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Digital quantum simulation of quantum dynamics and control

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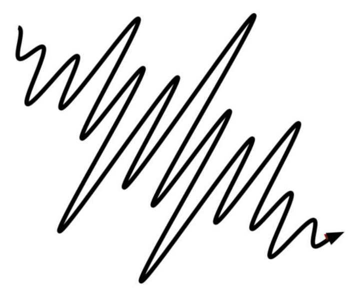
Background

Goal:
Explore applications of quantum computers for quantum optimal control simulations

The aim of quantum optimal control is to design a field $f(t)$, $t \in [0,T]$, to steer a quantum system towards a desired control target at time T by optimizing over a set of control parameters $\{\theta_i\}$.

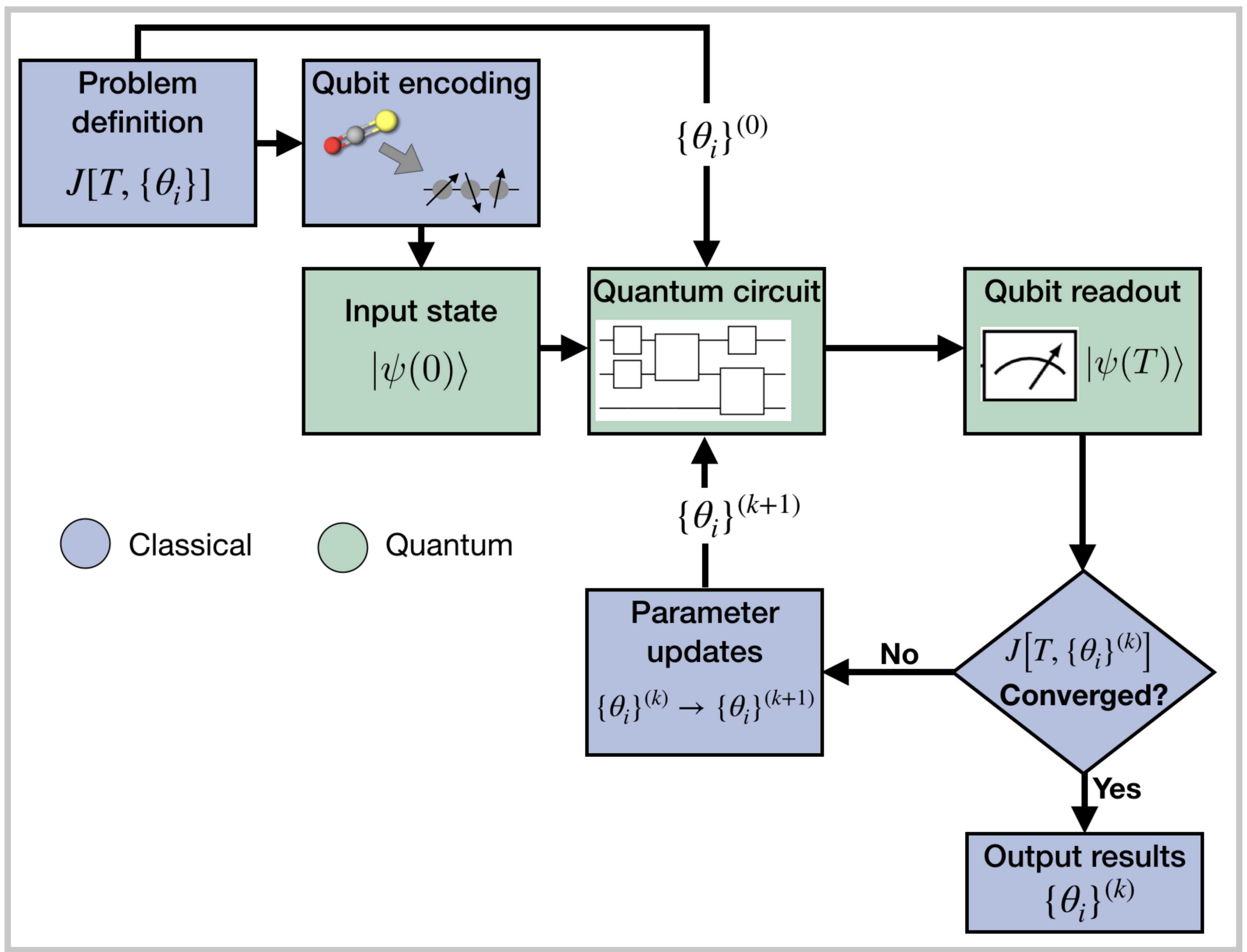
Problem is posed as the search for

$$\max_{\{\theta_i\}} J[T,\{\theta_i\}]$$



where $J[T,\{\theta_i\}]$ is the control objective functional

Simulation framework



Illustration, continued

Standard binary mapping for qubit encoding

Mapping from vibrational states to qubit states:

$$|v\rangle \to |q\rangle$$
$$|0\rangle \to |0\rangle|0\rangle\cdots|0\rangle|0\rangle|0\rangle$$
$$|1\rangle \to |0\rangle|0\rangle\cdots|0\rangle|0\rangle|1\rangle$$
$$|2\rangle \to |0\rangle|0\rangle\cdots|0\rangle|1\rangle|0\rangle$$
$$|3\rangle \to |0\rangle|0\rangle\cdots|0\rangle|1\rangle|1\rangle$$

d level system $\to \log_2(d)$ qubits

M degrees of freedom with d levels each $\to M\log_2(d)$ qubits

Mapping to qubit operators:

$$H = \sum_{v,v'} a_{v,v'}|v\rangle\langle v| \to \sum_{q,q'} a_{q,q'}|q\rangle\langle q'|$$

Projectors expressed as products of:

$$|1\rangle\langle 1| = \frac{I-Z}{2} \quad |0\rangle\langle 0| = \frac{I+Z}{2} \quad |0\rangle\langle 1| = \frac{X+iY}{2} \quad |1\rangle\langle 0| = \frac{X-iY}{2}$$

Product formulas for quantum simulation of driven dynamics

Time evolution of initial state $|\psi(0)\rangle$ to terminal state $|\psi(T)\rangle$ simulated as

$$|\psi(T)\rangle = U(T,0)|\psi(0)\rangle$$

Discretize time into steps of length Δt & assume Hamiltonian is piecewise-constant over each step:

$$U(T,0) = U(T,T-\Delta t)\cdots U(2\Delta t,\Delta t)\,U(\Delta t,0)$$
$$\approx U_{PF}(T,T-\Delta t)\cdots U_{PF}(2\Delta t,\Delta t)\,U_{PF}(\Delta t,0)$$

Time evolution over each Δt approximated using product formulas, e.g.:

$$U_{PF1}(t+\Delta t,t) = \left(e^{-iH_1(t)\Delta t/n}e^{-iH_2(t)\Delta t/n}\cdots e^{-iH_L(t)\Delta t/n}\right)^n$$

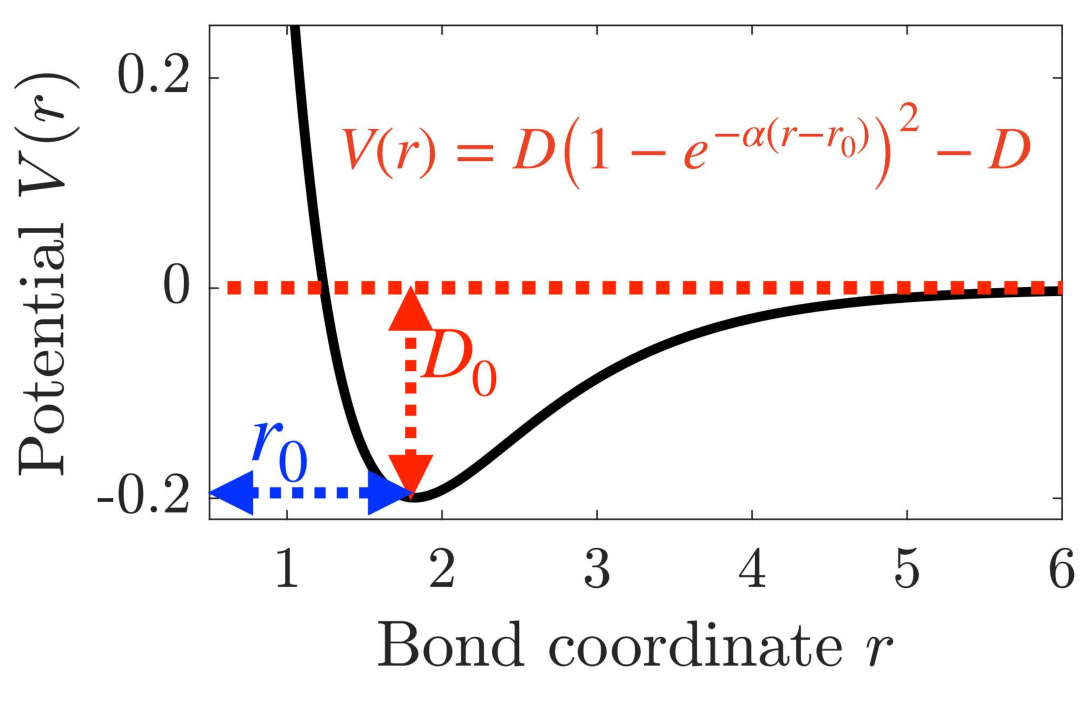
"Trotter number"
exact as $n \to \infty$

Errors reduced by going to higher order product formulas

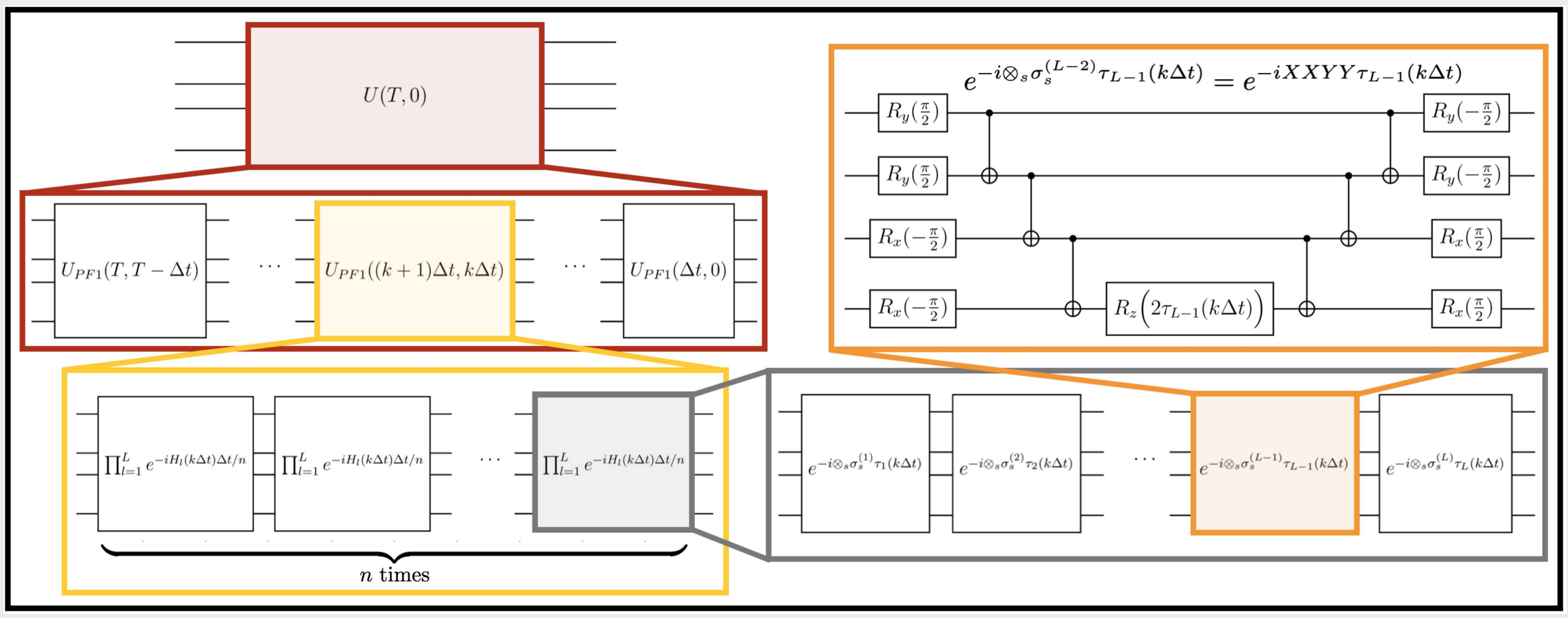
Illustration: Control of bond displacement in diatomic molecule

$$J[T,\{\theta_i\}] = \left(\langle\psi(T)|r|\psi(T)\rangle - \gamma\right)^2$$

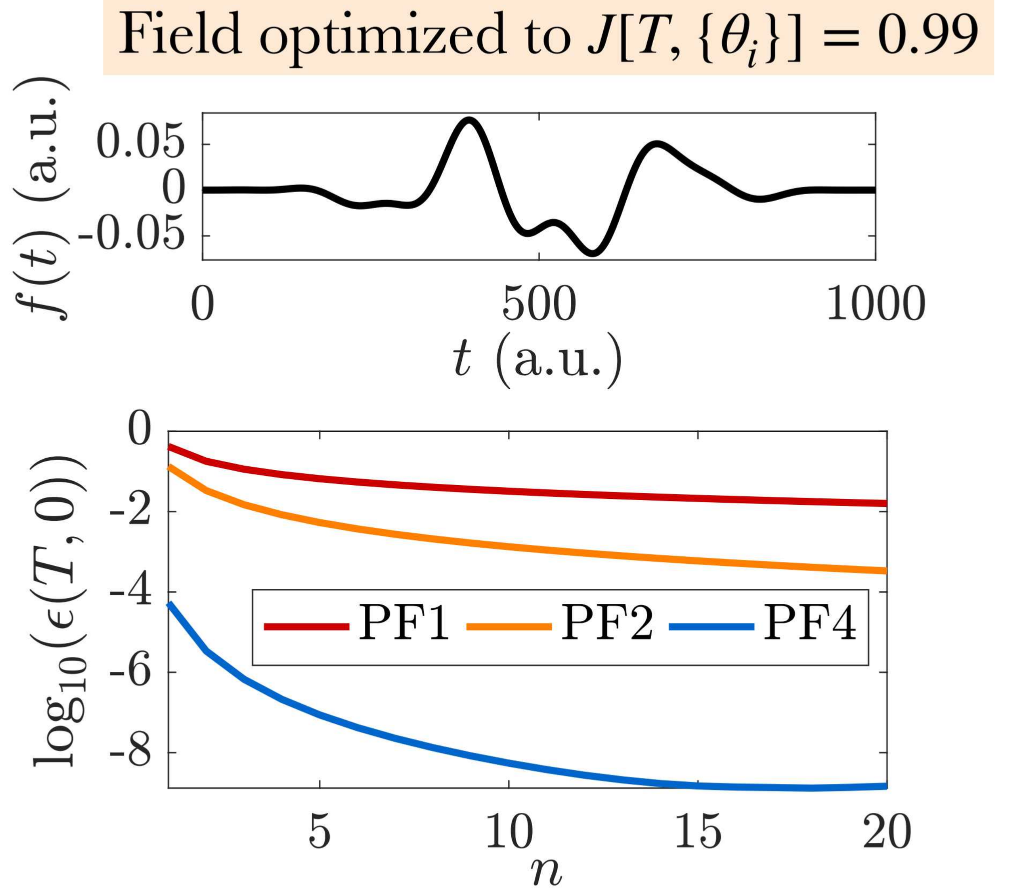
Goal: Identify set of control parameters $\{\theta_i\}$ describing field $f(t)$ that drives bond to target stretch $\gamma = 1.5r_0$ at time $T = 1{,}000$ a.u. ≈ 24 fs



Control parameters $\{\theta_i\}$ are amplitudes, phases, and detunings of set of frequency components in $f(t)$



Field optimized to $J[T,\{\theta_i\}] = 0.99$



Outlook

- Illustration 2: control of state preparation in a model for a light harvesting complex
- Estimation of the quantum resources necessary for DOE mission-relevant quantum control applications

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