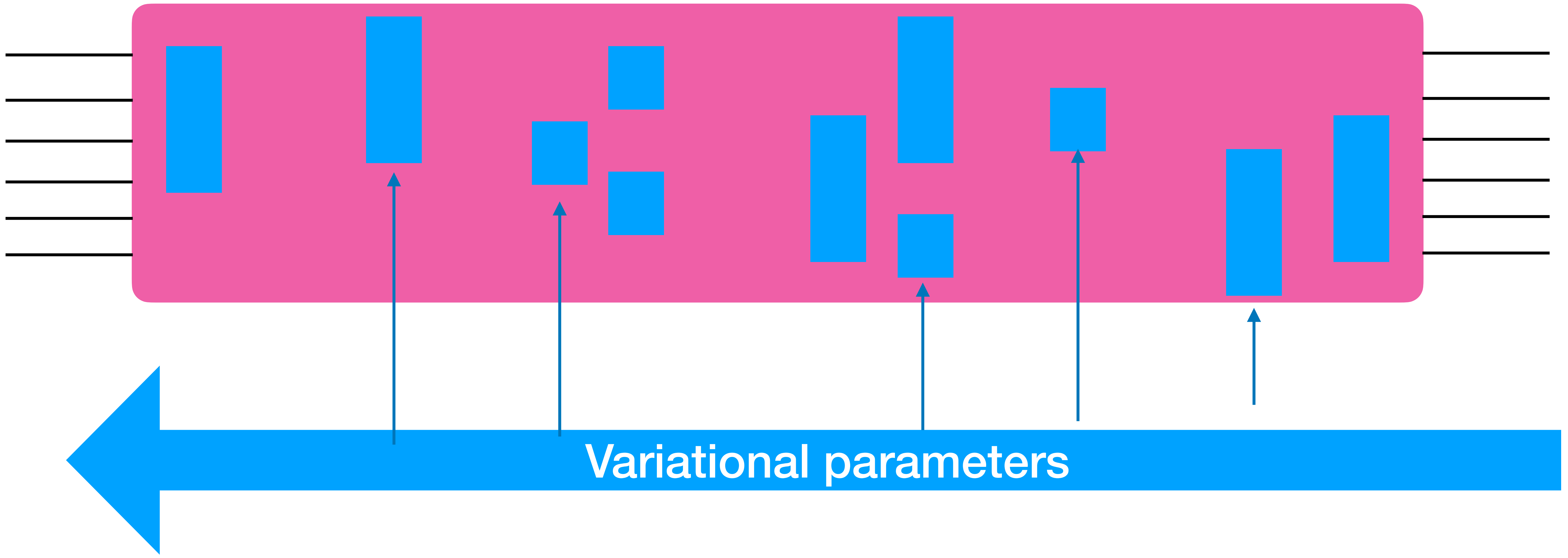
Model identification with AI
(C3 - Combined Control and Characterization)



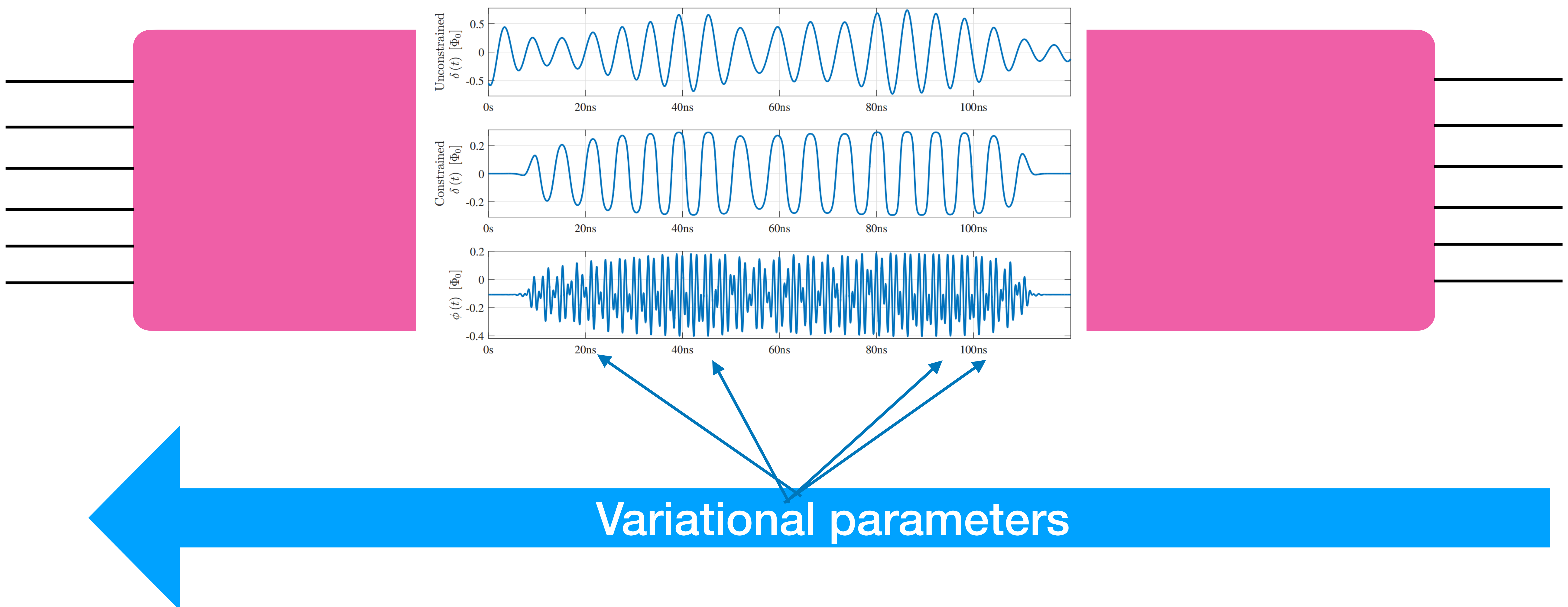
S. Machnes, N. Wittler, F. Roy, K. Pack, A.S. Roy, M. Werninghaus, D.J. Egger, S. Filipp, FKW
in preparation

Programming a variational quantum processor

Many ways to write an algorithm



Gate-based algorithm
Universal gate set
Tuneup of gates
Deal with junk DOFs



Optimal control
Controllability
Analogue programming
Reduce controls

Statements for discussion

- Disruptive programming for quantum computers closely integrates software on and for quantum computers
- Adiabatic quantum computing, gate model, and quantum controls are three initial programming paradigms motivated by physics, computer science, and chemistry
- We have not found the best paradigm to program quantum computers yet
- Co-Design of algorithms and hardware continues to be necessary - you are missing out be being all-purpose