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Finding quantum controls efficiently

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Finding quantum controls efficiently

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Quantum control theory: control theory applied to quantum systems

- Spins, atoms, molecules, etc

Why control quantum systems?

- Chemical reaction control, development of quantum computers, sensors, simulators, etc

How can we do it?

- Need external controls that can interact with quantum systems on their native length/time scales
    - Tailored laser fields

Finding quantum controls efficiently

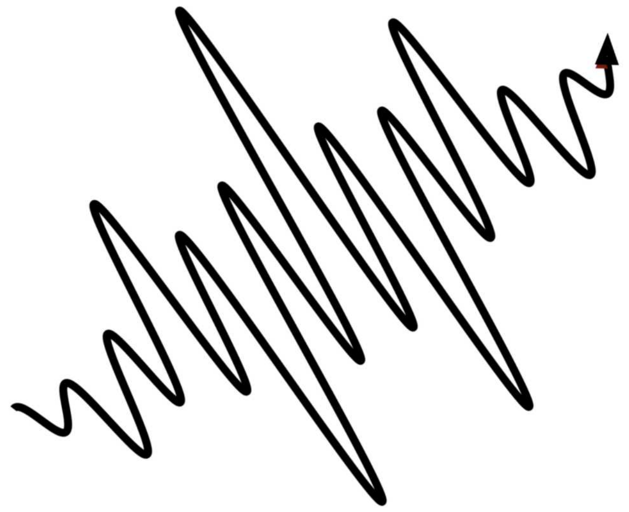
How can we find laser fields that achieve a desired control objective in a quantum system?

- Quantum optimal control (1980s)
  - Seek field that minimizes a control objective functional using iterative optimization
  - Promising experimental demonstrations starting late 1990s

Assion *et. al*., Science **282** (1998).
Vogt *et. al*., Phys. Rev. Lett. **94** (2005).

Why haven't optimally shaped laser fields become a widely used tool in chemistry (and chemical engineering)?

- A crucial issue is the lack of theoretical support
  - Simulations often prohibitively expensive due to:
    1. **Iterative field optimization procedure**
    2. **Exponential cost of simulating quantum systems**



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Part I:

➡ Review quantum tracking control, an iteration-free approach for quantum control simulations

➡ Illustrate its utility for identifying fields to control the orientation of molecules

Part II:

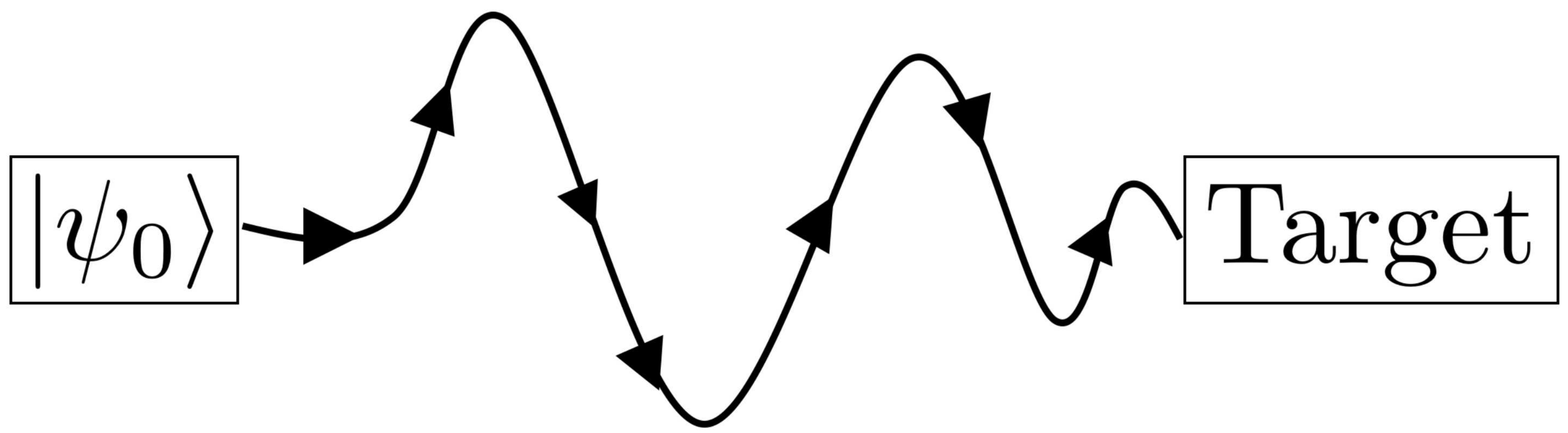
➡ Introduce digital quantum simulation as a polynomial-time approach for simulating controlled quantum systems

Part I:

Quantum tracking control of molecular orientation

Tracking control concept

Goal of tracking control:
- Specify a path in time for the observable
- Find field that drives system along this path



Approach:
- Invert observable dynamical equation to obtain expression for field $\varepsilon(t)$
- Plug in desired path for observable

$$\frac{d\langle O\rangle(t)}{dt} = i\Big\langle \big[H_0 - \mu\varepsilon(t), O\big] \Big\rangle(t) \quad \Rightarrow \quad \varepsilon(t) = \frac{i\frac{d\langle O\rangle_d(t)}{dt} + \big\langle [H_0, O] \big\rangle(t)}{\big\langle [\mu, O] \big\rangle(t)}$$

Advantages:
computationally attractive
(no iterative optimization)
entire time trajectory can be specified

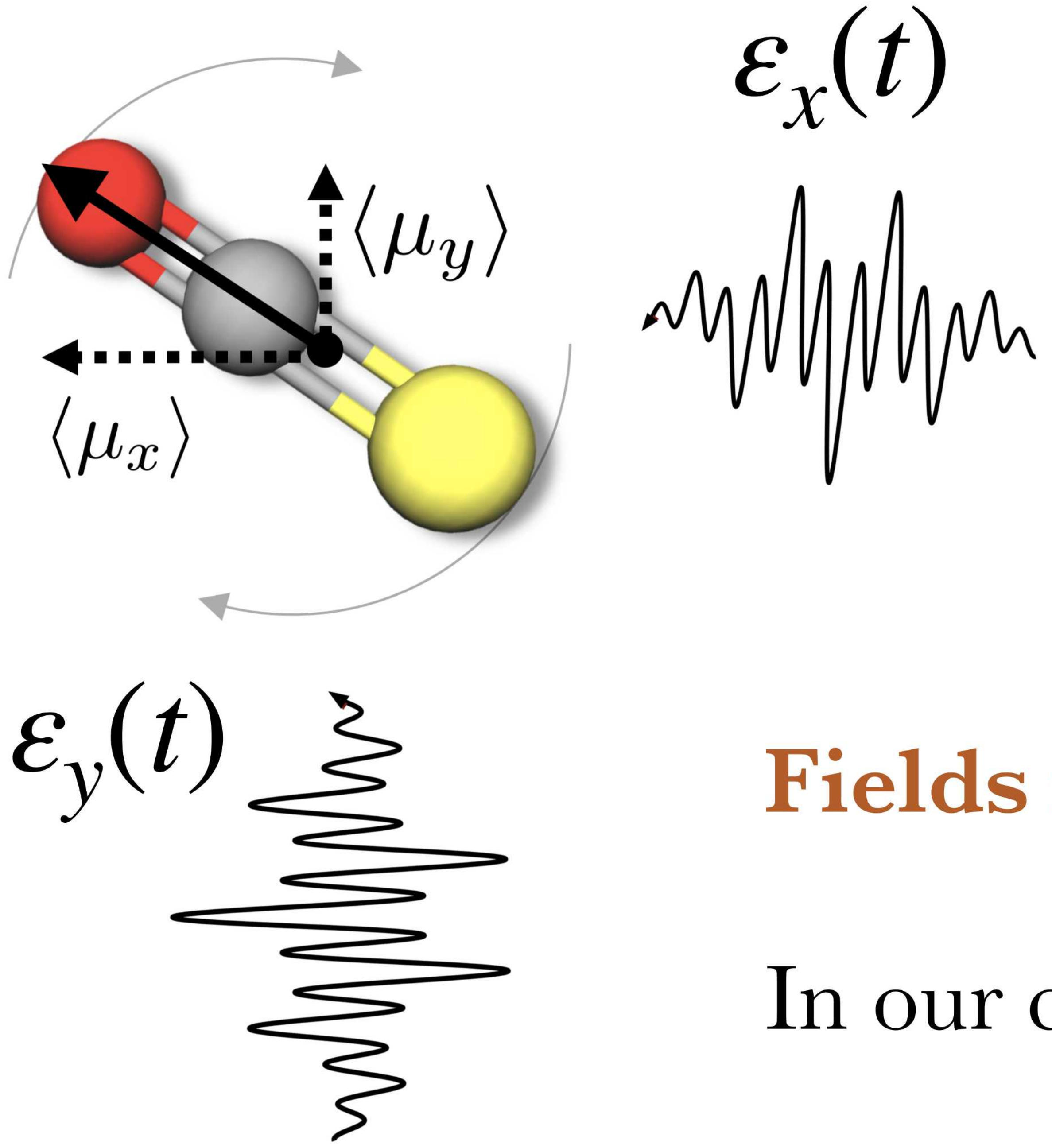
Disadvantages:
control fields can contain singularities

Application: molecular orientation

Goal:

Control the x and y orientations of a polar linear molecule rotating in a plane,

$\mu_x = \cos\varphi \qquad \mu_y = \sin\varphi$



We first write coupled dynamical equations for $\langle\mu_x\rangle(t)$ and $\langle\mu_y\rangle(t)$ in form $\mathbf{A}(t)\mathbf{E}(t) = \mathbf{b}(t)$, where $\mathbf{E}(t) = \left(\varepsilon_x(t),\ \varepsilon_y(t)\right)^T$

We then solve for the two fields: $\mathbf{E}(t) = \mathbf{A}(t)^{-1}\mathbf{b}(t)$

Fields free of singularities if $\det(\mathbf{A}(t))$ nonzero $\forall t$.

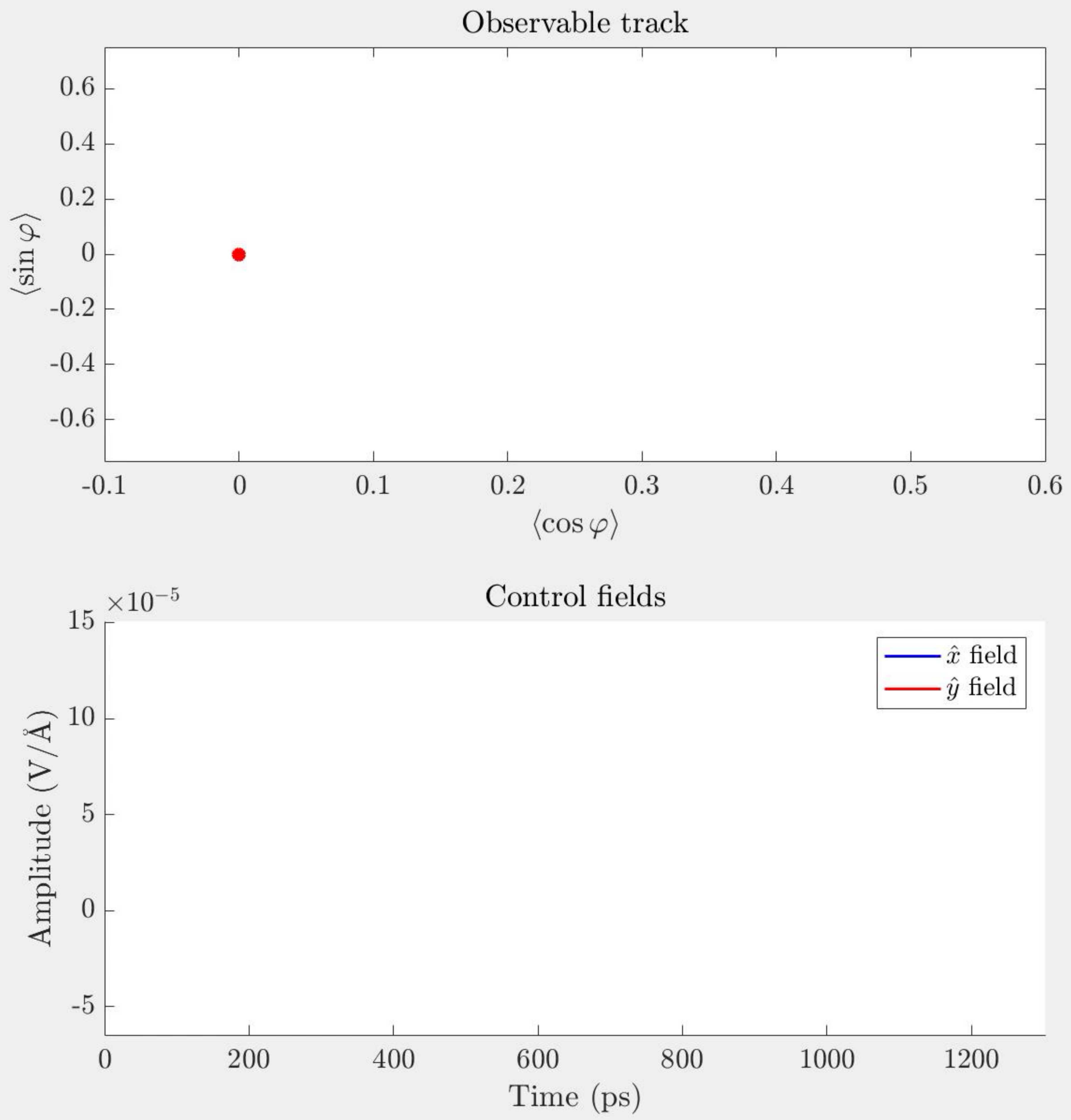
In our case, we have

$$\det\left(\mathbf{A}(t)\right) = \left(\langle\sin^2\varphi(t)\rangle\right)\left(\langle\cos^2\varphi(t)\rangle\right) - \left(\langle\sin\varphi\cos\varphi(t)\rangle\right)^2 \geq 0$$

Cauchy-Schwarz, $\langle a|a\rangle\langle b|b\rangle \geq |\langle a|b\rangle|^2$

Quantum tracking control of molecular orientation = singularity-free

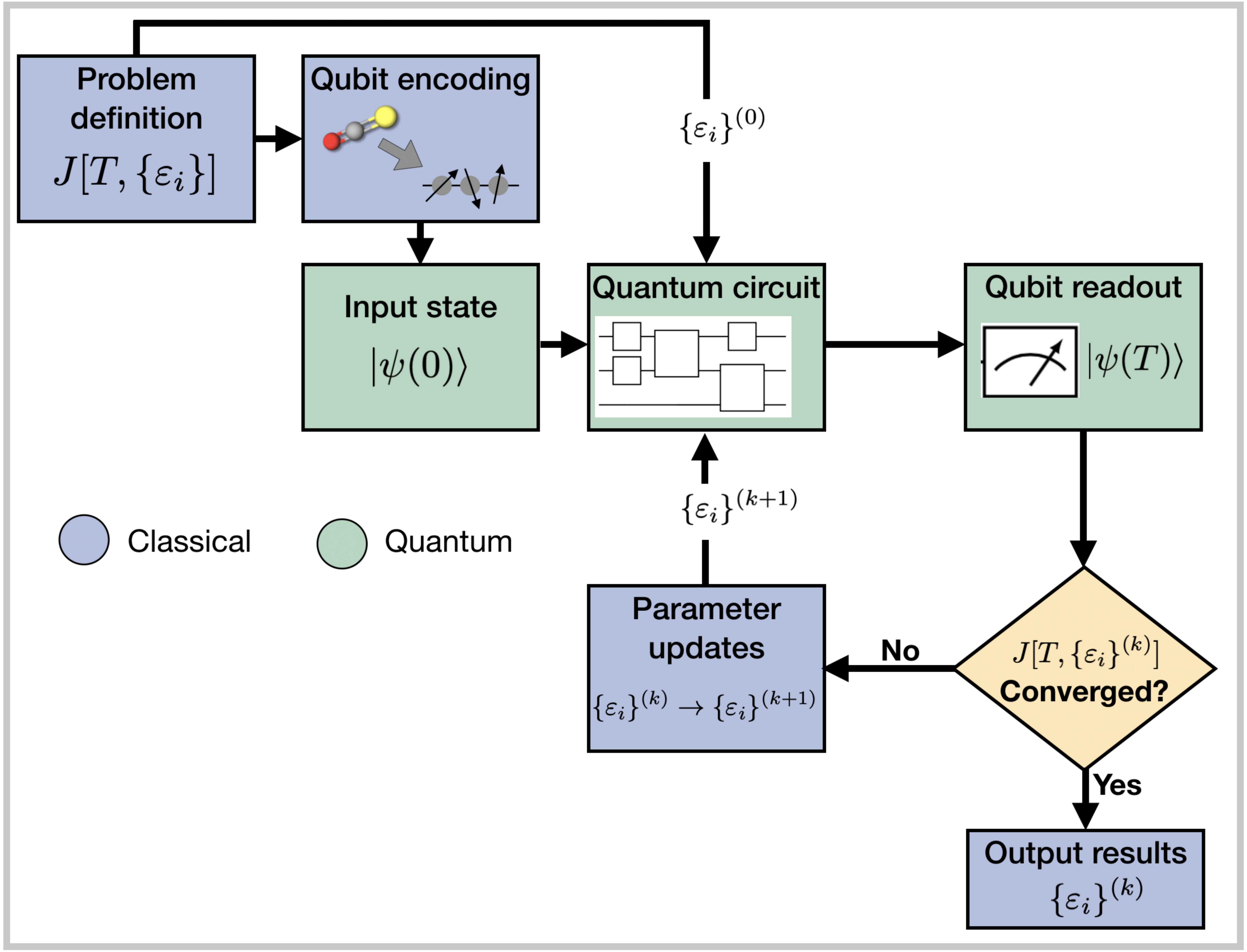
Numerical illustration



Part II:

Digital quantum simulation of quantum control

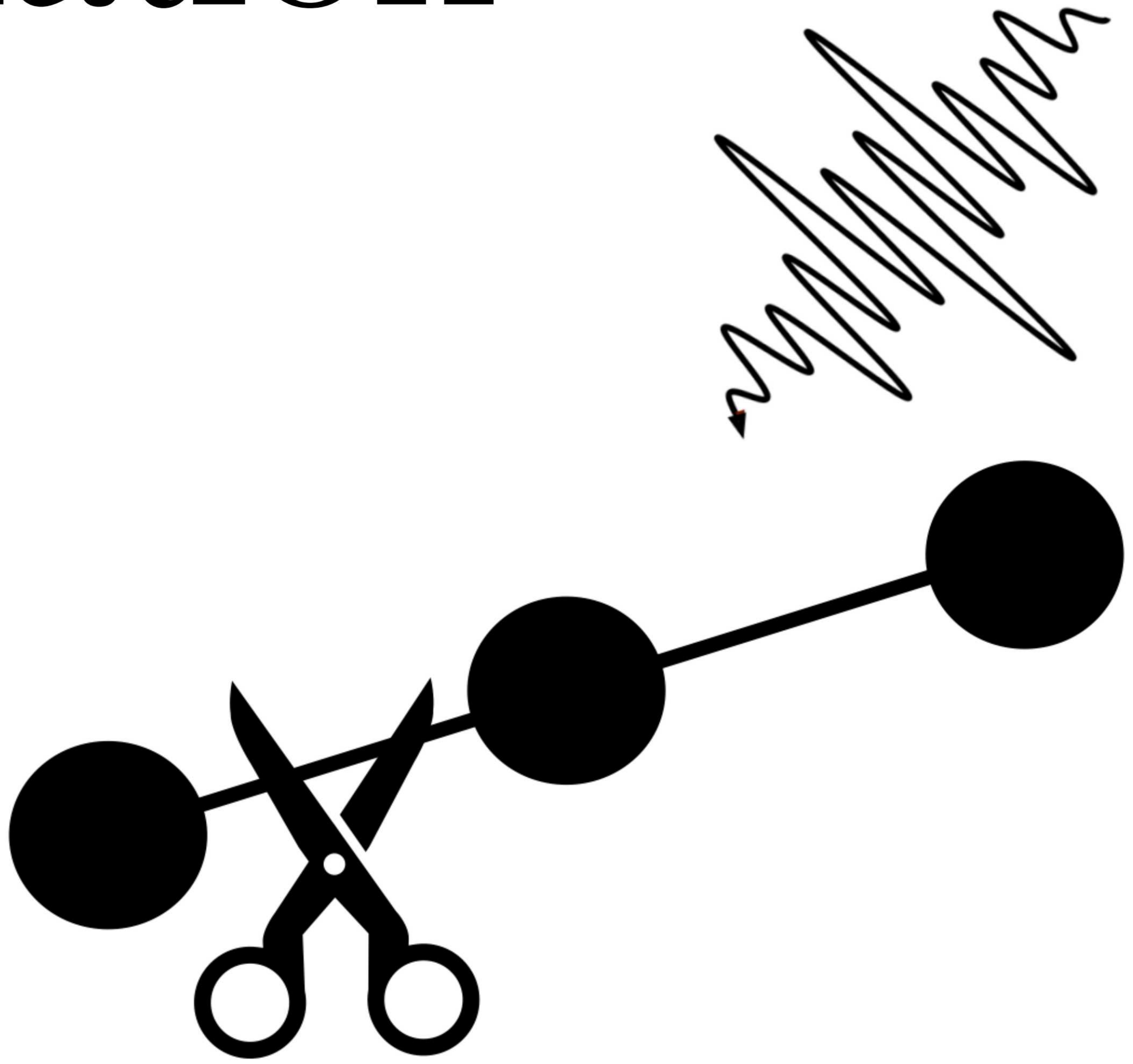
Concept

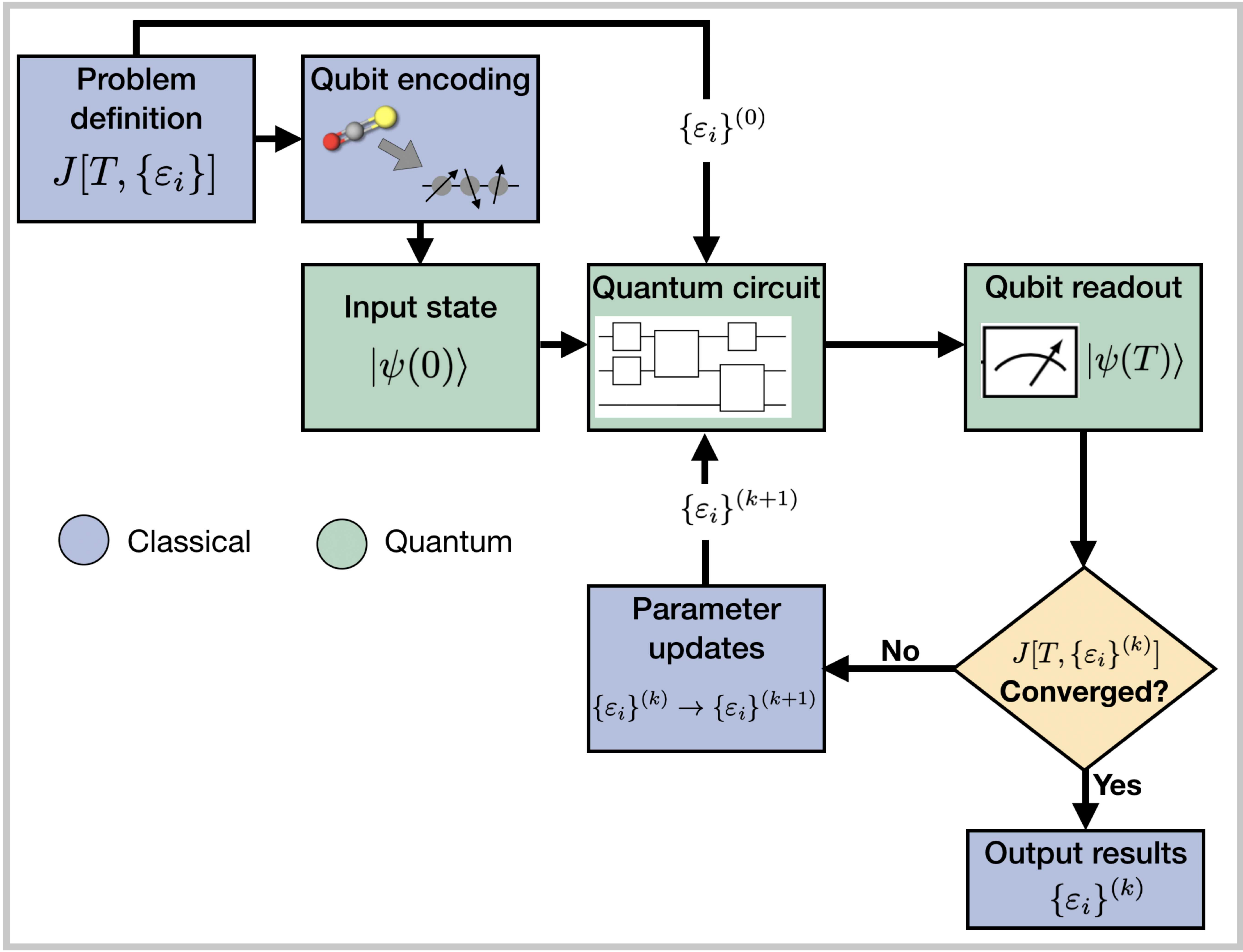


Problem definition
$J[T, \{\varepsilon_i\}]$
Qubit encoding
$\{\varepsilon_i\}^{(0)}$
Input state
$|\psi(0)\rangle$
Quantum circuit
Qubit readout
$|\psi(T)\rangle$
$\{\varepsilon_i\}^{(k+1)}$
Classical
Quantum
Parameter updates
$\{\varepsilon_i\}^{(k)} \to \{\varepsilon_i\}^{(k+1)}$
No
$J[T, \{\varepsilon_i\}^{(k)}]$
Converged?
Yes
Output results
$\{\varepsilon_i\}^{(k)}$

Application:

Control of selective dissociation in triatomic molecule

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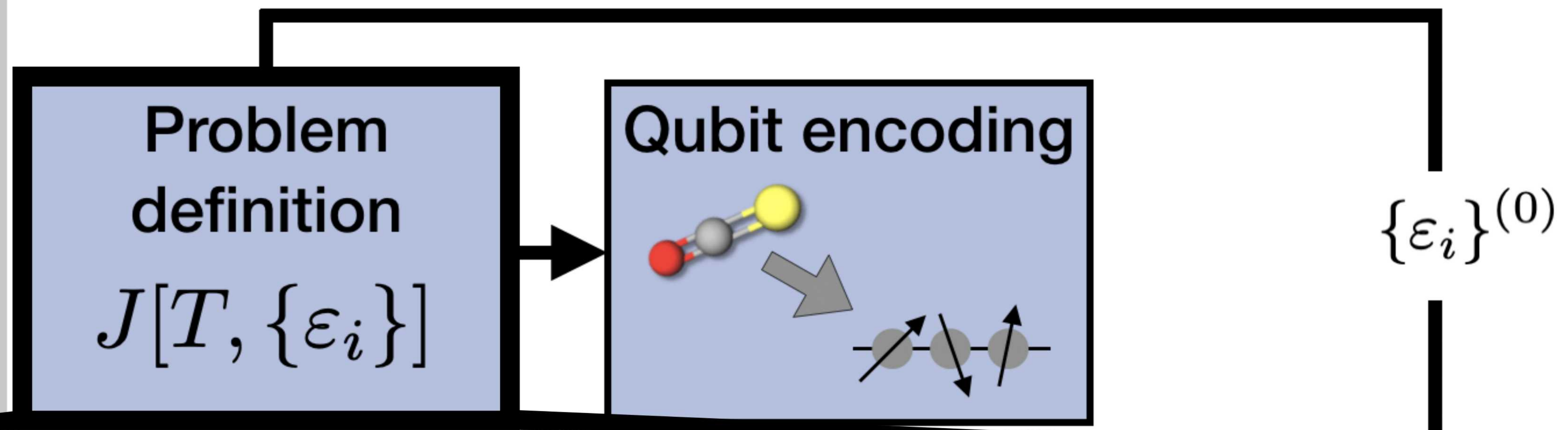
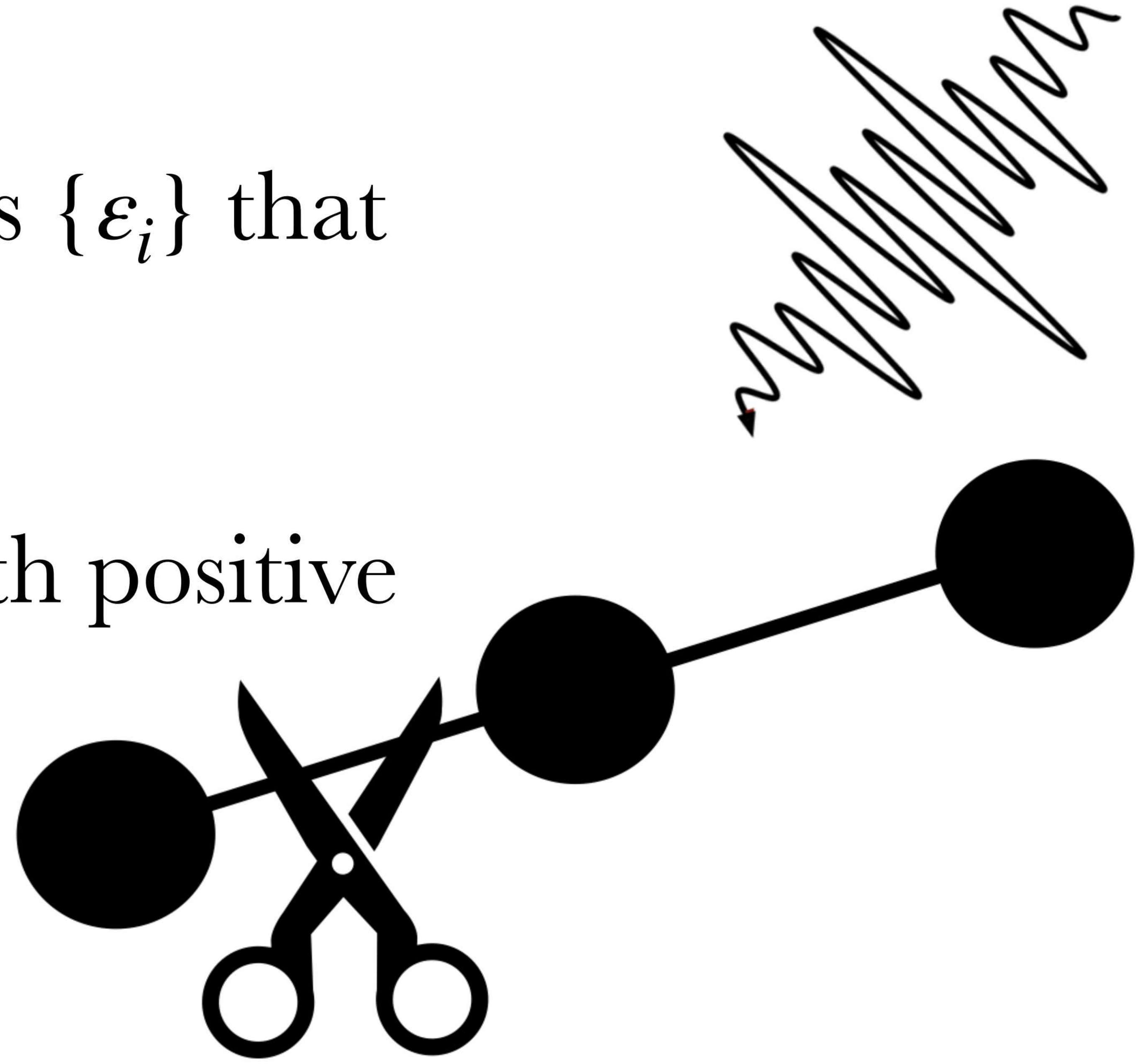


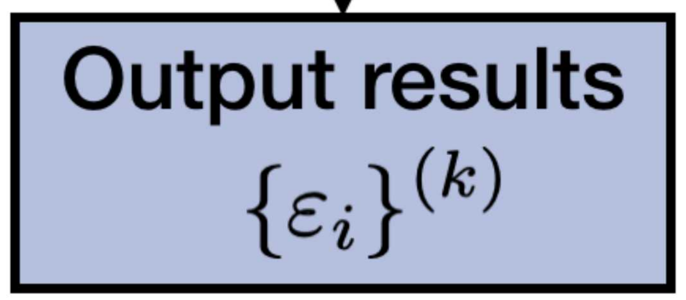
Goal: identify field to selectively dissociate bond 1.

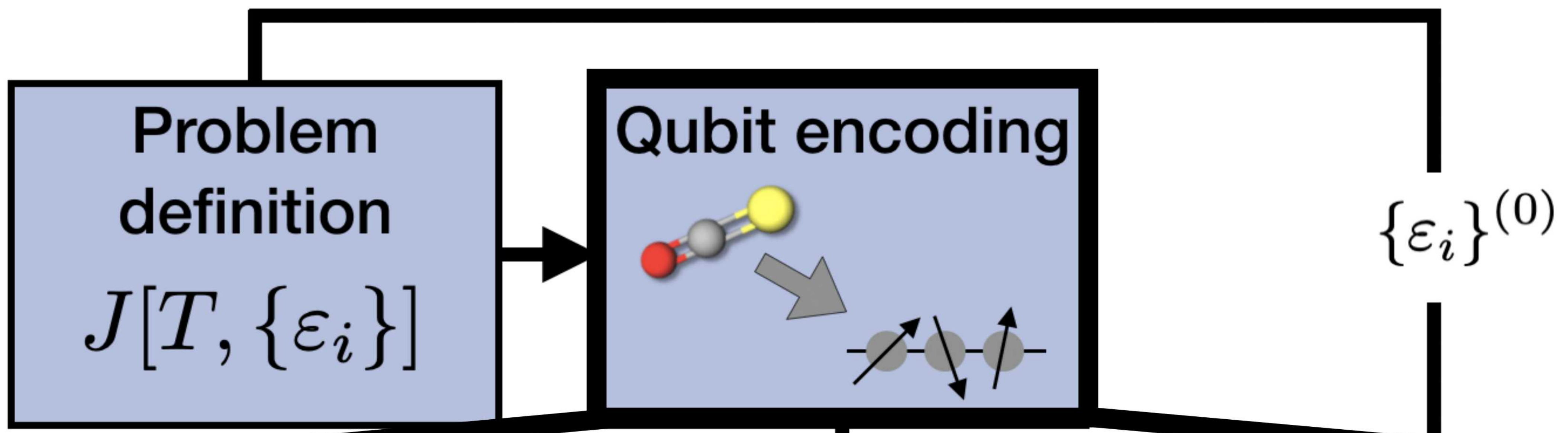
This is posed as the search for the control parameters $\{\varepsilon_i\}$ that minimize an objective functional $J[T, \{\varepsilon_i\}]$

$J[T, \{\varepsilon_i\}]$ chosen to seek bond 1 in a target stretch with positive (outgoing) momentum

Shi and Rabitz, Comput. Phys. Commun, **63** (1991).







Perform qubit encoding in harmonic oscillator eigenbasis truncated to *d* eigenfunctions

S. McArdle *et. al.*, arXiv:1811.04069 (2018)

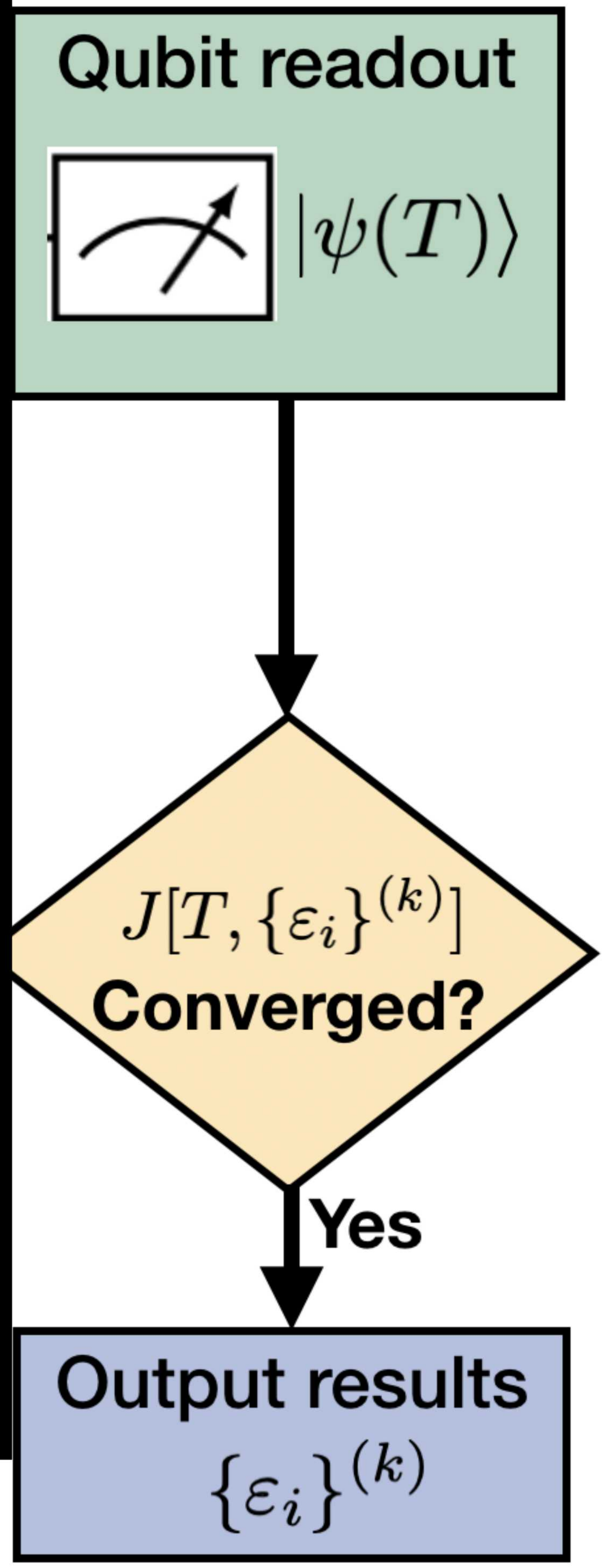
R. Somma *et. al.*, arXiv:0304063 (2003).

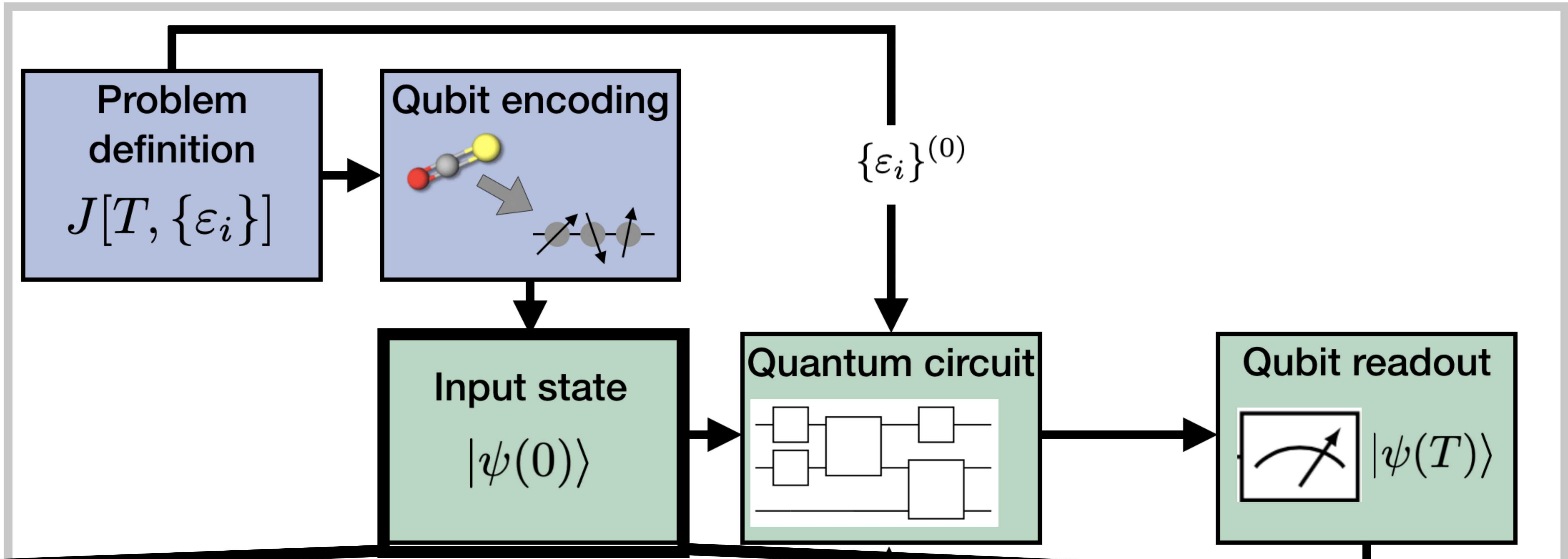
Encode *s*th vibrational eigenstate as:

$$|s\rangle = |0\rangle_0 |0\rangle_1 \cdots |0\rangle_{s-1} |1\rangle_s |0\rangle_{s+1} |0\rangle_{s+2} \cdots |0\rangle_{d-1}$$

Encode operators as:

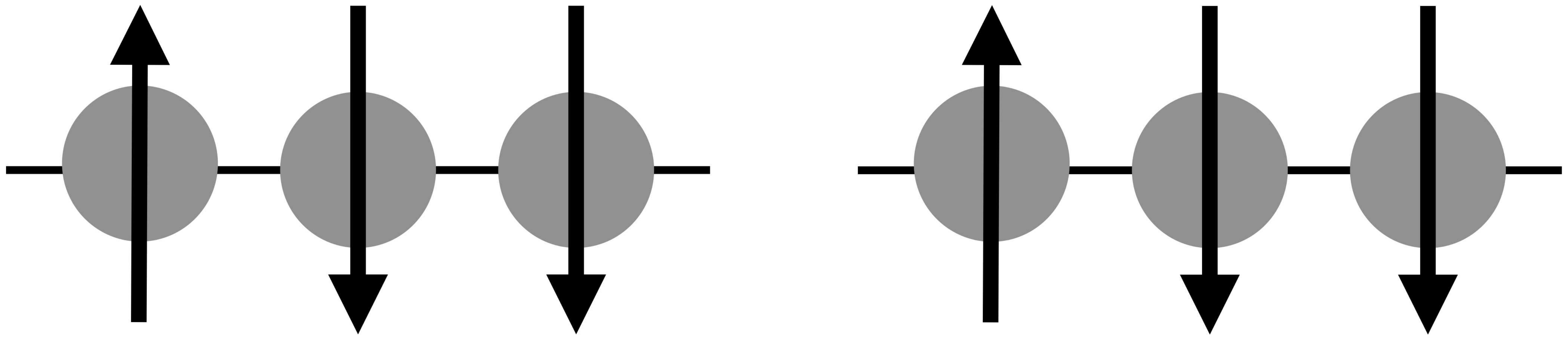
$$a^\dagger = \sum_{s=0}^{d-2} \sqrt{s+1} \left(\sigma_-^s \sigma_+^{s+1}\right) \qquad a^\dagger a = \sum_{s=0}^{d-1} s \left(\frac{\sigma_z^s + 1}{2}\right)$$

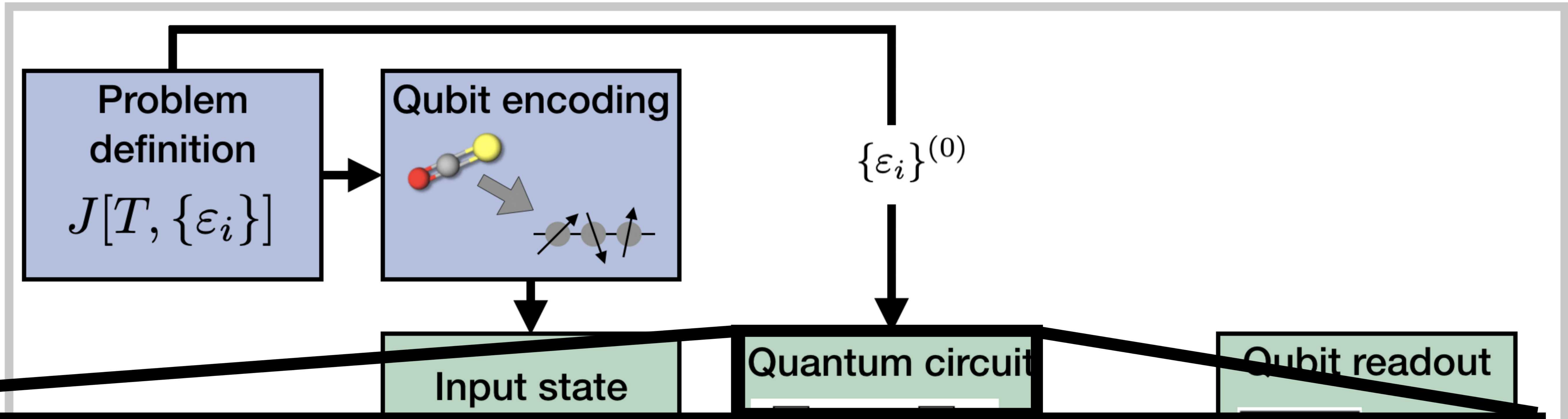




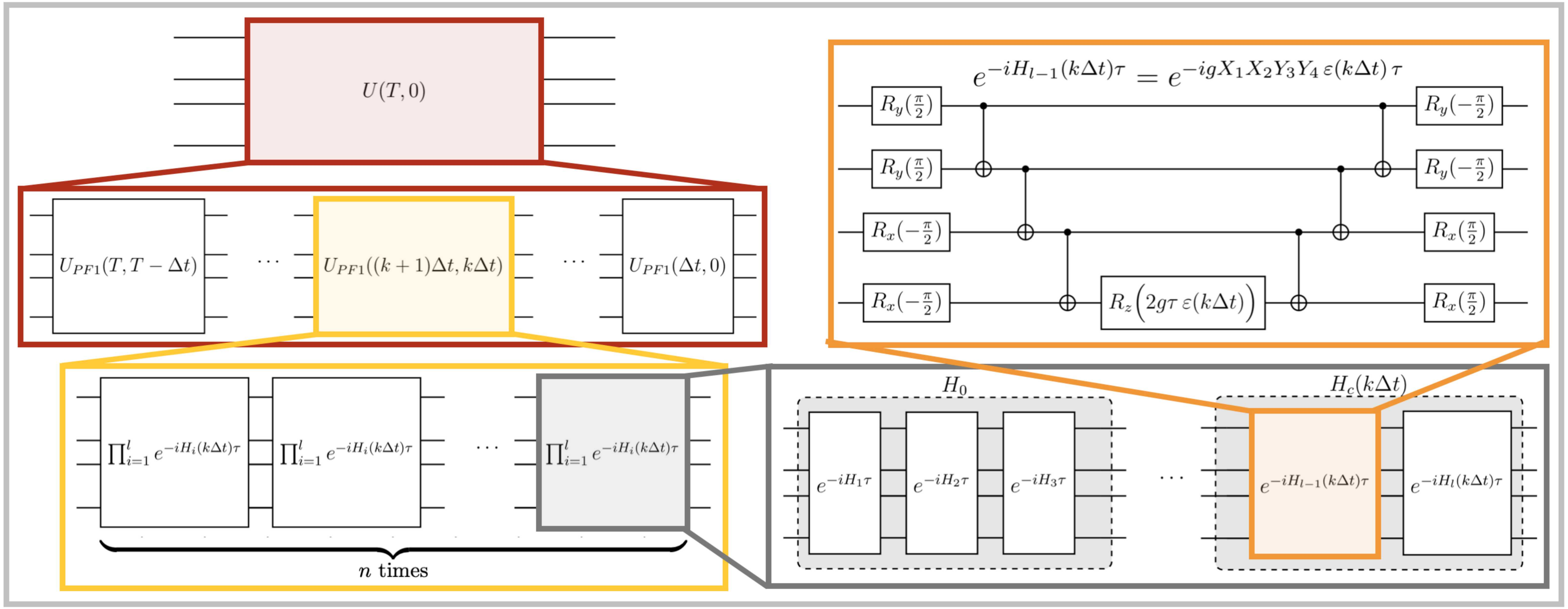
- Qubits initialized in encoded $|\psi(0)\rangle$ state

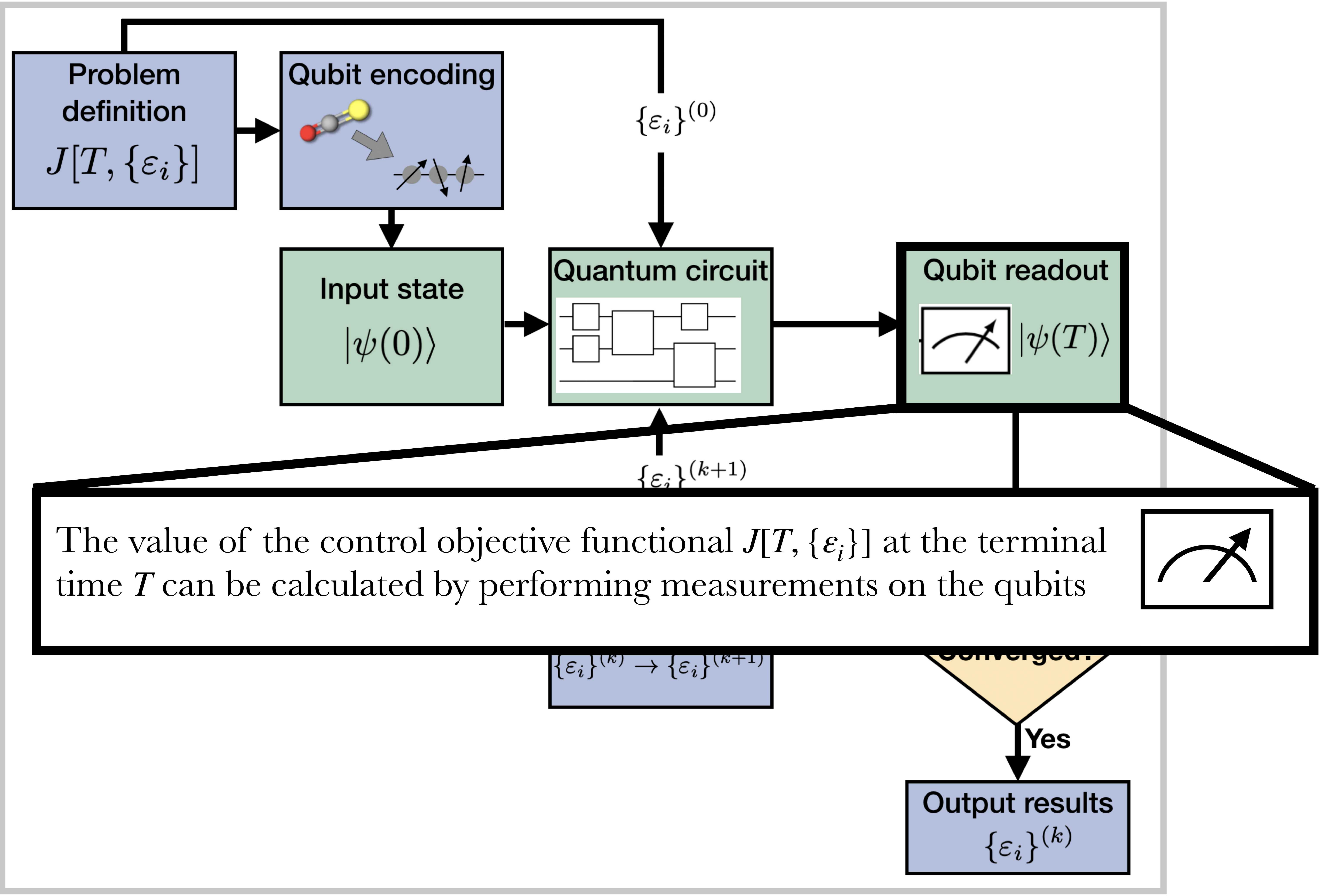
- This is taken as the product state $|0\rangle_1|0\rangle_2$ whose encoding is given by $\left(|1\rangle_0|0\rangle_1|0\rangle_2\cdots|0\rangle_{d-2}|0\rangle_{d-1}\right)_1\left(|1\rangle_0|0\rangle_1|0\rangle_2\cdots|0\rangle_{d-2}|0\rangle_{d-1}\right)_2$





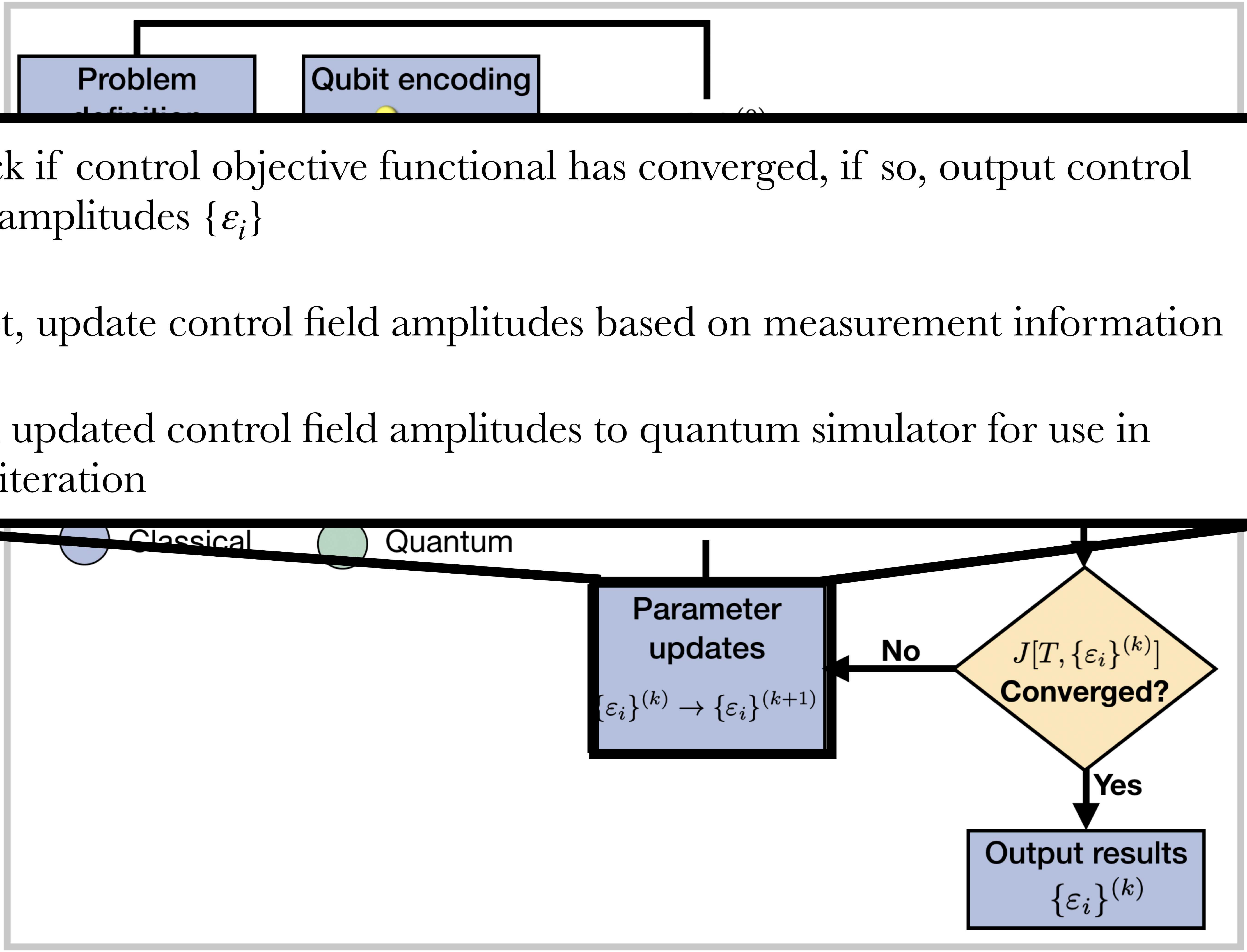
Goal: quantum circuit to find $|\psi(T)\rangle = U(T,0)|\psi(0)\rangle$





The value of the control objective functional $J[T, \{\varepsilon_i\}]$ at the terminal time T can be calculated by performing measurements on the qubits

- Check if control objective functional has converged, if so, output control field amplitudes $\{\varepsilon_i\}$
- If not, update control field amplitudes based on measurement information
- Send updated control field amplitudes to quantum simulator for use in next iteration



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Thank you

Herschel Rabitz

Tak-San Ho

Matthew Grace

Mohan Sarovar