Simulating Physical Phenomena with a Quantum Computer

"What is really important about quantum computers is that they show us that there's a deep and unsuspected connection between physics and computation."
David Deutsch

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Simulation of Physical Systems

C.J. Negrevergne: NMR Experiment

Feynman's Unfinished Legacy

$$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

"...The question is, If we wrote a Hamiltonian which involved only these [Pauli] operators, locally coupled to corresponding operators on the other space-time points, could we imitate every quantum mechanical system which is discrete and has a finite number of degrees of freedom? I know, almost certainly, that we could do that for any quantum mechanical system which involves Bose particles. I'm no sure whether Fermi particles could be described by such a system. So, I leave that open..."

Richard P. Feynman

(Simulating Physics with Computers (1982))

Simulating Physical Phenomena

What is the problem?

Quantum phenomena is too complex for classical computers.

What is the challenge?

Simulate quantum phenomena using a number of resources that scales polynomially with the number of degrees of freedom of the physical system involved.

What kind of physical phenomena can be imitated?

Time-dependent phenomena, correlation functions, spectral problems, thermodynamics.

How does a QIPD imitate?

Design quantum algorithms.

What are the limitations?

Decoherence, absence of efficient quantum algorithms

Classical Simulations of Quantum Phenomena

- Deterministic: Exponential "catastrophe."
- Probabilistic: Feynman's answer is NO. However, probabilistic simulations are perfomed with the Monte Carlo method that uses random walks.

$\oplus$ Real-time Dynamics: (e.g., scattering)

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = H|\Psi\rangle$$

solved by incrementally propagating the initial state via

$$|\Psi(t)\rangle = \underbrace{e^{-i\Delta t H/\hbar} e^{-i\Delta t H/\hbar} \cdots e^{-i\Delta t H/\hbar}}_{M \text{ factors}} |\Psi(0)\rangle \ .$$

— Problem: Always

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$\oplus$ Imaginary-time Dynamics: (e.g., ground state or thermodynamics)

$$\frac{\partial |\Psi\rangle}{\partial \tau} = -H|\Psi\rangle$$

solved by incrementally propagating the initial state via

$$|\Psi(\tau)\rangle = \underbrace{e^{-\Delta\tau H} e^{-\Delta\tau H} \cdots e^{-\Delta\tau H}}_{M \text{ factors}} |\Psi(0)\rangle \ .$$

— Problem: Sometimes (liquid He^4 has been a success!), but most of the time...

$$\Downarrow$$

$\boxed{\text{Origin: Negative and Complex Probabilities}}$

The million-dollar question

- Dynamical Sign Problem: real-time dynamics; any particle statistics
- Fermion Sign(Phase) Problem: imaginary-time dynamics; almost any particle statistics ($e^{i\Phi} = \pm 1$)

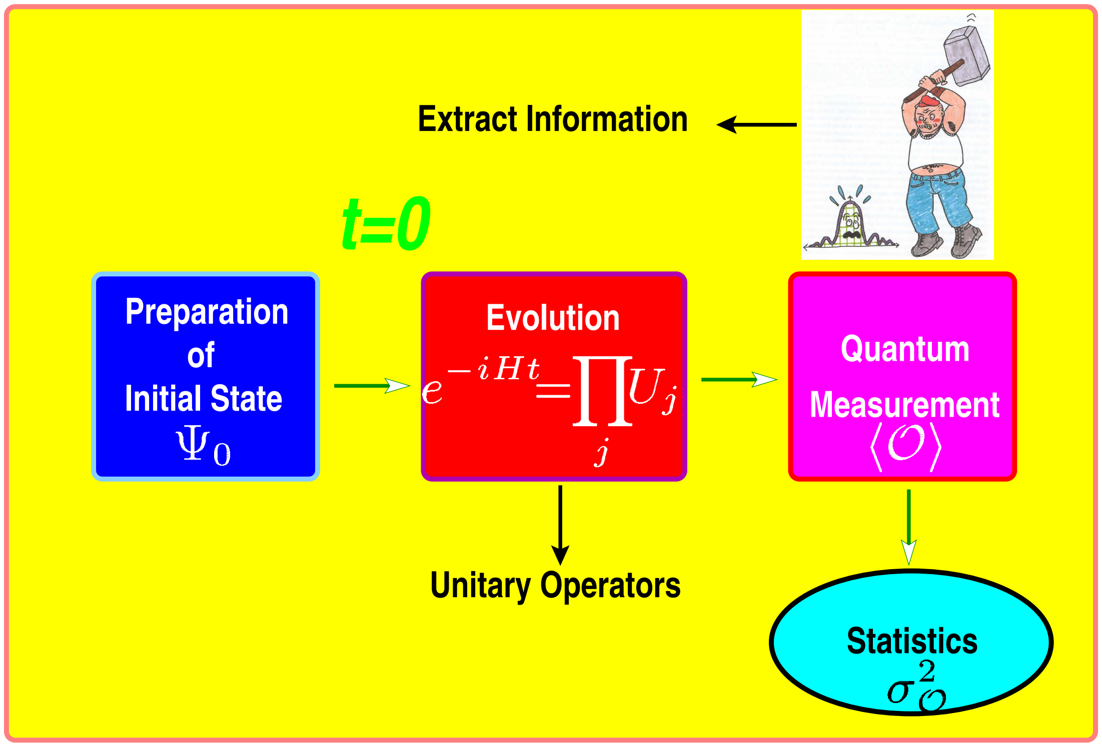
Will a quantum computer solve these problems?

Layman's reasoning

Naive argument: A quantum computer is a physical system and physical systems have no dynamical or fermion sign problems.

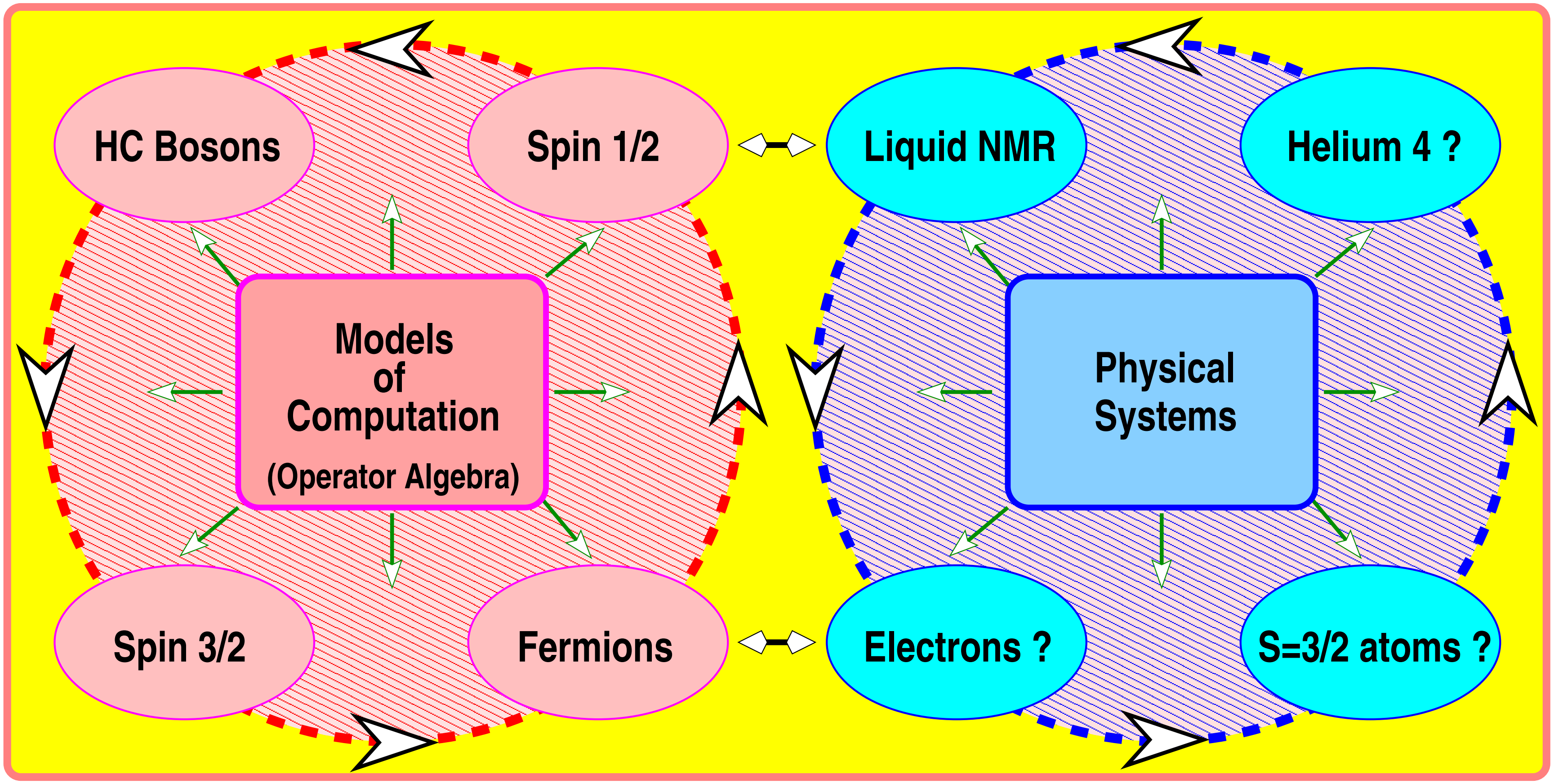
However: A quantum computer suffers from limited accuracy.

One has to show that:

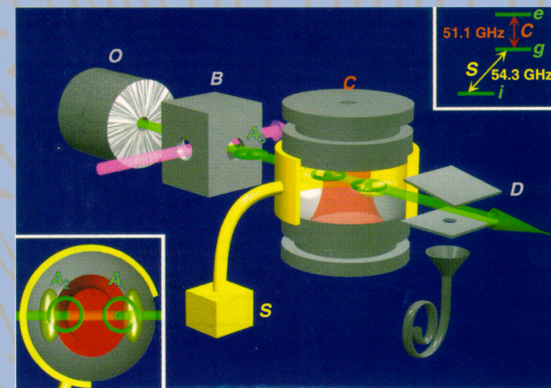


can be done with polynomial complexity

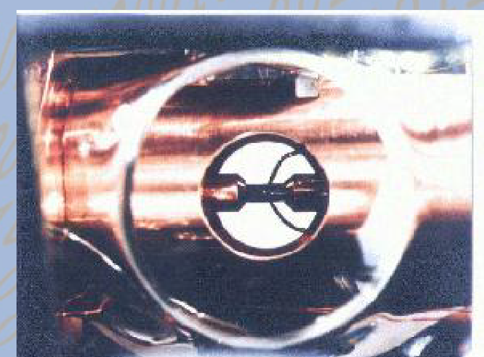
Models of Computation and Physical Systems

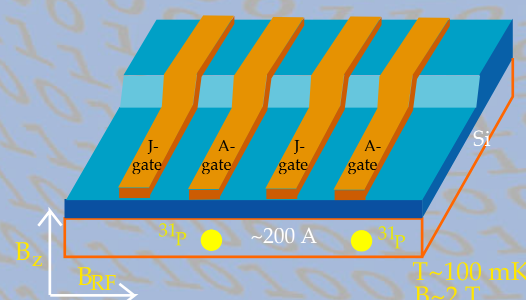


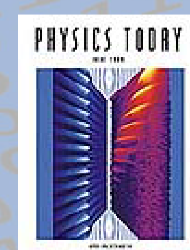
Devices for Quantum Information Processing



- Atom traps
- Cavity QED
- Electron floating on helium
- Electron trapped by surface acoustic waves
- LANL P — Ion traps
- LANL CSS-T — Nuclear Magnetic Resonance
- LANL CSS-T — Quantum Optics
- Quantum dots
- LANL MST — Solid state
- LANL CSS-MST-T — Spintronics
- Superconducting Josephson junctions







Specifying a Model of Computation

§1. What is the state space?

§2. What is the initial state?

§3. How can states be manipulated; how do states evolve?

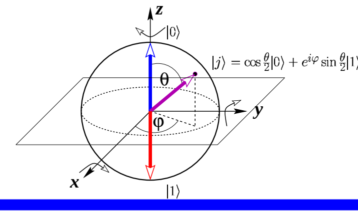
§4. How do we gain information about a state? (Readout)

Models of Quantum Computation

A model requires physical systems that can be controlled by modulating the parameters of the system Hamiltonian H_P (*quantum control*)

The method for defining a model of quantum computation consists of giving an algebra of operators (acting on the qubits) with Hermitian conjugation together with the set of controllable Hamiltonians (Hermitian operators in the algebra), the set of measurable observables, and an initial state. In the simplest case, projective (von Neumann) measurements of the observables may be assumed, and the initial state is an expectation of the algebra's operators.

Standard Model



Operator algebra: For each qubit j,

$$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

For a *quantum register* with n qubits: $\sigma_\mu^j = \mathbb{1} \otimes \mathbb{1} \otimes \cdots \otimes \underbrace{\sigma_\mu}_{j^{th} \text{ factor}} \otimes \cdots \otimes \mathbb{1}$.

Control Hamiltonians: For universal computation

$$H_P(t) = \sum_j [\alpha_{x_j}(t)\, \sigma_x^j + \alpha_{y_j}(t)\, \sigma_y^j] + \sum_{i,j} \alpha_{ij}(t)\, \sigma_z^i \sigma_z^j,$$

where the $\alpha_\mu(t)$, and $\alpha_{i,j}(t)$ are controllable.

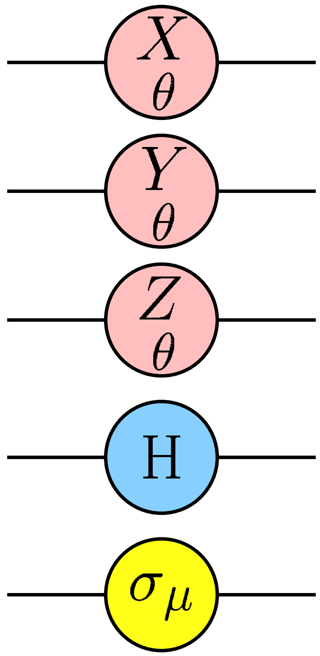
<u>Theorem</u>: Single qubit rotations + Two qubits interaction is sufficient to build any unitary operation.

$\oplus$ Universal set of gates:

$$e^{i\theta_1 \sigma_x^i}\; , \; e^{i\theta_2 \sigma_y^i}\; , \; e^{i\theta_3 \sigma_z^i \sigma_z^j}$$

The Language of Quantum Networks

One qubit:



$e^{i\theta\sigma_x}$

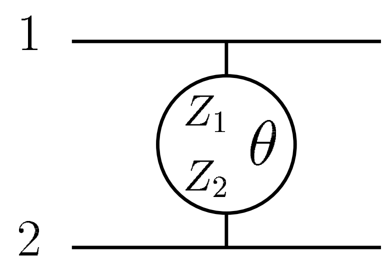
$e^{i\theta\sigma_y}$

$e^{i\theta\sigma_z}$

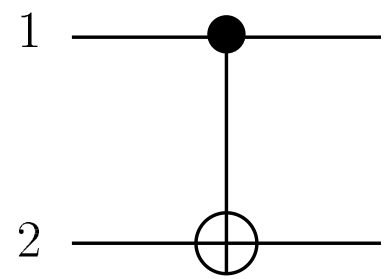
$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$

σ_μ

Two qubit:

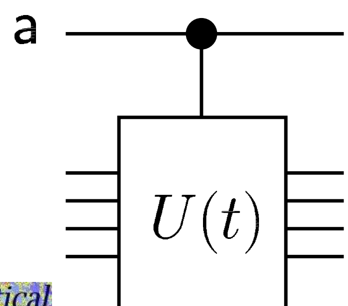


$e^{i\theta\sigma_z^1\sigma_z^2}$

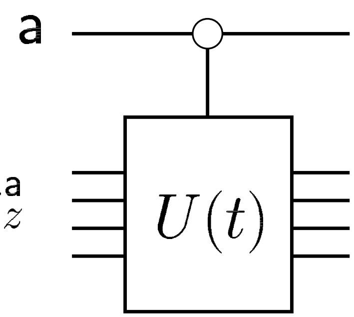


$$\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{pmatrix}$$

Controlled-U:



$U(\frac{t}{2})U(\frac{t}{2})^{-\sigma_z^{a}}$



$U(\frac{t}{2})U(\frac{t}{2})^{\sigma_z^{a}}$

Fermion Model: Grassmann Chip

Operator algebra: Generators $(a_j, a_j^\dagger)$ of a $*$-algebra of dimension 2^{2n} $(j = 1, \cdots, n)$ satisfying

$$
\begin{aligned}
\{a_i, a_j\} &= 0 \\
\{a_i, a_j^\dagger\} &= \delta_{ij} \ ,
\end{aligned}
$$

A basis of operators is: $1, a_j, a_j^\dagger, a_j^\dagger a_j = n_j$

Control Hamiltonians: For universal computation

$$H_P = \sum_j \left[\alpha_j(t) a_j + \tilde{\alpha}_j(t) a_j^\dagger\right] + \sum_{ij} \alpha_{ij}(t) \left(a_i^\dagger a_j + a_j^\dagger a_i\right) + \beta_{ij}(t)\, a_i^\dagger a_i a_j^\dagger a_j$$

$\oplus$ Universal set of gates:

$$e^{i\theta_1 (a_i^\dagger + a_i)} \ , \ e^{i\theta_2 n_i} \ , \ e^{i\theta_3 n_i n_j}$$

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Fermion Computation via the Standard Model

Given a fermion model algorithm, can we efficiently obtain an standard model algorithm that produces the desired result?

If it is possible to efficiently simulate the fermion model by the standard model then these two models of computation are equivalent

Modus Operandi: Map the fermion Hamiltonian to the standard model operators. Provided that the number of terms is polynomially bounded in the number n of qubits and provided that each term can be polynomially simulated, the simulation is efficient in n and 1/error.

Spin-Particle Connection

Spin language is mapped onto particle language in any spatial dimension and for any particle statistics*

* C.D. Batista and G. Ortiz, PRL 86, 1082 (2001)

$$\text{Standard Model} \mapsto \text{Grassmann Chip Model}$$

$$\Downarrow$$

$$S = \frac{1}{2} \mapsto \text{spinless fermions}$$

From the $2n$ matrices γ_μ (of dimension $2^n \times 2^n$, $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$)

$$\begin{aligned} \gamma_1 &= \sigma_x^1, & \gamma_2 &= \sigma_y^1 \\ \gamma_3 &= \sigma_z^1 \sigma_x^2, & \gamma_4 &= \sigma_z^1 \sigma_y^2 \\ \gamma_5 &= \sigma_z^1 \sigma_z^2 \sigma_x^3, & \gamma_6 &= \sigma_z^1 \sigma_z^2 \sigma_y^3 \end{aligned}$$

$$\vdots$$

$$\gamma_{2n-1} = [\prod_{j=1}^{n-1} \sigma_z^j] \sigma_x^n, \qquad \gamma_{2n} = [\prod_{j=1}^{n-1} \sigma_z^j] \sigma_y^n \ .$$

$$a_j \ \rightarrow \ \left(\prod_{i=1}^{j-1} - \sigma_z^i \right) \sigma_-^j = (-1)^{j-1} \ \sigma_z^1 \sigma_z^2 \cdots \sigma_z^{j-1} \sigma_-^j = (-1)^{j-1} \ \frac{\gamma_{2j-1} - i\gamma_{2j}}{2}$$

$$a_j^\dagger \ \rightarrow \ \left(\prod_{i=1}^{j-1} - \sigma_z^i \right) \sigma_+^j = (-1)^{j-1} \ \sigma_z^1 \sigma_z^2 \cdots \sigma_z^{j-1} \sigma_+^j = (-1)^{j-1} \ \frac{\gamma_{2j-1} + i\gamma_{2j}}{2}$$

"$S = \frac{1}{2}$ $d = 1$ Jordan-Wigner transformation"

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Evolution

In general, if $H_c = \sum_j H_c(j)$, and $[H_c(j), H_c(j')] \neq 0$, one needs a Trotter breakup

Consider $H_c = a_1 a_j^\dagger + a_j a_1^\dagger$ ($j \in$ odd) $\longrightarrow e^{-i\Delta t H_c/\hbar}$

$$H_c = \frac{(-1)^j}{2}[\sigma_x^1\sigma_z^2 \cdots \sigma_z^{j-1}\sigma_x^j + \sigma_y^1\sigma_z^2 \cdots \sigma_z^{j-1}\sigma_y^j] = H_x + H_y$$

How do we write a $U = U_1 \ldots U_k$ such that $H_c = U^\dagger H U$? (each U_i must be of the form $e^{-i\Delta t H_P/\hbar}$)

Procedure: $H = \sigma_z^1$

$$U_1 = e^{i\frac{\pi}{4}\sigma_y^1} = \frac{1}{\sqrt{2}}\left[\hat{\mathbb{1}} + i\sigma_y^1\right]$$

takes $\sigma_z^1 \rightarrow \sigma_x^1$

$$U_2 = e^{i\frac{\pi}{4}\sigma_z^1\sigma_z^2} = \frac{1}{\sqrt{2}}\left[\hat{\mathbb{1}} + i\sigma_z^1\sigma_z^2\right]$$

takes $\sigma_x^1 \rightarrow \sigma_y^1\sigma_z^2$

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$$\vdots$$

$$U_j = e^{i\frac{\pi}{4}\sigma_z^1\sigma_z^j}$$

takes $\sigma_y^1\sigma_z^2\cdots\sigma_z^{j-1} \rightarrow (-1)^{\left[\frac{j-1}{2}\right]}\sigma_x^1\sigma_z^2\cdots\sigma_z^j$

$$U_{j+1} = e^{i\frac{\pi}{4}\sigma_y^j}$$

will bring the control operator to the desired one H_x

$$\Downarrow$$

$$\boxed{\text{The number of steps scales polynomially with the complexity}}$$

Preparation of Initial State

Any (Perelomov-Gilmore) generalized coherent state can be prepared with polynomial complexity

A generic N_e-fermion state can be written ($N_e \leq n$)

$$|\Psi(t=0)\rangle = \sum_{\alpha=1}^{N} \mathsf{a}_\alpha \, |\Phi_\alpha\rangle \ ,$$

where the integer N is a finite and small number (not $\begin{pmatrix} n \\ N_e \end{pmatrix}$)

$$|\Phi_\alpha\rangle = \prod_{j=1}^{N_e} b_j^\dagger \, |0\rangle$$

is a Slater determinant and ($\vec{a}^\dagger = (a_1^\dagger, \cdots, a_n^\dagger)$)

$$b_j^\dagger = \sum_{i=1}^{n} a_i^\dagger P_{ij} = e^{iM} \vec{a}^\dagger, \quad M \in (n \times n) \text{ Hermitian}$$

Preparation of $|\Phi_\alpha\rangle$:

$$\text{Given } |\phi\rangle = \prod_{i=1}^{N_e} a_i^\dagger\ |0\rangle, \quad e^{i\frac{\pi}{2}(a_i + a_i^\dagger)}|0\rangle \rightsquigarrow a_i^\dagger\ |0\rangle \text{ (up to } e^{i\frac{\pi}{2}})$$

$\Downarrow$ Thouless's theorem implies

$$\boxed{|\Phi_\alpha\rangle = e^{i\vec{a}^\dagger M \vec{a}}\ |\phi\rangle}$$

With $N+1$ ancilla qubits and conditional operations one builds $|\Psi(t=0)\rangle$

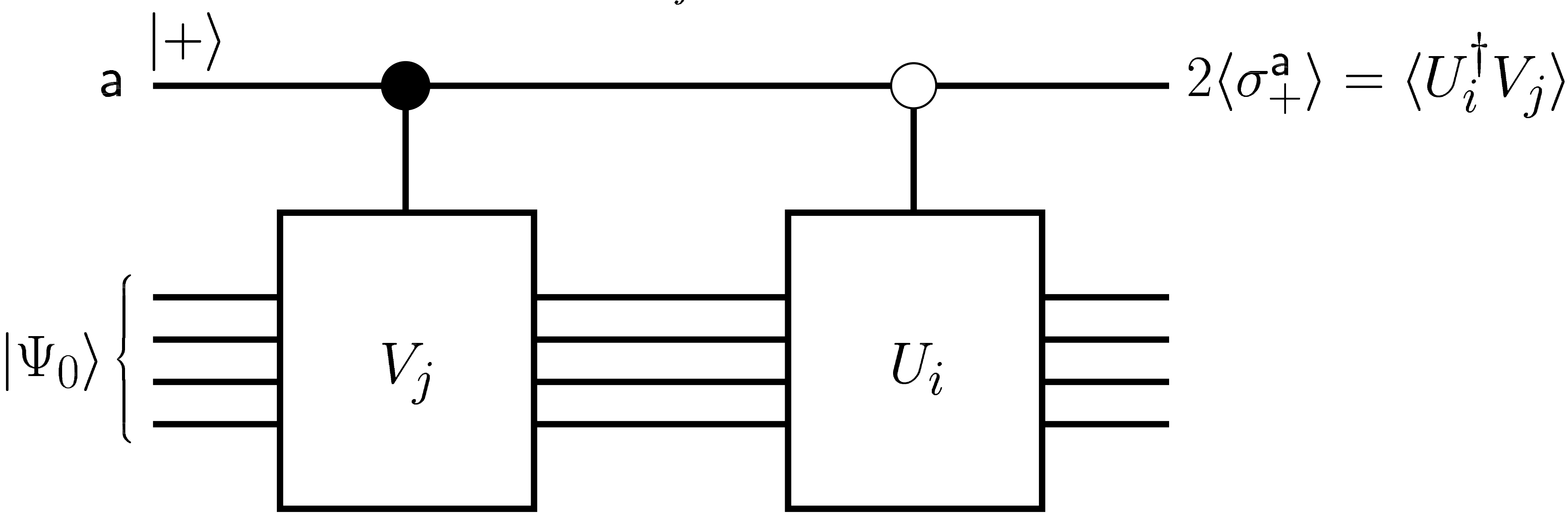
$$\Downarrow$$

Complexity to build $|\Psi(t=0)\rangle$ scales as $\mathcal{O}(N^2 n N_e) \leq \mathcal{O}(N^2 n^2)$

Measurement: Dynamical correlation function

$$C_{AB}(t) = \langle \Psi_0 | A(t) B(0) | \Psi_0 \rangle = \langle e^{iHt} A e^{-iHt} B \rangle$$

$$A(0) = \sum_{i=1}^{m_A} \alpha_i A_i \text{ and } B(0) = \sum_{j=1}^{m_B} \beta_j B_j \ , \quad \text{with } A_j \text{ and } B_j \in \text{unitary}$$



Step 1: $|0\rangle_{\mathsf{a}}\langle 0| \otimes \mathbb{1} + |1\rangle_{\mathsf{a}}\langle 1| \otimes V_j , \quad V_j = B_j$

Step 2: $|0\rangle_{\mathsf{a}}\langle 0| \otimes U_i + |1\rangle_{\mathsf{a}}\langle 1| \otimes \mathbb{1}, \quad U_i = e^{iHt} A_i^\dagger e^{-iHt}$

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Measurement Noise Control

§1. Gate Imperfections:

Quantum Error Correction and Fault Tolerant Computation

$$\Downarrow$$

Effects of physical noise can in principle be ignored

§2. Discretization error:

Trotter decomposition

$$\Downarrow$$

$$(\Delta t)^m$$

§3. Measurement Statistics:

$C_{AB}(t)$ is a sum of $\mathcal{O}(m_A m_B)$ bounded random variables r_{ij} with $|r_{ij}| \leq 1$

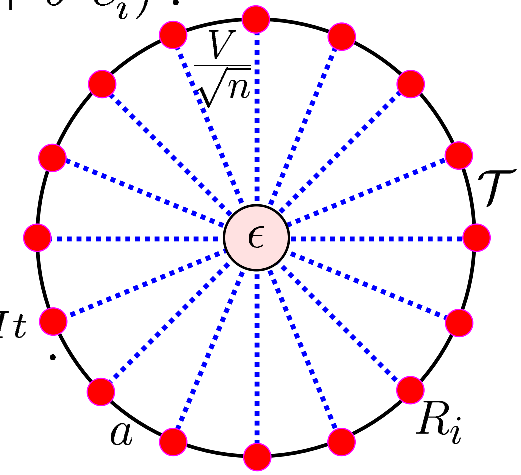
$$\Downarrow$$

Statistical noise $< \epsilon$, it suffices $N_{\rm meas}(r_{ij}) = \mathcal{O}(m_a m_b/\epsilon^2)$

Example: Resonant Impurity Scattering

A) System to simulate: $L = na$, $R_i = ia$ (n := # of modes, $c^\dagger_{i+n} = c^\dagger_i$)

$$H = -\mathcal{T} \sum_{i=1}^{n} (c^\dagger_i c_{i+1} + c^\dagger_{i+1} c_i) + \epsilon\, b^\dagger b + \frac{V}{\sqrt{n}} \sum_{i=1}^{n} (c^\dagger_i b + b^\dagger c_i)\ .$$



B) Property to compute: Probability to stay in $|\Psi(0)\rangle$

$$G(t) = \langle \Psi(0) | b(t) b^\dagger(0) | \Psi(0) \rangle\ ,\ b(t) = e^{iHt}\, b(0)\, e^{-iHt}\ .$$

C) Initial state: Fermi sea of $N_e \leq n$ fermions

$$|\Psi(0)\rangle = |FS\rangle = \prod_{i=0}^{N_e-1} c^\dagger_{k_i} |0\rangle\ ,\ c^\dagger_{k_i} = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} e^{ik_i R_j}\ c^\dagger_j$$

$k_j = k_j = \frac{2\pi n_j}{L}$, with n_j an integer ($-\frac{\pi}{a} < k \leq \frac{\pi}{a}$), $|0\rangle$:= vacuum

Quantum Algorithm to compute $G(t)$

Spin-Fermion Mapping: First Fourier-transformed modes

$$
\begin{aligned}
b &= \sigma_-^1 & b^\dagger &= \sigma_+^1 \\
c_{k_0} &= -\sigma_z^1 \sigma_-^2 & c_{k_0}^\dagger &= -\sigma_z^1 \sigma_+^2 \\
&\vdots & &\vdots \\
c_{k_{n-1}} &= (-1)^n \sigma_z^1 \sigma_z^2 \cdots \sigma_z^n \sigma_-^{n+1} & c_{k_{n-1}}^\dagger &= (-1)^n \sigma_z^1 \sigma_z^2 \cdots \sigma_z^n \sigma_+^{n+1} \, .
\end{aligned}
$$

Standard Model Hamiltonian: (2-qubit problem) $\mathcal{E}_{k_i} = -2\mathcal{T} \cos k_i a$

$$
2H = \left[\epsilon + \sum_{i=0}^{n-1} \mathcal{E}_{k_i} \right] \mathbb{1} + \epsilon \sigma_z^1 + \sum_{i=0}^{n-1} \mathcal{E}_{k_i} \sigma_z^{i+2} + V(\sigma_x^1 \sigma_x^2 + \sigma_y^1 \sigma_y^2) \, .
$$

Preparation Initial State: Same as before

Physical Quantity: $G(t) = \langle \mathcal{A}(t) \rangle$

$$\mathcal{A}(t) = b(t)b^\dagger(0) = e^{i\bar{H}t}\sigma_-^1 e^{-i\bar{H}t}\sigma_+^1 \ .$$

$$\bar{H} = \frac{\epsilon}{2}\sigma_z^1 + \frac{\mathcal{E}_{k_0}}{2}\sigma_z^2 + \frac{V}{2}(\sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2) \ .$$

Exact Unitary Mapping: $e^{-i\bar{H}t} = U e^{-iH_{P1}t} U^\dagger$

$$U = e^{i\frac{\pi}{4}\sigma_x^2} e^{-i\frac{\pi}{4}\sigma_y^1} e^{-i\frac{\theta}{2}\sigma_z^1\sigma_z^2} e^{i\frac{\pi}{4}\sigma_y^1} e^{i\frac{\pi}{4}\sigma_x^1} e^{-i\frac{\pi}{4}\sigma_x^2} e^{-i\frac{\pi}{4}\sigma_y^2} e^{i\frac{\theta}{2}\sigma_z^1\sigma_z^2} e^{-i\frac{\pi}{4}\sigma_x^1} e^{i\frac{\pi}{4}\sigma_y^2} \ ,$$

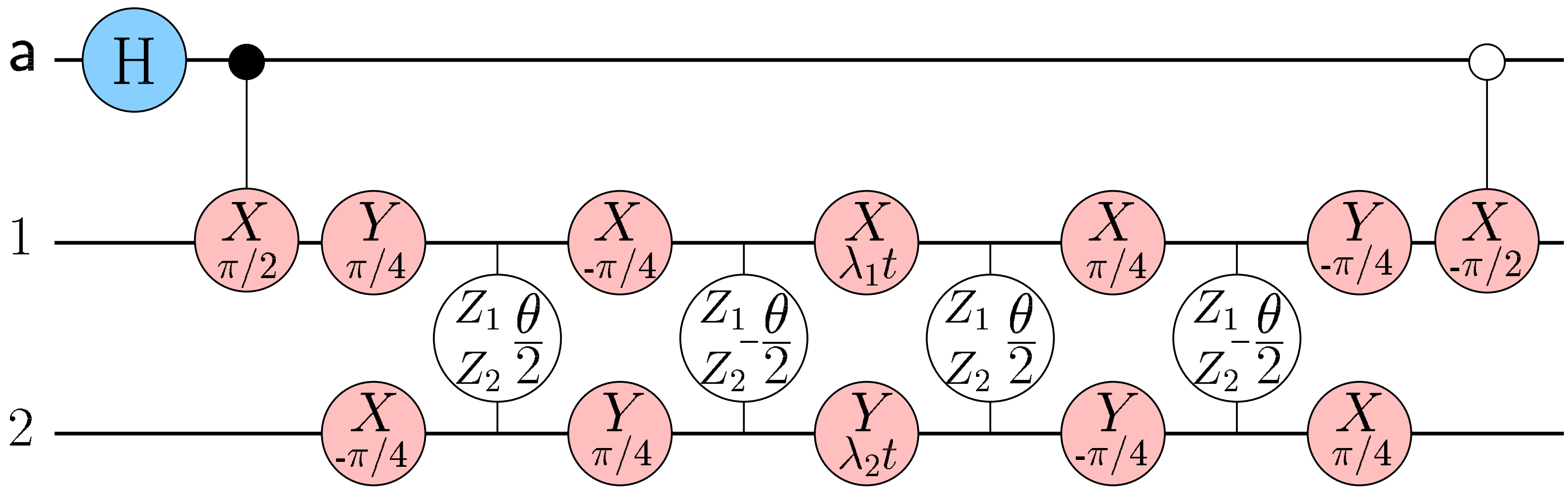
$$H_{P1} = \frac{1}{2}(E - \sqrt{\Delta^2 + V^2})\sigma_z^1 + \frac{1}{2}(E + \sqrt{\Delta^2 + V^2})\sigma_z^2 \ ,$$

Approximate Unitary Mapping: Trotter breakup

$$e^{i\bar{H}t} = \left[e^{i\bar{H}s}\right]^M = \left[e^{i\bar{H}_z s} e^{i\bar{H}_{xy} s} + \mathcal{O}(s^2)\right]^M \ , \ \bar{H} = \bar{H}_z + \bar{H}_{xy} \ .$$

Quantum Network for Resonant Scattering

$$|\Psi(0)\rangle = |0\rangle_{\mathsf{a}} \otimes |1\rangle_1 \otimes |0\rangle_2$$



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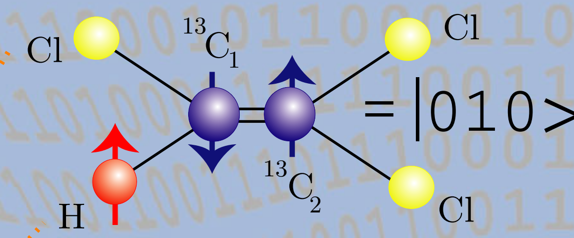
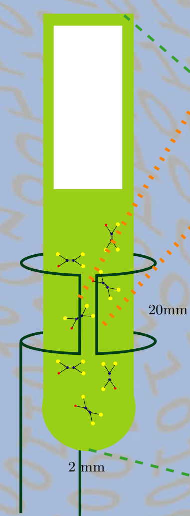
Liquid State NMR

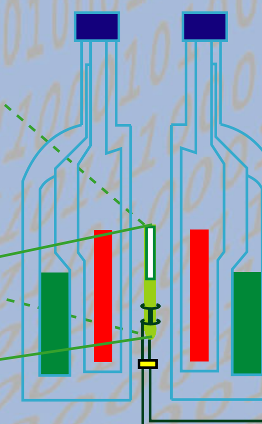
Cory & Havel PNAS, 64, 1634, 1997
Gershenfeld & Chuang, Science 275, 350, 1997

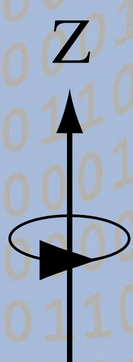
-Larmor Frequency~ 500MHz
-Single bit gate: 1/ ~ms
-Two qubit gate: ~ 10ms
z^1 z^2 interaction
-T2 ~ 1s
-T1 ~ 5-30s
- =e$^-$ H ~ 1- H

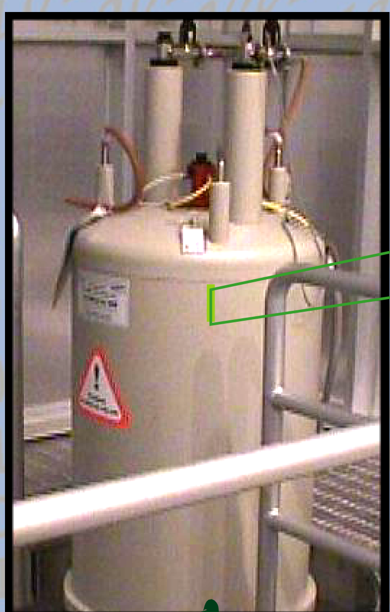


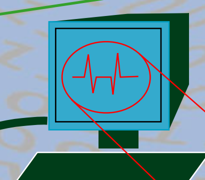
Trichloroethylene

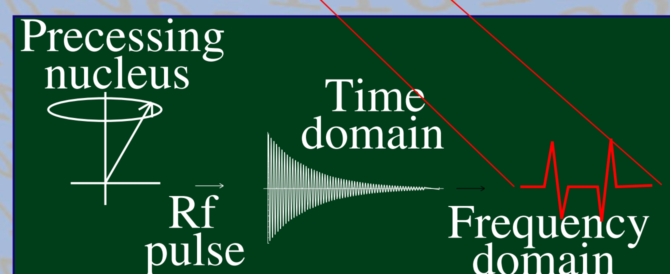






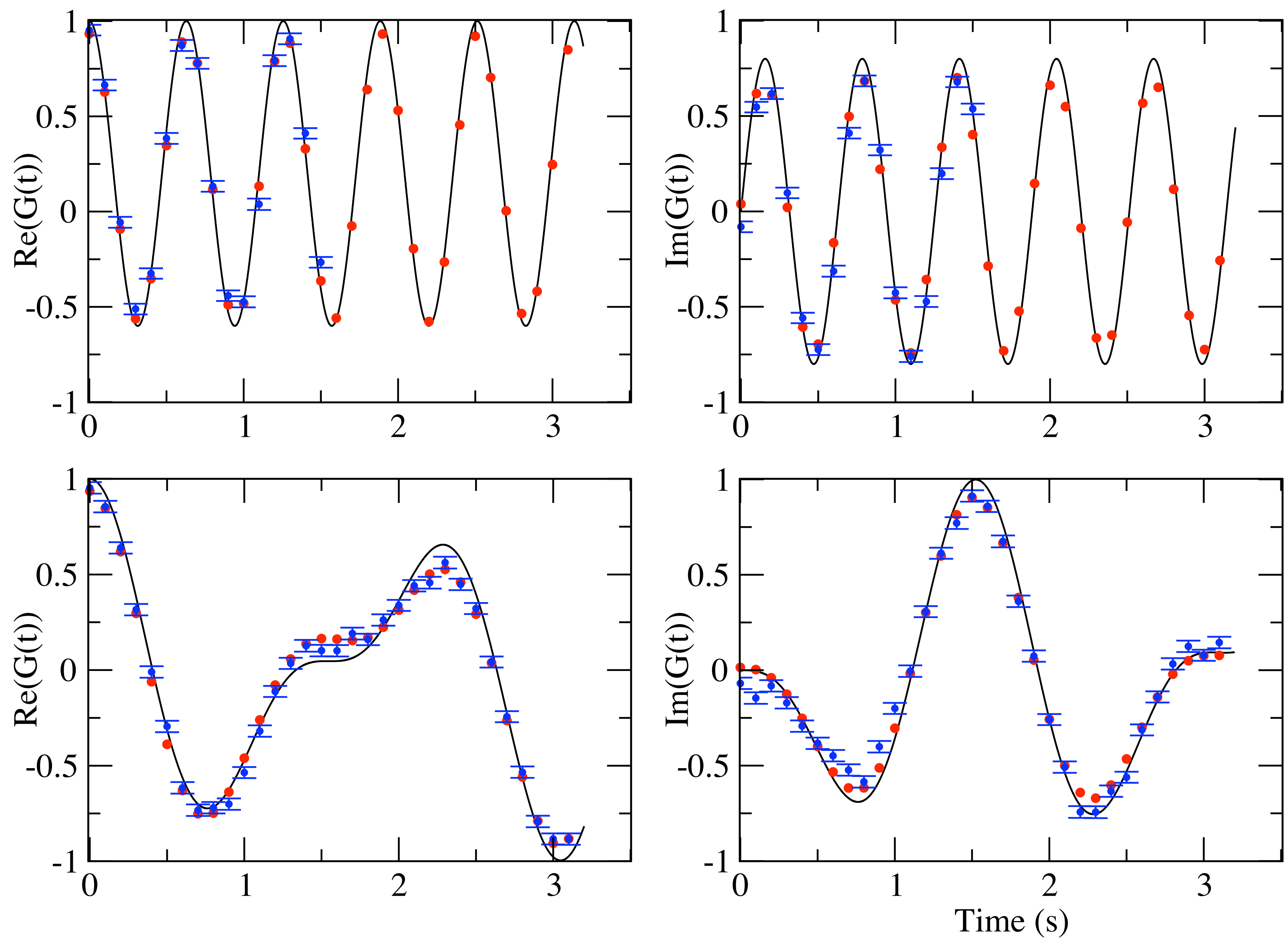

Bruker DRX-500





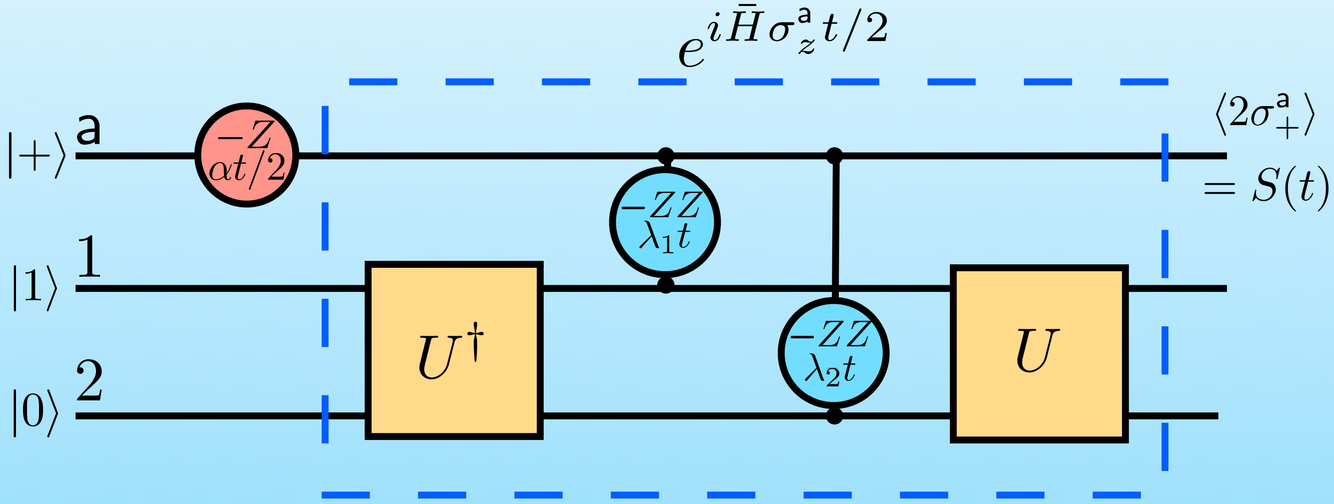
Green's function G(t)

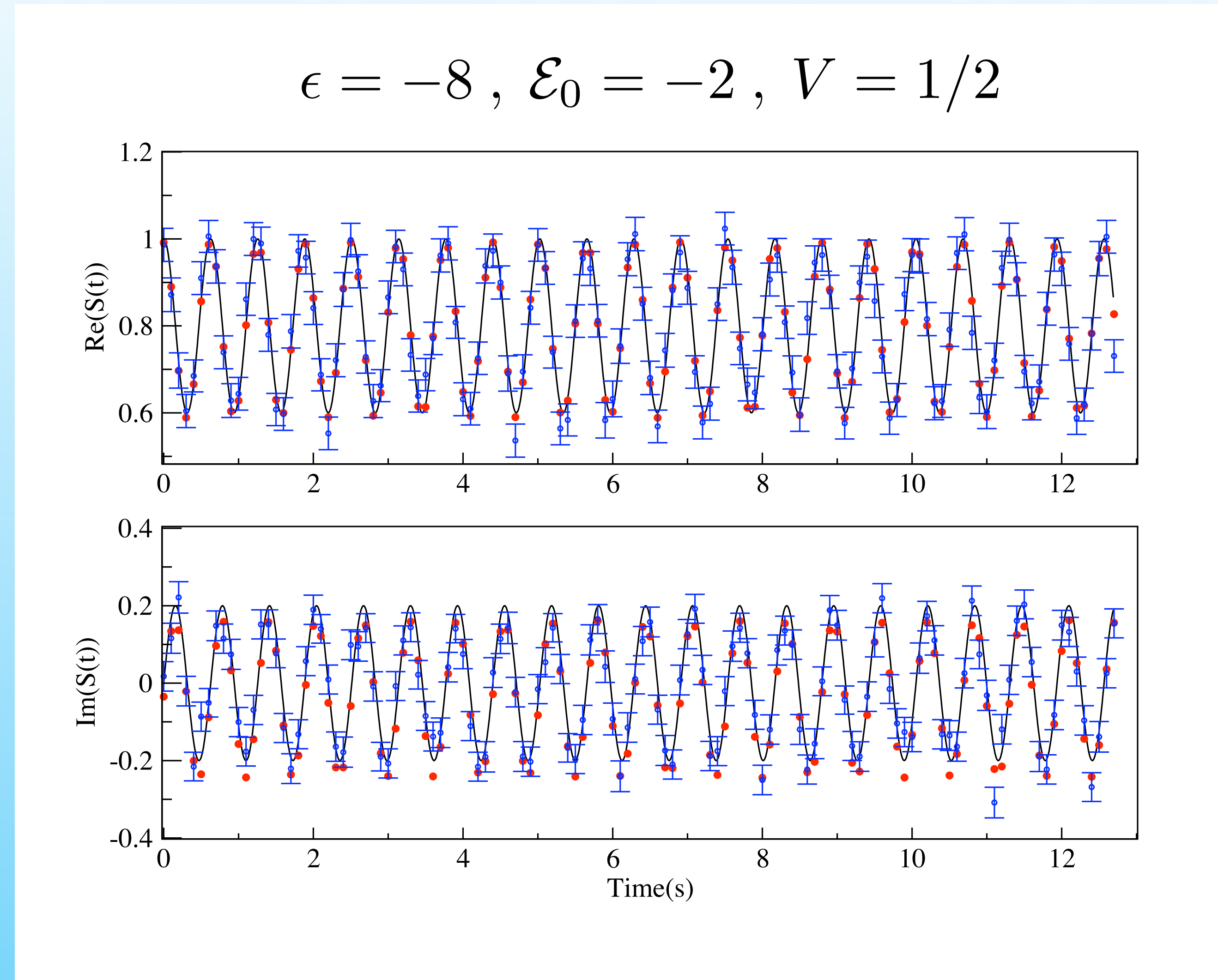
$$\epsilon = -8\ ,\ \mathcal{E}_0 = -2\ ,\ V = 4$$

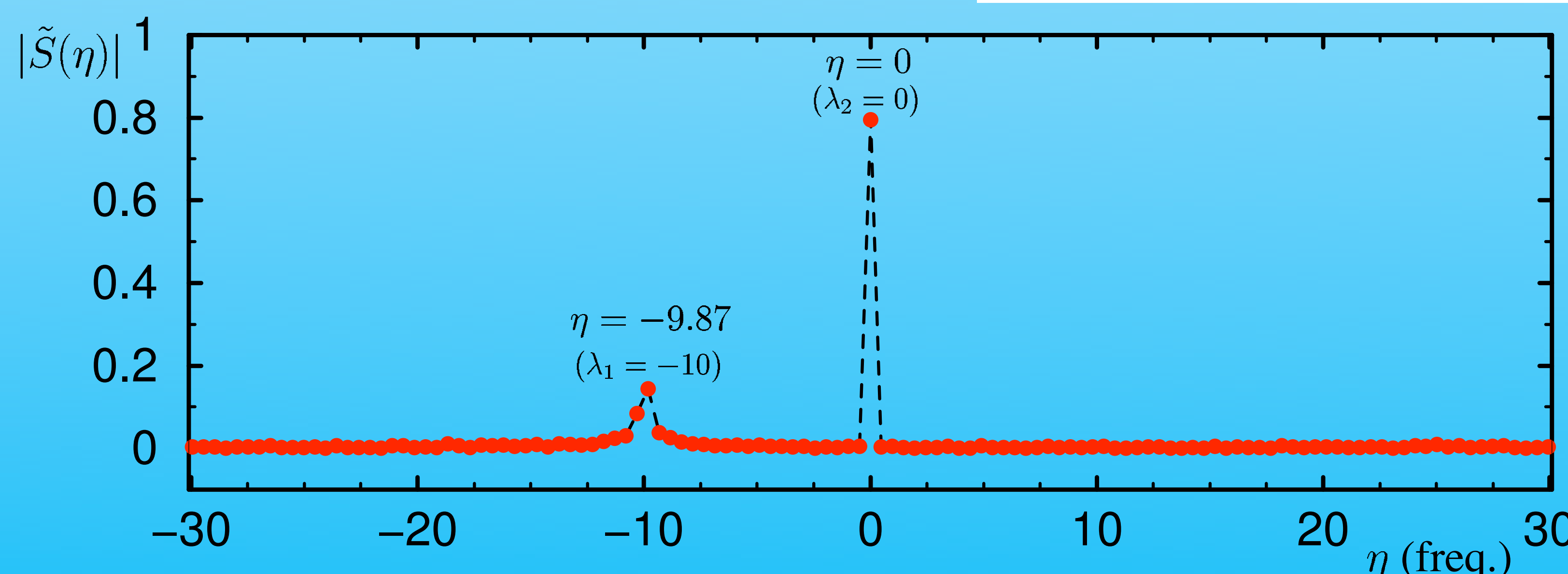


$$\epsilon = 0\ ,\ \mathcal{E}_0 = -2\ ,\ V = 4$$

Energy Spectrum







Main Messages

Physical Systems and Models of Computation:

A key fundamental concept in information theory is the realization that a model of computation is intimately connected to a physical system through an operator algebra. In other words, each physical system is associated to a certain language (e.g., spin 1/2) and thus to an algebra describing it (e.g., Pauli algebra). That particular algebra is a possible model of computation. Therefore, an arbitrary physical system can be simulated by another physical system (quantum computer) whenever there exists an isomorphic mapping between the different operator algebras representing each system.

Quantum Imitation and Efficiency:

It is this last connection that allows one to imitate quantum phenomena with a *quantum computer*. Imitation is realized through a quantum algorithm that consists of *unitary operations* and *measurements*. One of the objectives is to accomplish imitation *efficiently*, i.e, with polynomial complexity. The hope is that quantum imitation is *more* efficient (less resources) than classical imitation and there are examples that support such hope (Dynamical correlation functions).

Quantum Networks and Physical Phenomena:

All possible physical phenomena can be mapped onto a quantum network. (A quantum network is a set of elementary universal quantum gates.) Their realization is limited by the "ability of the programmer" and formulation of the "right questions."

Dynamical correlation functions	$\longrightarrow$	Exponential speed-up
Shor's factoring	$\longrightarrow$	Superpolynomial ($e^{n^{\frac{1}{2}}\cdots}$) speed-up
Grover's unstructured search	$\longrightarrow$	Quadratic speed-up

"If you had discrete quantum systems, what other discrete quantum systems are exact imitators of it, and is there a class against which everything can be matched? I believe it's rather simple to answer that question and to find the class, but I just haven't done it."

R.P. Feynman

What are the Big Challenges?

§1. Can we find an interesting physical problem (question) that a quantum computer can resolve impossible to address with a classical computer? (Let's say with $\mathcal{O}(100)$ qubits and $\mathcal{O}(10^4)$ gates)

§2. What computational resources are required to answer interesting questions?

— Confinement, etc. in QCD ?

— $N > 12$ nuclei ?

— $\ldots$

§3. Quantum Control: Is there any physical limitation to what can be really achieved?

• Developed efficient quantum networks for the evaluation of the physical properties of an arbitary system.

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