Efficient Unitary Method for Simulation of Driven Quantum Information Systems

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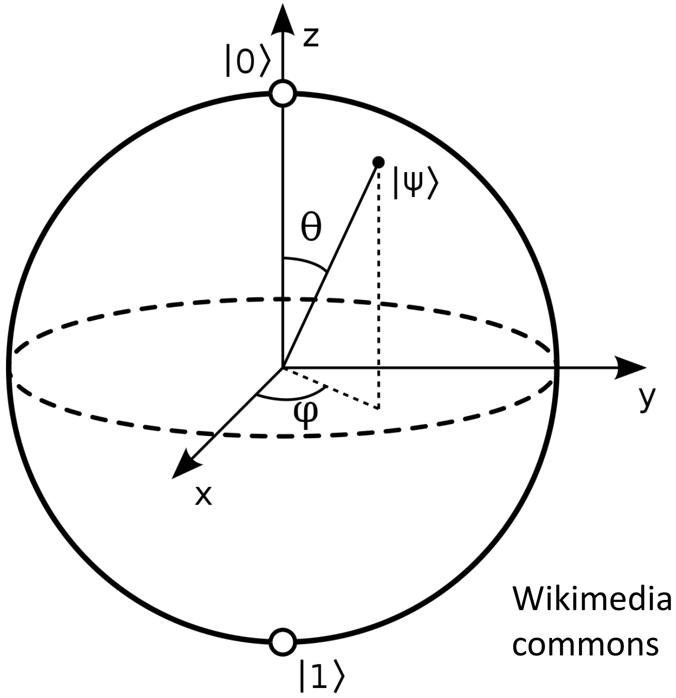
Motivation: Quantum Information



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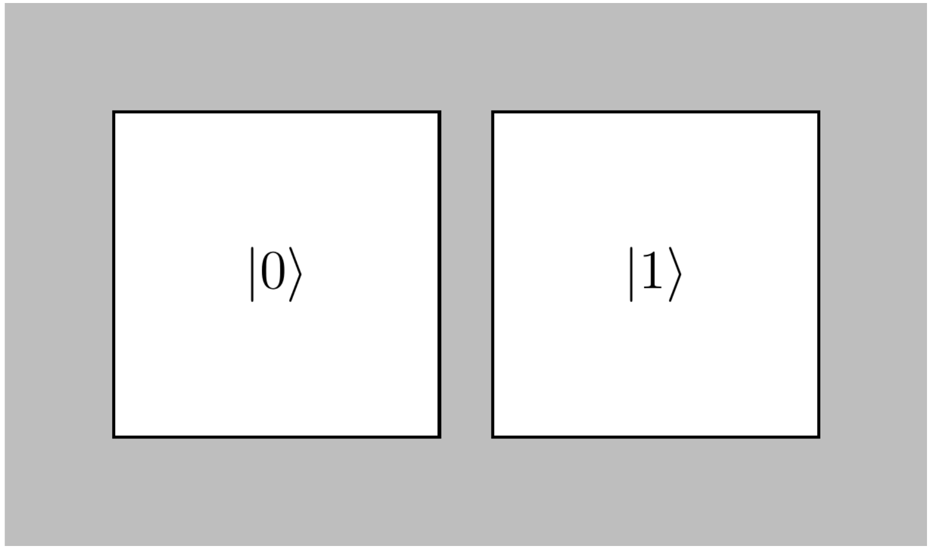
- Qubits
  - Two-state systems, with $|0\rangle$ and $|1\rangle$
  - Information is $|\psi(t)\rangle = c_0(t)|0\rangle + c_1(t)|1\rangle$
- Example degrees of freedom
  - Spin, $|S_z^+\rangle$ and $|S_z^-\rangle$
  - Charge, $|\text{Left}\rangle$ and $|\text{Right}\rangle$

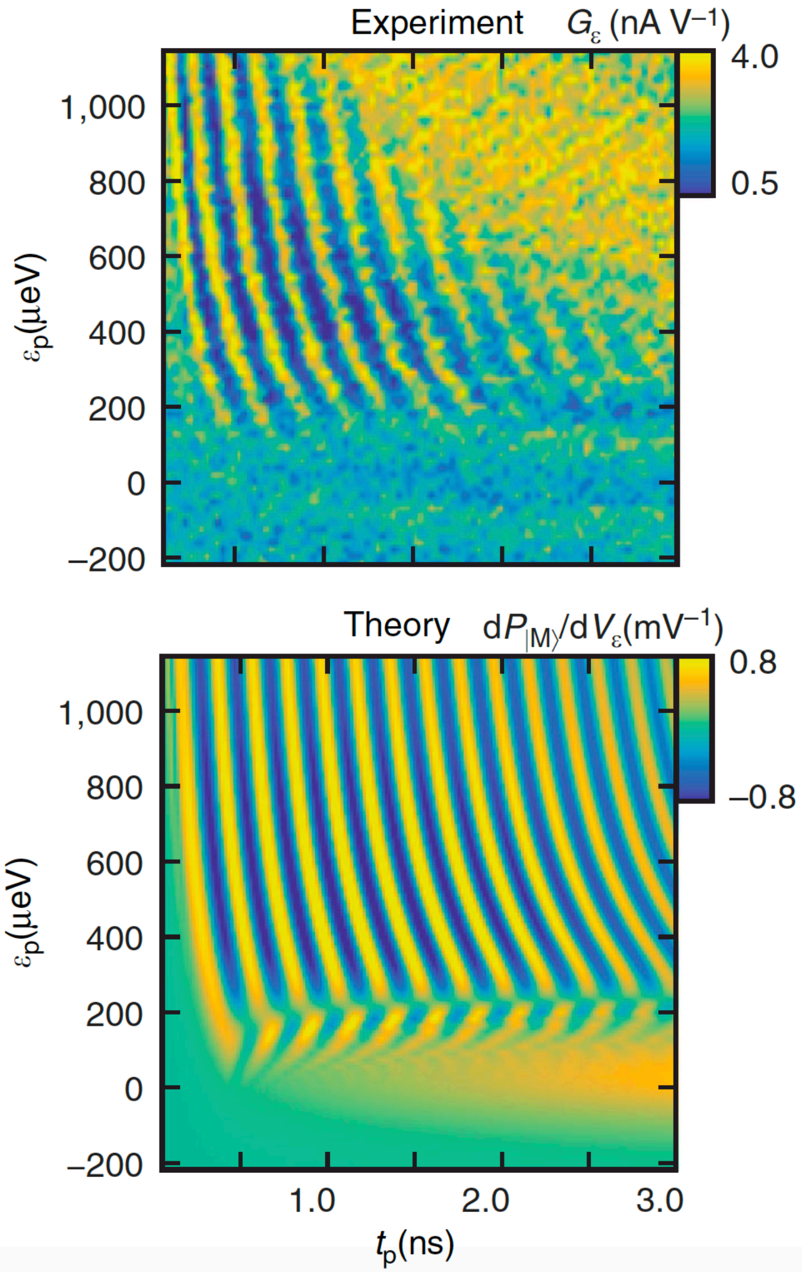


Motivation: Quantum Control

1. Encoding
   - Drive the system into a desired state
2. Storage
   - Account for time-evolution of state while encoded
3. Readout
   - Measure transconductance as driven to readout state

- Ex. Drive a charge qubit by varying gate voltages

Readout Transconductance



Schoenfield, *et al.* Nat. Commun. **5**, 64 (2017)

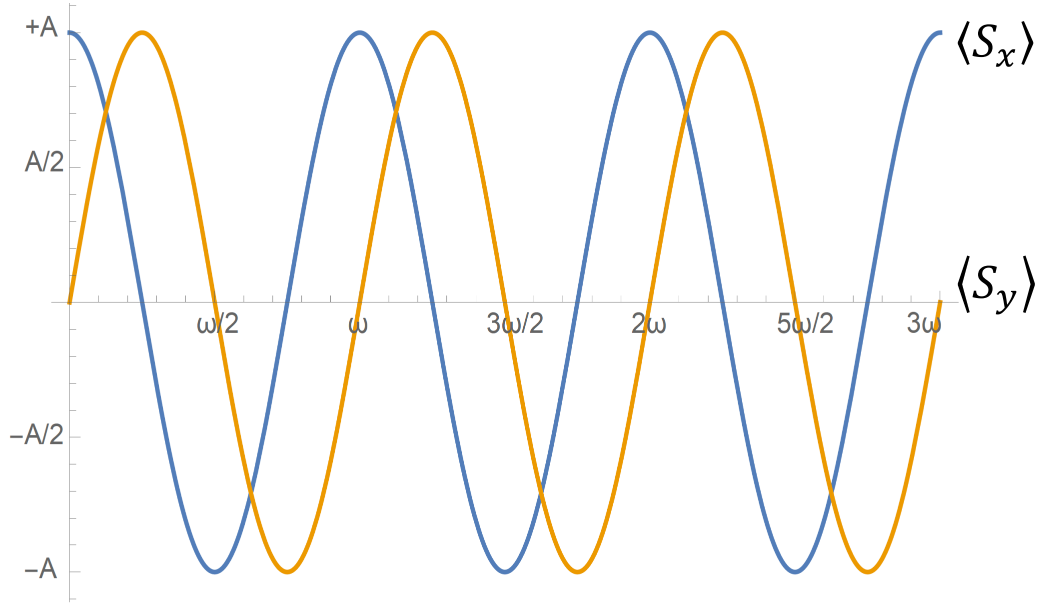
Background: Larmor Precession

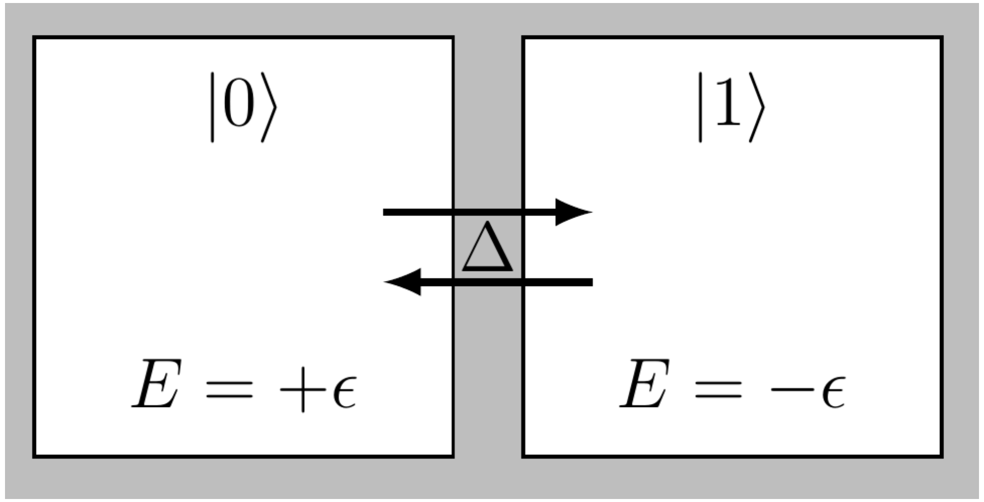
- Ex. spin-1/2 particle with gyromagnetic ratio γ in a magnetic field $\mathbf{B} = \mathrm{B}\,\hat{\mathbf{z}}$

$$H = \gamma \mathrm{B}\,\sigma_z, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Mathematically similar to any two-state system with splitting 2ε and tunneling Δ

$$H = \varepsilon(t)\sigma_z + \Delta\sigma_x$$





Experimental Considerations

- Charge-based semiconductor quantum dot qubits
- Benefit
  - Existing materials science technology
- Complicating factors
  - Device geometry, ex. dot location
  - Pulse generation, ex. multiple gates, physical constraints
  - Material properties, ex. pseudospin states
- Need more complex $H(t)$ and $\varepsilon(t)$ to model system

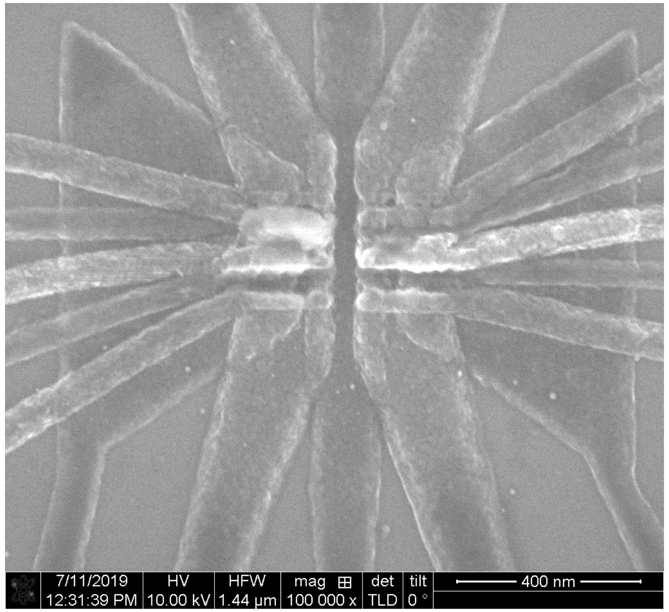


Image credit: J.D. Rooney

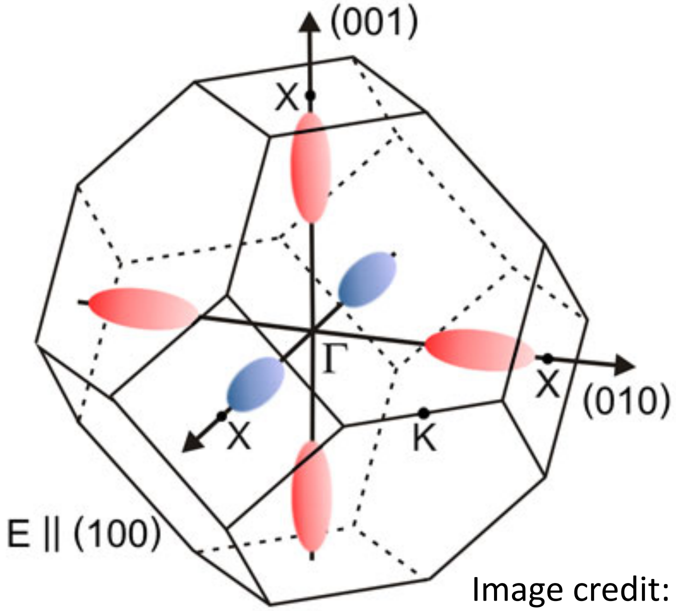


Image credit: J. Isberg

Simulation of Driven Quantum Systems

- Density matrix evolution
  - Dominant method used in quantum information
  - Solve $\partial_t \rho(t) = -i[H(t), \rho(t)]/\hbar + (\text{other terms})$, using RK4 or similar
  - Robust and extensible but slow, e.g. **1 hour** for one 100x100 image

- Unitary time evolution
  - Uncommonly used in quantum information
  - Compute the time evolution operator $U(t)$ for $|\psi(t)\rangle = U(t)|\psi(0)\rangle$
  - Fast but more focused, e.g. **30 sec** for one 100x100 image

Assumptions for Unitary Method

1. Energy is conserved in the system
2. Particle number is conserved
3. Hamiltonians at different times commute

- On short time scales, environmental coupling (1) and relaxation (2) are less important, so these assumptions are reasonable

Computational Method

- Begin with the expression:

$$U(t) = \exp\left[-\frac{i}{\hbar}\int_0^t dt'\, H(t')\right]$$

- Discretize time from 0 to t in N intervals with $t_n \in \{t_0, t_1, \dots, t_N\}$, letting $\Delta t_n = t_n - t_{n-1}$, we approximate the operator:

$$U(t) = \prod_{n=0}^{N} \exp\left[-\frac{i}{\hbar}\Delta t_n\, H(t_n)\right]$$

- With carefully chosen t_n we can compute this quickly and accurately

Optimization

1. If a region is time-independent, calculate that region in one step

2. If we are interested in the time evolution of an expectation value, proceed iteratively:

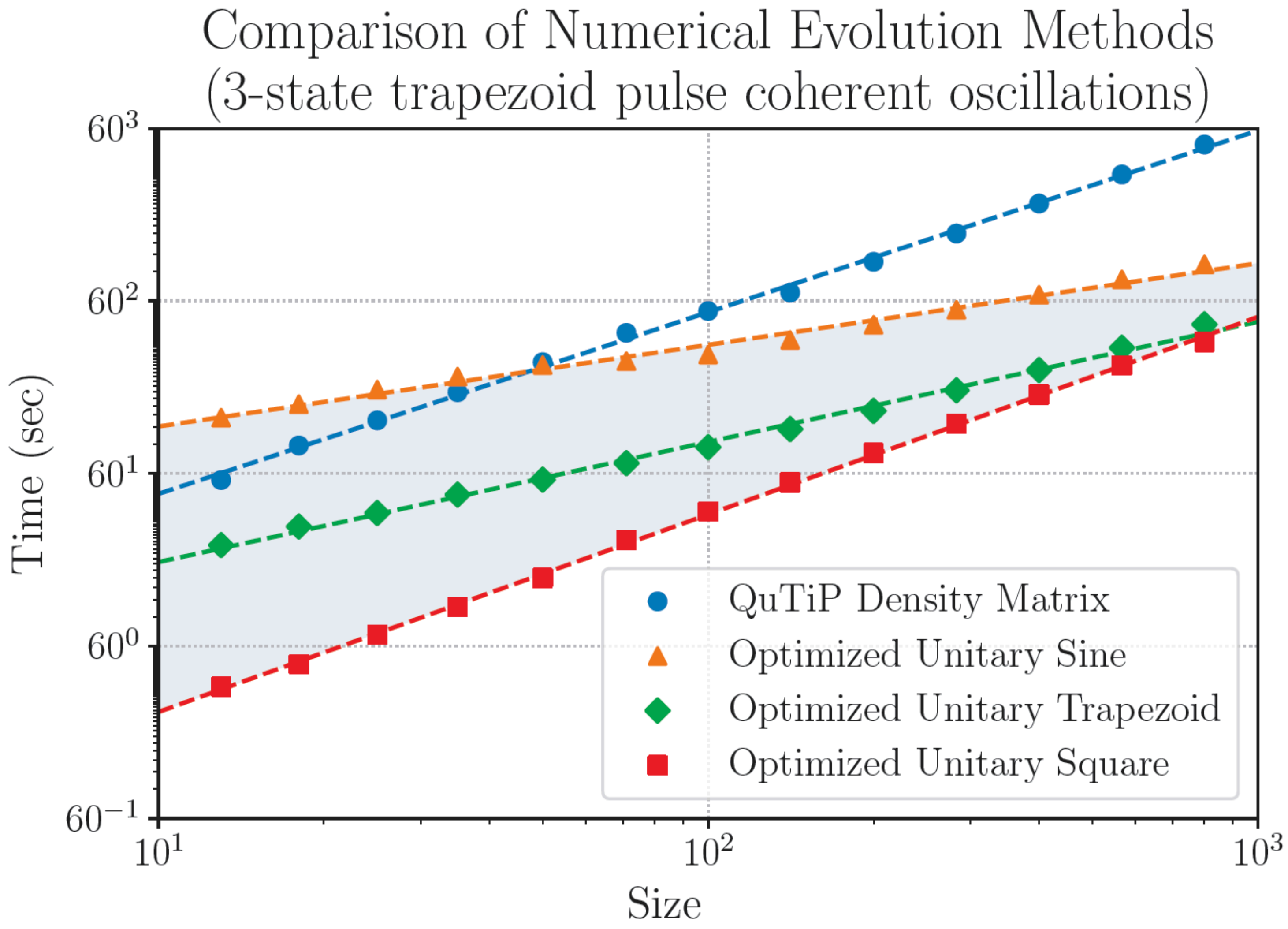
$$|\psi(t_n)\rangle = U(t_n, t_{n-1})|\psi(t_{n-1})\rangle$$

1. If driving features repeat, separate and store these features. Ex:

$$U_{\text{total}} = U_{\text{readout}}\, U_{\text{storage}}\, U_{\text{encode}}$$

Speed Comparison

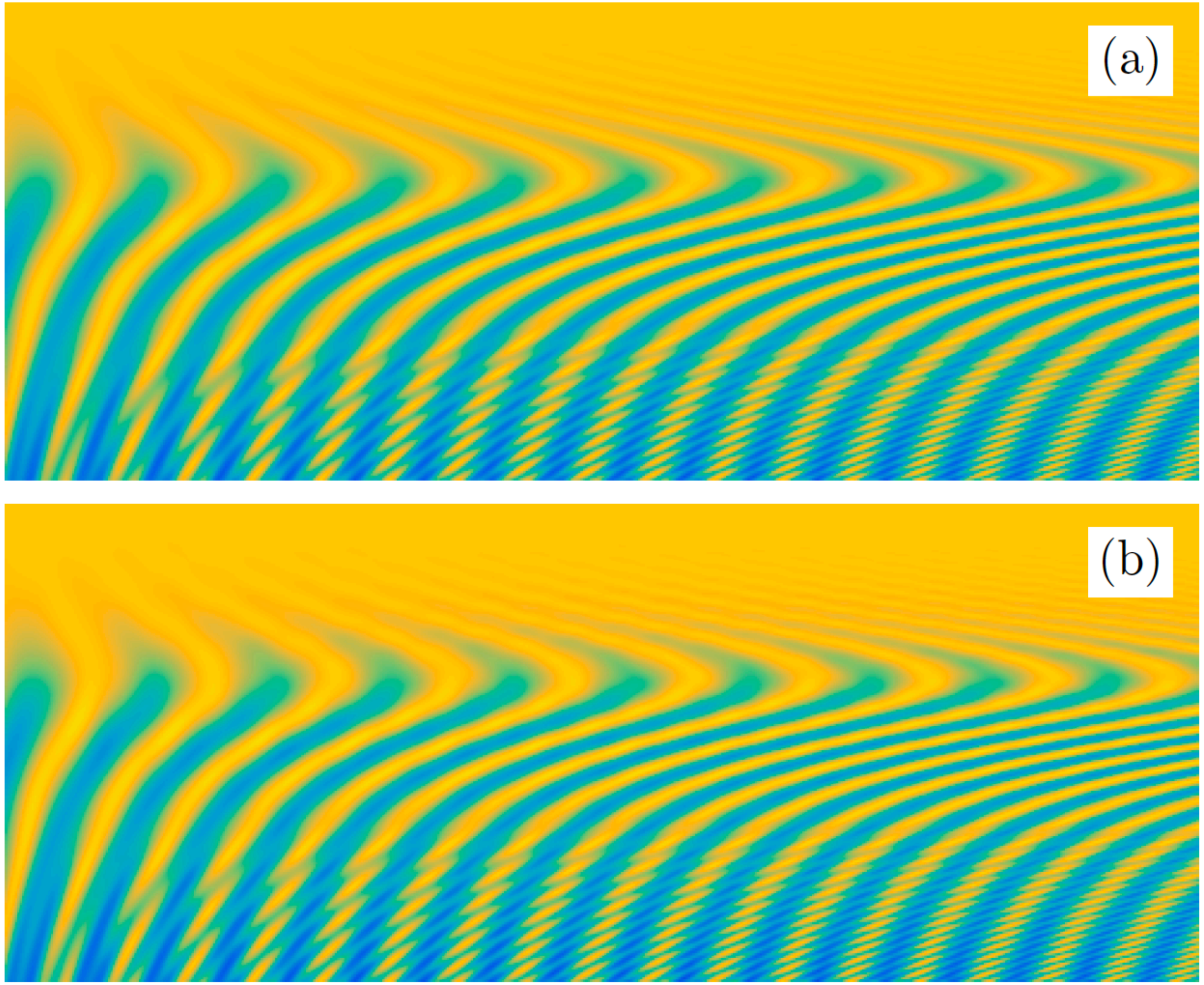
- Compare our method (in Python) to the Python module QuTiP for a variety of driving pulses, as used to make images of oscillations
- This plot underestimates the speedup of the unitary methods by approximately a factor of 5 over the density matrix methods (due to different accuracies)



Ex 1. QD Qubit with Pseudospin States

- (a) QuTiP took 6 hours
- (b) Unitary method took 3 mins

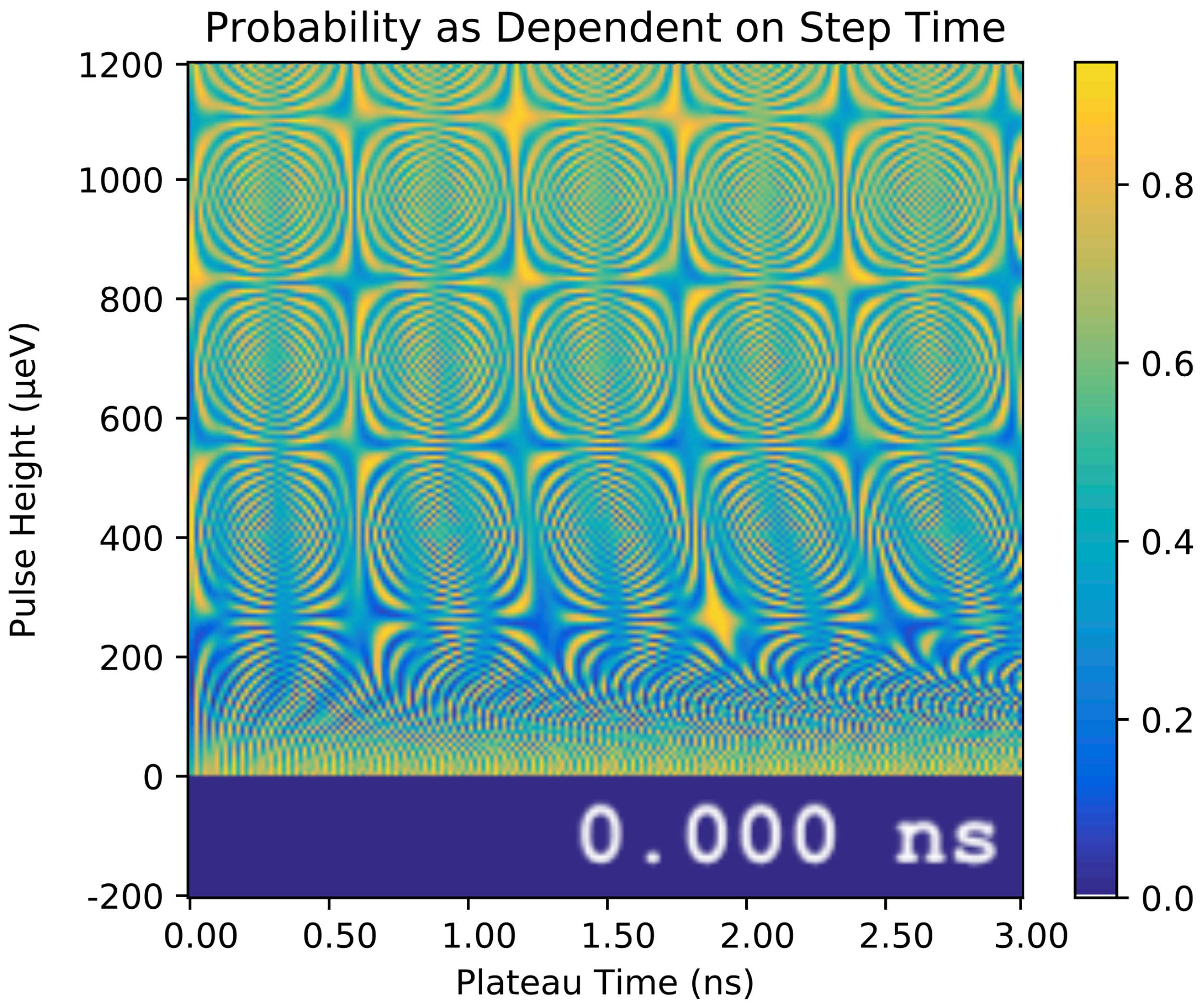
- Hamiltonian from Z. Shi, et al., Nat. Commun. **5**, 3020 (2014)



Talkington, and Jiang. arXiv:1909.02532.

Ex 2. QD Qubit with Two-Axis Driving

- 200 images in 3 hours
- Hamiltonian from Penthorn, *et al.* Quantum Inf., accepted (2019)



Talkington, and Jiang. arXiv:1909.02532.

With Faster Simulations…

- Experiment
  - Explain results more quickly and explore parameter spaces
  - Can study other systems too, ex. spin qubits, superconducting qubits, etc.

- Theory
  - Exploration of diabatic transitions that have no exact solution (Landau-Zener)
  - Study periodically driven systems (Floquet systems)

Acknowledgements

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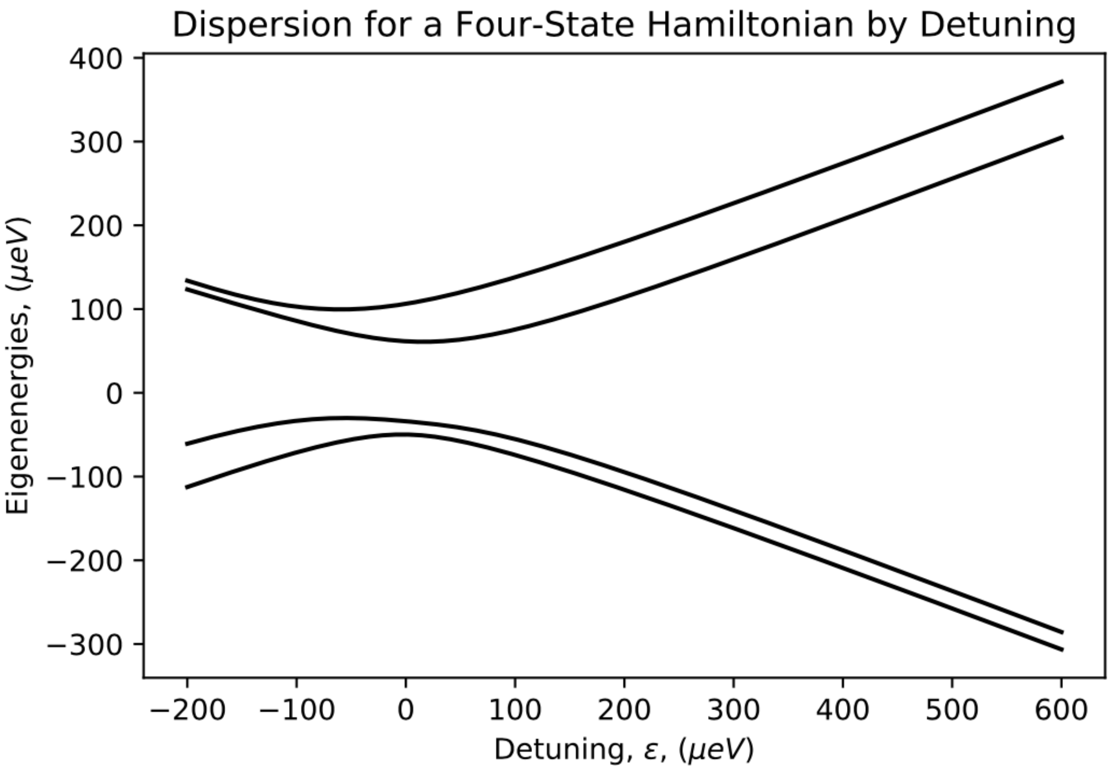
Questions?

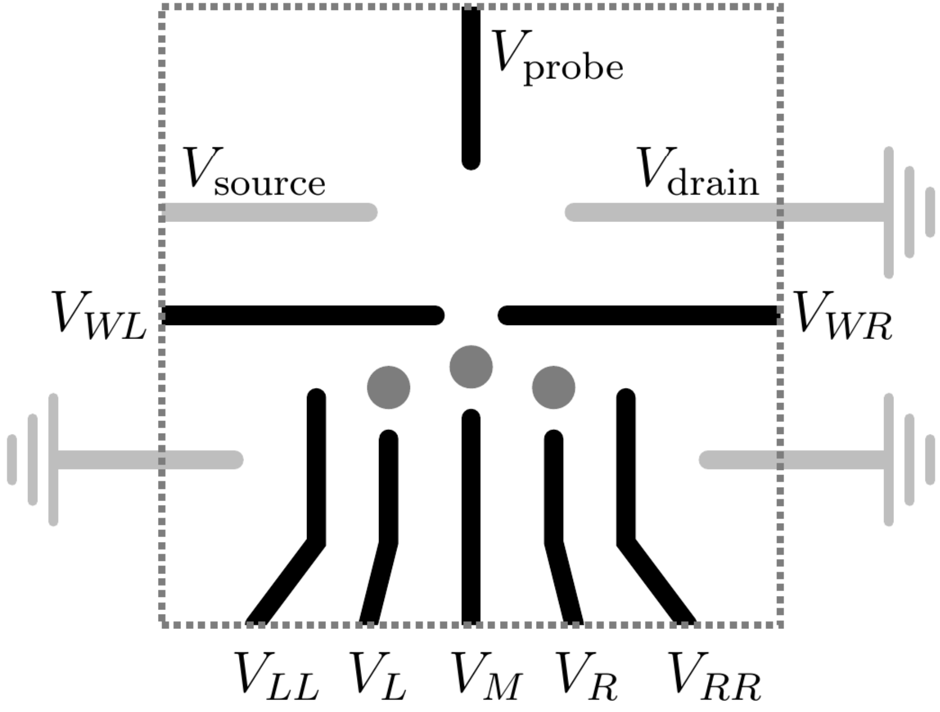
Additional slides

Charge-Based Quantum Dot Qubits

- Discarding all but the charge-tunneling degrees of freedom yields a 4x4 Hamiltonian for time-evolution



Quantum Dot Qubit Device



The charge-tunneling Hamiltonian

Detuning $(U_L - U_R)$

Inter-dot tunnelings

$$H = \begin{pmatrix} \epsilon/2 & 0 & \Delta_1 & -\Delta_2 \\ 0 & \epsilon/2 + \delta_L & -\Delta_3 & \Delta_4 \\ \Delta_1 & -\Delta_3 & -\epsilon/2 & 0 \\ -\Delta_2 & \Delta_4 & 0 & -\epsilon/2 + \delta_R \end{pmatrix}$$

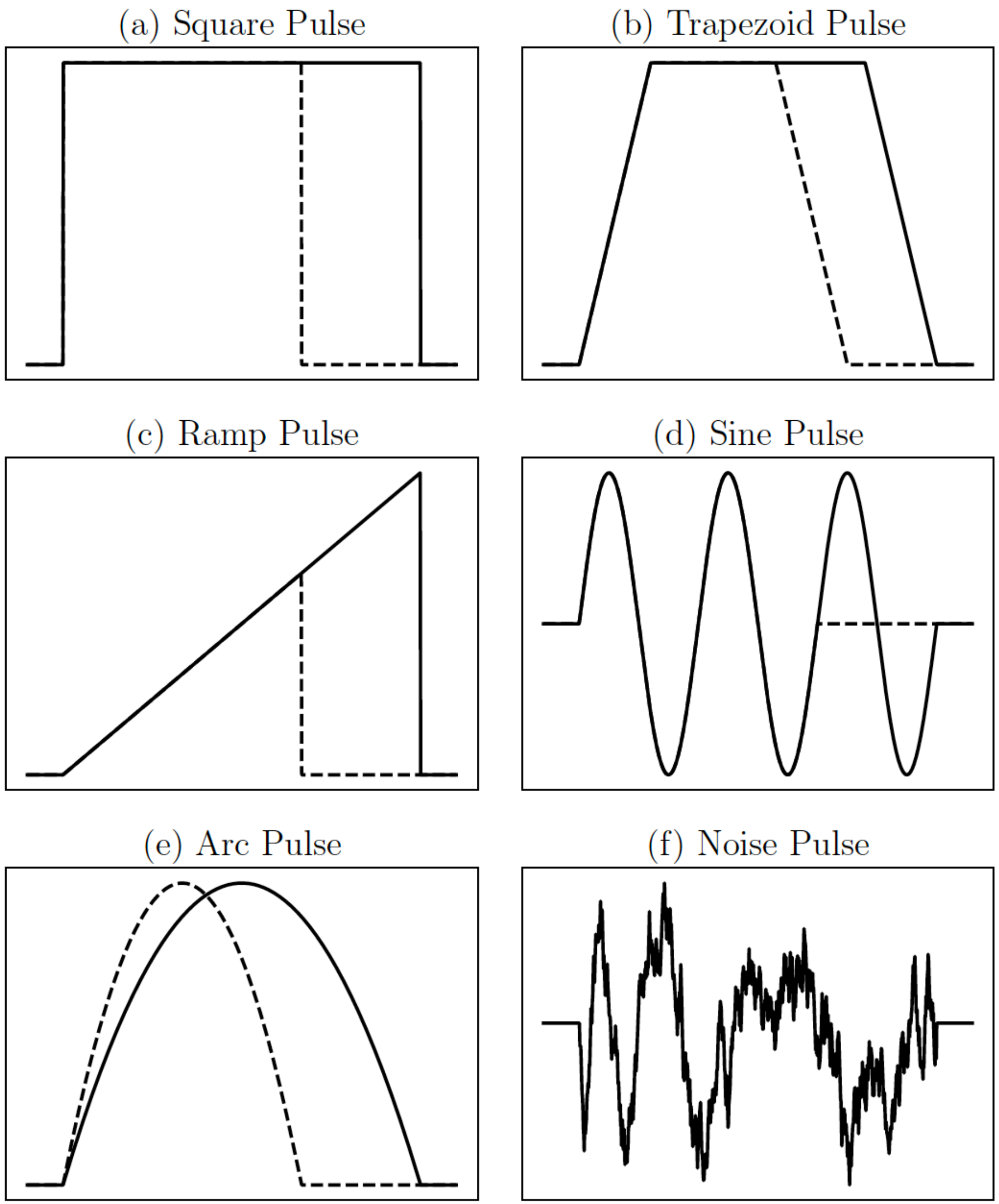
Valley splittings

Driving with Pulses

- Systems are driven by electric pulses

$$U_{site} = qE_{site}$$

- Optimizations are possible in the unitary regime assuming forms of the driving pulse



Evolution of Quantum States

Density Matrices

- Solve a differential equation

A density matrix, ρ has $\mathrm{tr}(\rho) = 1$, in particular, for states $|\psi_i\rangle$, and positive real numbers p_i:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

The von Neumann equation gives time evolution:

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho]$$

There are other useful properties and applications of density matrices, but they are not relevant here.

Unitary Evolution

- Evaluate an integral

When particle number $\langle\psi|\psi\rangle$ is conserved, quantum states evolve with a unitary time-evolution operator:

$$|\psi(t)\rangle = \mathscr{U}(t, 0)\,|\psi(0)\rangle$$

So long as Hamiltonians of different times commute the time-evolution unitary may be found using the formula:

$$\mathscr{U}(t, 0) = \exp\left[-\frac{i}{\hbar}\int_0^t d\bar{t}\ H(\bar{t})\right]$$

Simulation of Driven Quantum Systems

- Density matrix evolution through differential equation solving is the dominant method used in quantum information
  - Solve $\partial_t \rho(t) = -i[H(t), \rho(t)]/\hbar + (\text{other terms})$, using RK4 or similar
  - (+) robust, it works for many systems with little code modification needed
  - (+) extensible, e.g. to systems with relaxation and coupling to environment
  - (−) slow, e.g. **1 hour** for one 100x100 image
- Unitary time evolution
  - Compute the time evolution operator $U(t)$ for $|\psi(t)\rangle = U(t)|\psi(0)\rangle$
  - (−) delicate, more code modification is often necessary to be faster than dm
  - (−) focused, only practical for certain systems and driving behaviors
  - (+) fast, e.g. **30 sec** for one 100x100 image

Assumptions for Unitary Method

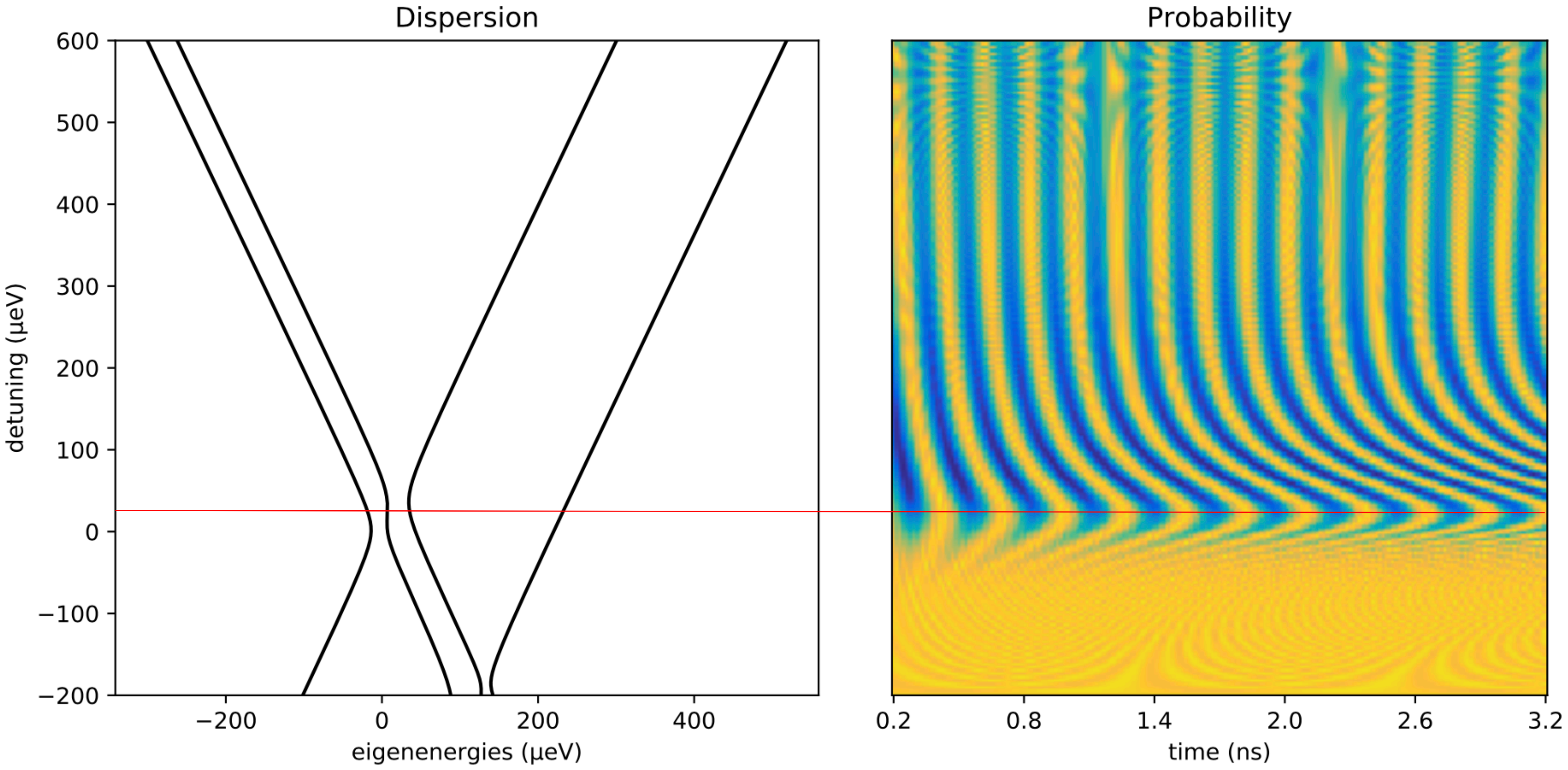
- Energy is conserved in the system, so no coupling to the environment
- Particle number is conserved, i.e. $H^\dagger = H$, so no relaxation of states
- Hamiltonians at different times commute, $\left[H(t_i), H\left(t_j\right)\right] = 0$

- These are often reasonable assumptions
  - On short time frames environmental noise and relaxation are less important
  - We can still make quantitative predictions for encoding states, and predict the period (but not amplitude) of stored states. Readout results are less reliable.

Time Complexity

Pulse	Matrix Exponentials	Calculated[a]	Measured[b]
Square	N^2	4 sec	7 sec
Trapezoid	$N^2 + N(t_r + t_f)/\tau$	84 sec	98 sec
Ramp/Sine	$N(t_{\max}/\tau)$	1280 sec	1306 sec
Arc/Noise	$N^2(t_{\min} + t_{\max})/2\tau$	68000 sec	73648 sec

Coherent Oscillations



Background: Larmor Precession (Oscillations)

- Ex. A spin-1/2 particle with gyromagnetic ratio γ in a magnetic field $\mathbf{B} = \|\mathbf{B}\|\,\hat{\mathbf{z}}$

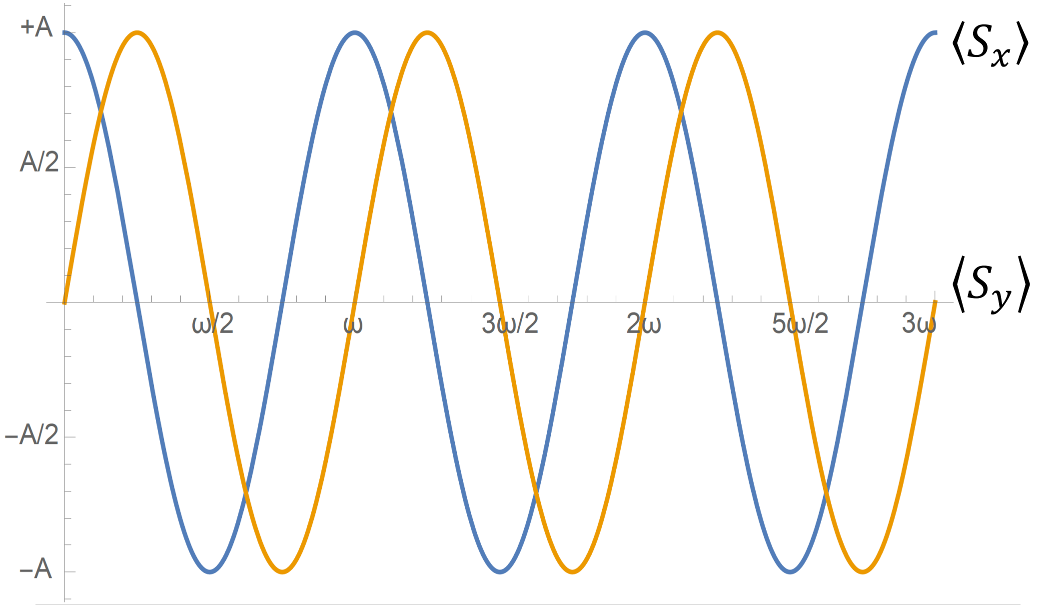
$$H = \gamma \|\mathbf{B}\| \sigma_z, \text{ where, } \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

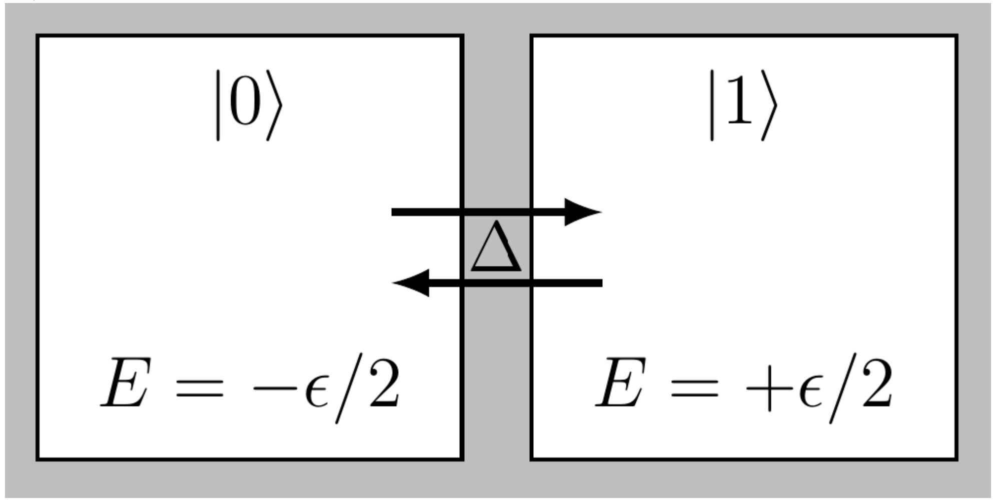
- We find $\langle S_x \rangle$ and $\langle S_y \rangle$ oscillate in time

- Mathematically similar to any two-state system with splitting ε and tunneling Δ

$$H = \varepsilon(t)\sigma_z + \Delta\sigma_x$$

- Both exhibit "coherent oscillations"





Optimization

1. If a region is time-independent, calculate that region in one step
    1. Ex. The storage region in a trapezoidal driving pulse
    2. Ex. The step regions in a two-axis driving pulse
2. If we are interested in the time evolution of an expectation value, proceed iteratively: $|\psi(t_n)\rangle = U(t_n, t_{n-1})|\psi(t_{n-1})\rangle$
    1. Ex. Plotting $\langle S_x \rangle$ as a function of time for $\mathbf{B}(t) = \mathrm{B}\,\hat{\mathbf{z}}$ in Larmor precession
    2. Ex. Plotting $\langle 0 \rangle$ as a function of time for $\varepsilon(t)$ with no evolution at readout
3. If driving features repeat, separate and store these features. Ex:

$$U_{\text{total}} = U_{\text{readout}}\, U_{\text{storage}}\, U_{\text{encode}}$$