The Challenge of Quantum Computer Simulation of Physical Phenomena

Gerardo Ortiz

Theoretical Division (T-11)

Los Alamos National Laboratory

J.E. Gubernatis

E. Knill

R. Laflamme

} Simulation of Physical Systems

R. Somma: "Quantum Simulator," Lattice Systems, Experiment

C.J. Negrevergne: NMR Experiment

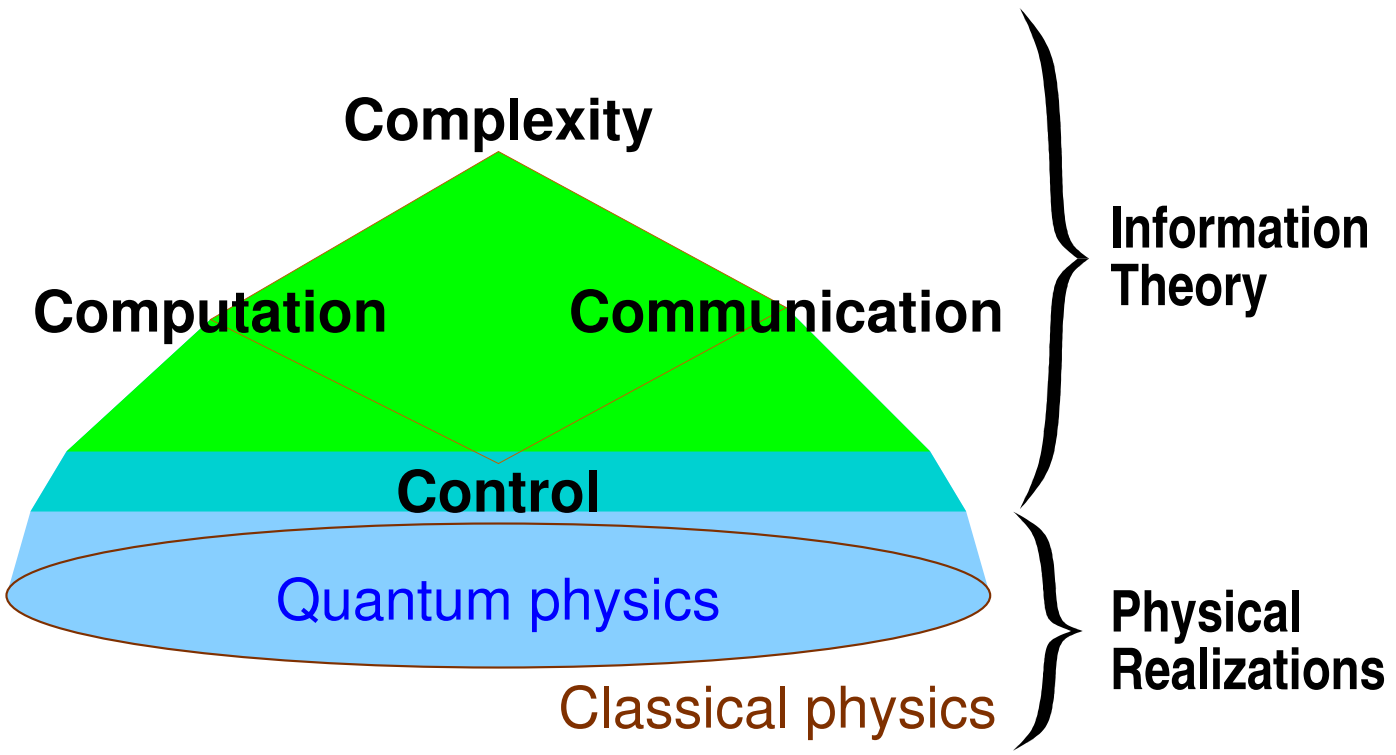
Theoretical Division

Los Alamos NATIONAL LABORATORY

Quantum Information Processing

QUANTUM INFORMATION PROCESSING, SCIENCE OF - The theoretical, experimental and technological areas covering the use of quantum mechanics for communication and computation.

Kluwer Encyclopedia of Mathematics, Supplement III



Outline

§1. What is the Challenge?:

— Can quantum systems be (*deterministically, probabilistically*) simulated by a classical computer?

— Can quantum systems be simulated by a quantum computer?

Feynman suggested that q. prob. are too complex for a c. comp.

§2. Simulation of Physical Phenomena: Fermions

— Models of quantum computation $\Longleftrightarrow$ Algebra of operators

— Spin-particle connection

— Solving some fermion "sign(phase) problems"

Exponential complexity $\mapsto$ Polynomial complexity

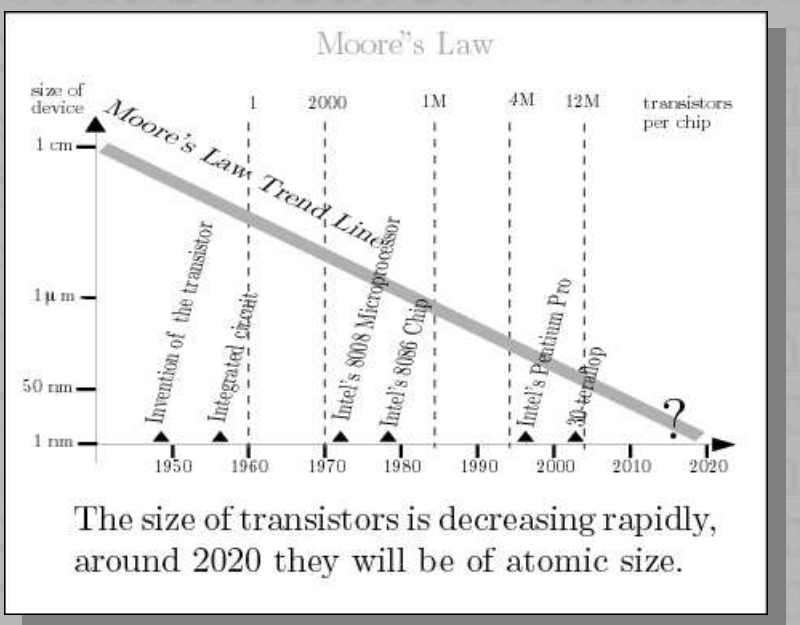
§3. Example of a Quantum Algorithm: Resonant impurity scattering

$\rightarrow$ Simulation in a REAL quantum computer

§4. Conclusions + Next steps

Why Quantum Computation?

We are advancing towards the quantum scale:



The size of transistors is decreasing rapidly, around 2020 they will be of atomic size.

www.sciencemag.org SCIENCE VOL 285 24 SEPTEMBER 1999 207

SCIENCE'S COMPASS

PERSPECTIVES: DEVICE PHYSICS

Pushing the Limits

Paul A. Packan

For the past 30 years, the semiconductor industry has followed Moore's law, which states that transistor performance and density double every 3 years (*1*). Although not truly a law, Gordon Moore's statement has yet to be violated. But now it seems to be in serious danger. Fundamental thermodynamic limits are being reached in critical areas, and unless new, innovative solutions are found, the current rate of improvement cannot be maintained.

The dominant electronic device used today in integrated circuits is the silicon-

silicon lattice. In silicon, each
is covalently bonded to the
neighbors in the lattice. Add
atom with five valence electr
the mobile charge concentrat
ing an unbound electron. A
with only three valence elect
accept an extra electron to substitute a sili-
con atom; the localized trapping of the extra electron effectively creates a positive free charge referred to as a "hole." Transistor scaling requires an increase in the concentration of these donor and acceptor atoms to maintain a constant total charge

These fundamental issues have not previously limited the scaling of transistors and represent a considerable challenge for the semiconductor industry. There are currently no known solutions to these problems. To continue the performance trends of the past 20 years and maintain Moore's law of improvement will be the most difficult challenge the semiconductor industry has ever faced.

References

1. G. Moore, *IEDM Tech. Dig.* (1975), p. 11 .
2. R. H. Denard *et al.*, *IEEE J. Solid-State Circuits* **SC-9**,

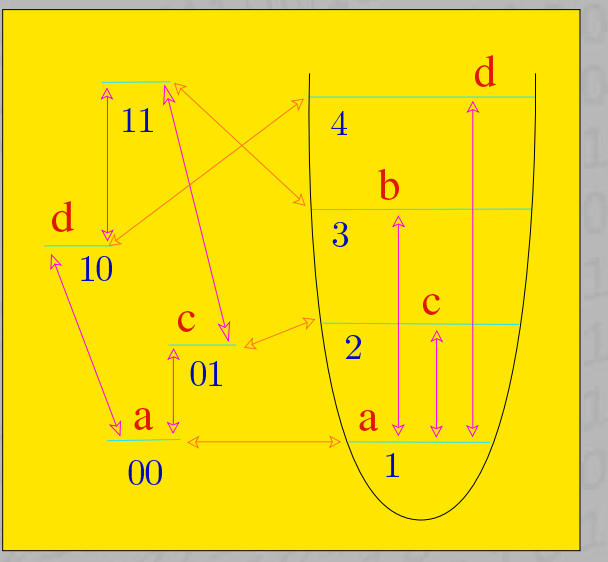
The author is at Intel Corporation, 5200 NE Elam Parkway, Hillsboro, OR 97124, USA. E-mail: paul.a.packan@intel.com

Why quantum computation?

Problems where quantum mechanics is useful:

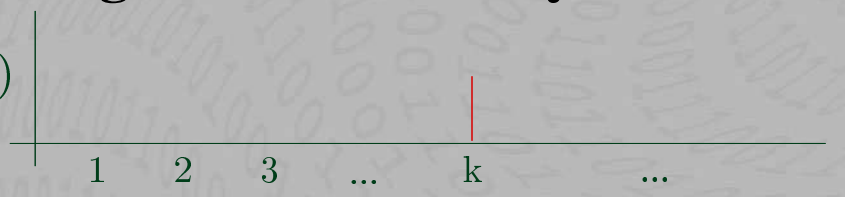
- **Quantum physics simulation:**
  simulation of
  n spin 1/2 systems $2^n \Rightarrow n$

  Feynman, J.O.S. of A, 1984



- **Search: finding a needle in a haystack**

Grover, PRL79, 1997



Classical algorithm ~n Quantum algorithm ~$n^{1/2}$

- **Communication problems such as scheduling**

  Burhman, Cleve, Widgerson, 1998; Raz 1999

- **Factoring a number n=pq**

  Shor, Proc. of the 35'th Annual Symposium on Foundations of Computer Science, 1994

RSA Data Security.
A Security Dynamics Company

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))

Promises of a Quantum Computer

- Are QCs capable of performing any computation which a (deterministic or probabilistic) classical CC may do? (Toffoli gate)
- Can we find a task that a QC can perform better than a CC?

  Q Resources: Superposition + Entanglement + Unitary O

  (QFT:Shor, Deutsch-Jozsa; QSearch; QSimul)
- What can be done with a 100 qubit QC?

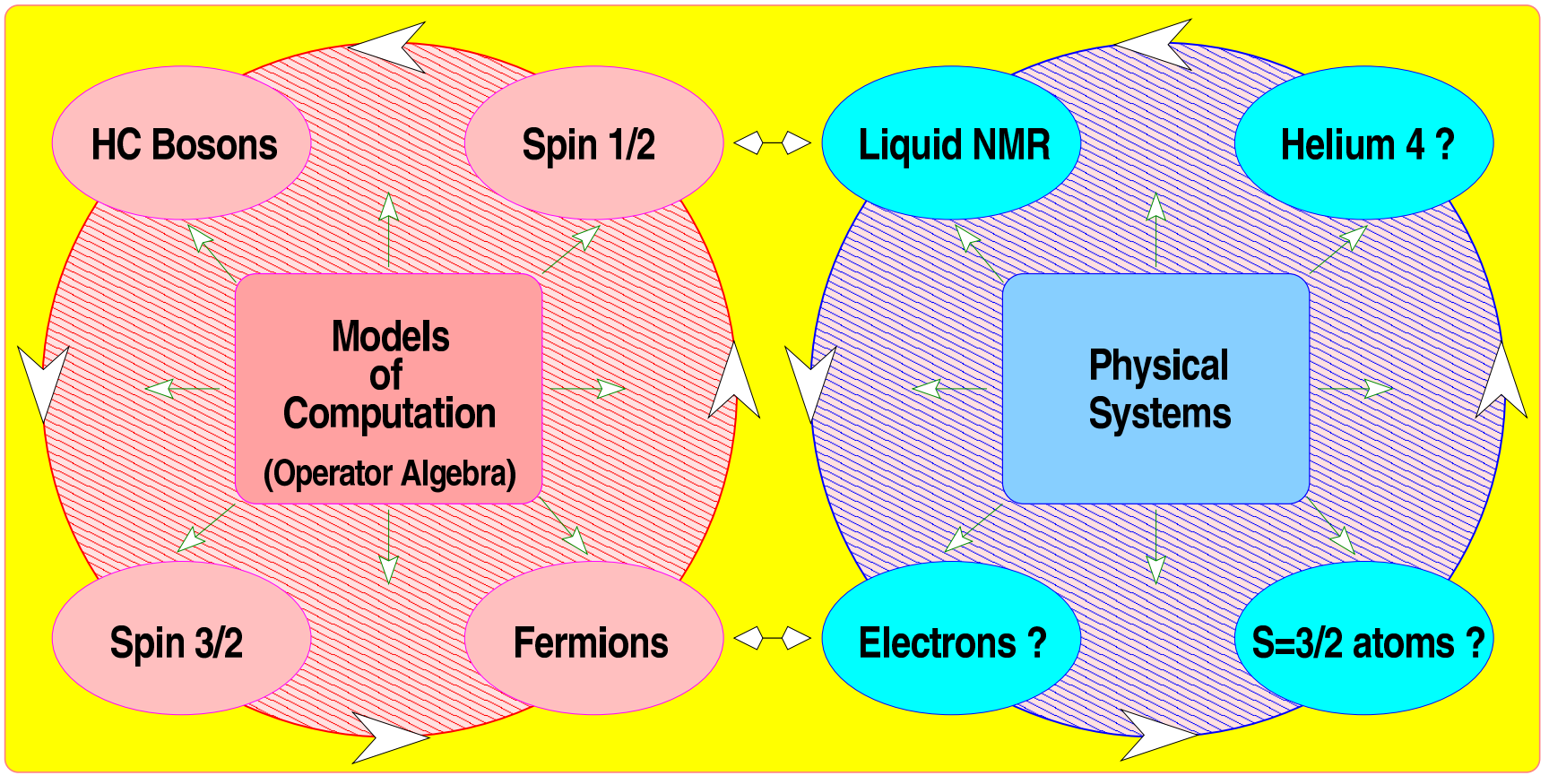
What is the sign problem ?

- The sign problem (SP) is a Disease that shows up when simulating physical systems in a probabilistic Classical computer. Even if the problem is computationally solvable, in principle, it is not solvable in practice.
- There are many kinds of SPs: Dynamic, Projective.
- Symptom: Exponential Complexity in time and number of degrees of freedom.

Can we solve the sign problem ?

- In general, although not rigorously proved, a classical computer (either deterministic or probabilistic) cannot cure the disease.
- One hopes that the problem becomes tractable on a quantum computer.

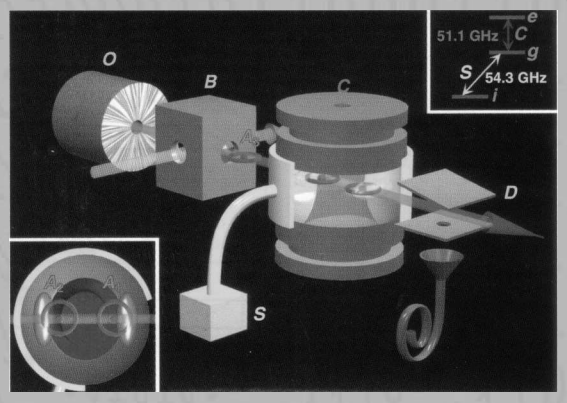
Models of Computation and Physical Systems



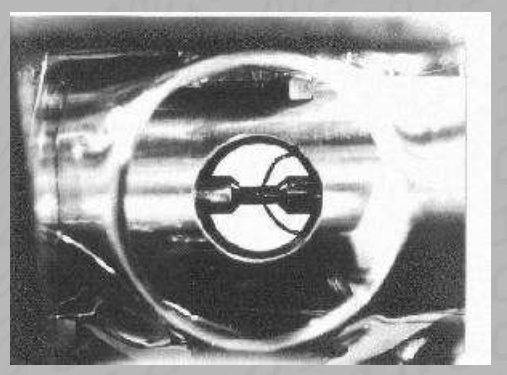
Theoretical Division

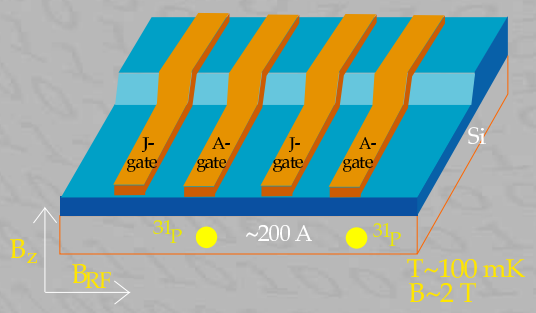
Los Alamos NATIONAL LABORATORY

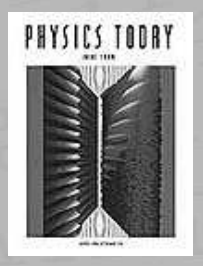
Devices for Quantum Information Processing



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







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.

Specifying a Model of Computation

- What is the state space?
- What is the initial state?
- How can states be manipulated; how do states evolve?
- How do we gain information about a state?

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 $\alpha_\mu(t)$ are controllable.
$\oplus$ Universal set of gates:

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

Initial State: Common eigenstate $|0\rangle$ with eigenvalue 1 of products of the σ_z^j operators. The state is completely determined by $\langle 0|\sigma_{\mu_i}^1 \otimes |0\rangle$

Measurement: Projective (von Neumann) measurement according to the observables σ_z^i. If it is desirable to learn the expectation of an observable at the end of an algorithm, one can accomplish this by repeating the algorithm and measurement and averaging over the measurement outcomes until the desired accuracy is achieved.

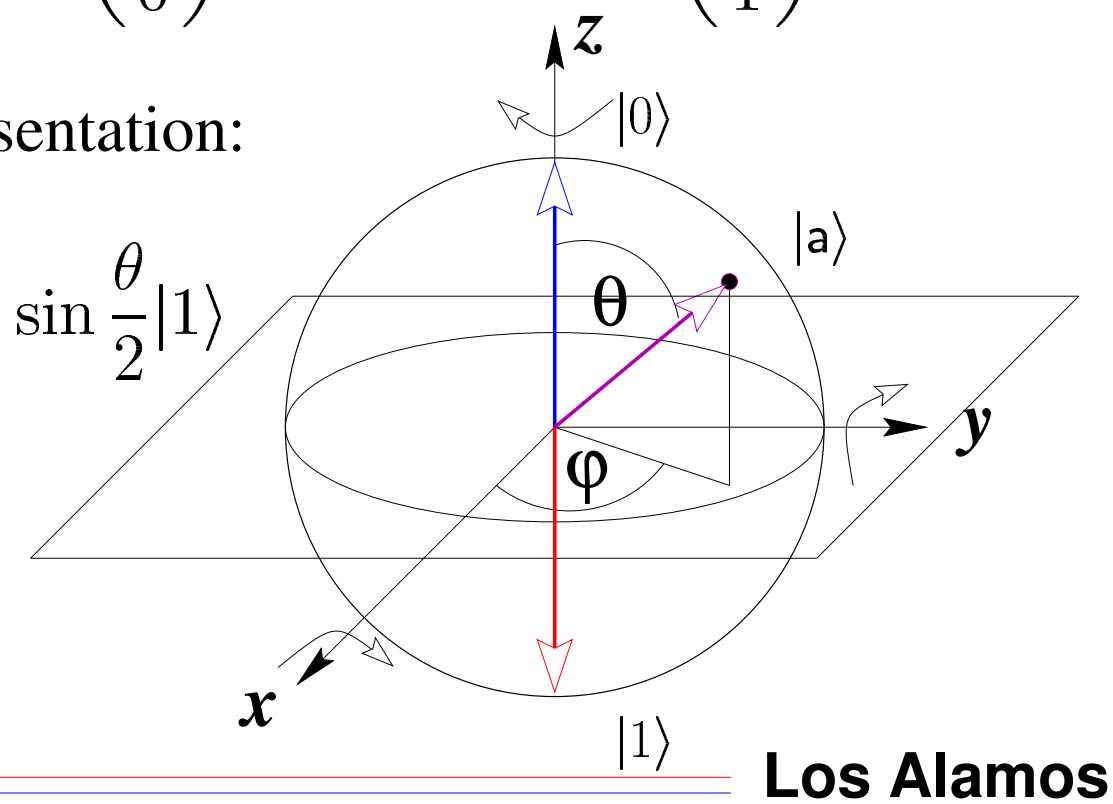
Quantum Bit Representation

Computational Basis:

$$|0\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \ , \ \ |1\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Bloch-sphere Representation:

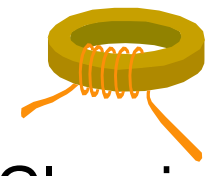
$$|\mathsf{a}\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$



Theoretical Division

Los Alamos NATIONAL LABORATORY

State Space

	1 bit	n bits
 Classical	$0, 1$	$000\ldots, 100\ldots,$ $010\ldots, 110\ldots,$ $001\ldots, \ldots$
Quantum	$\alpha\|0\rangle + \beta\|1\rangle$	$\alpha_{000\ldots}\|000\ldots\rangle +$ $\alpha_{100\ldots}\|100\ldots\rangle +$ $\alpha_{010\ldots}\|010\ldots\rangle +$ $\alpha_{110\ldots}\|110\ldots\rangle +$ $\alpha_{001\ldots}\|001\ldots\rangle + \ldots$

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:

$$e^{i\theta_1(a_i^\dagger a_j + a_j^\dagger a_i)} \ , \ e^{i\theta_2(a_i^\dagger a_j^\dagger + a_j a_i)} \ , \ e^{i\theta_3 n_i} \ , \ e^{i\theta_4 n_i n_j}$$

Initial State: We use the unit operator and the number operator $a_j^\dagger a_j$ such that

$$\langle 0 | a_j^\dagger a_j | 0 \rangle = 0,$$

for all j.

Measurement: It is possible to measure the observables $a_j^\dagger a_j$ for all j.

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)

Standard Model $\mapsto$ **Grassmann Chip Model**

$\Downarrow$

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

From the $2n$ matrices γ_μ (of dimension $2^n \times 2^n$)

$$\begin{aligned} \gamma_1 &= \sigma_x^1, & \gamma_2 &= \sigma_y^1 \\ \gamma_3 &= \sigma_z^1\sigma_x^2, & \gamma_4 &= \sigma_z^1\sigma_y^2 \\ \gamma_5 &= \sigma_z^1\sigma_z^2\sigma_x^3, & \gamma_6 &= \sigma_z^1\sigma_z^2\sigma_y^3 \\ & \vdots & & \\ \gamma_{2n-1} &= [\prod_{j=1}^{n-1}\sigma_z^j]\sigma_x^n, & \gamma_{2n} &= [\prod_{j=1}^{n-1}\sigma_z^j]\sigma_y^n \ . \end{aligned}$$

satisfying $\{\gamma_\mu,\gamma_\nu\}=2\delta_{\mu\nu}$

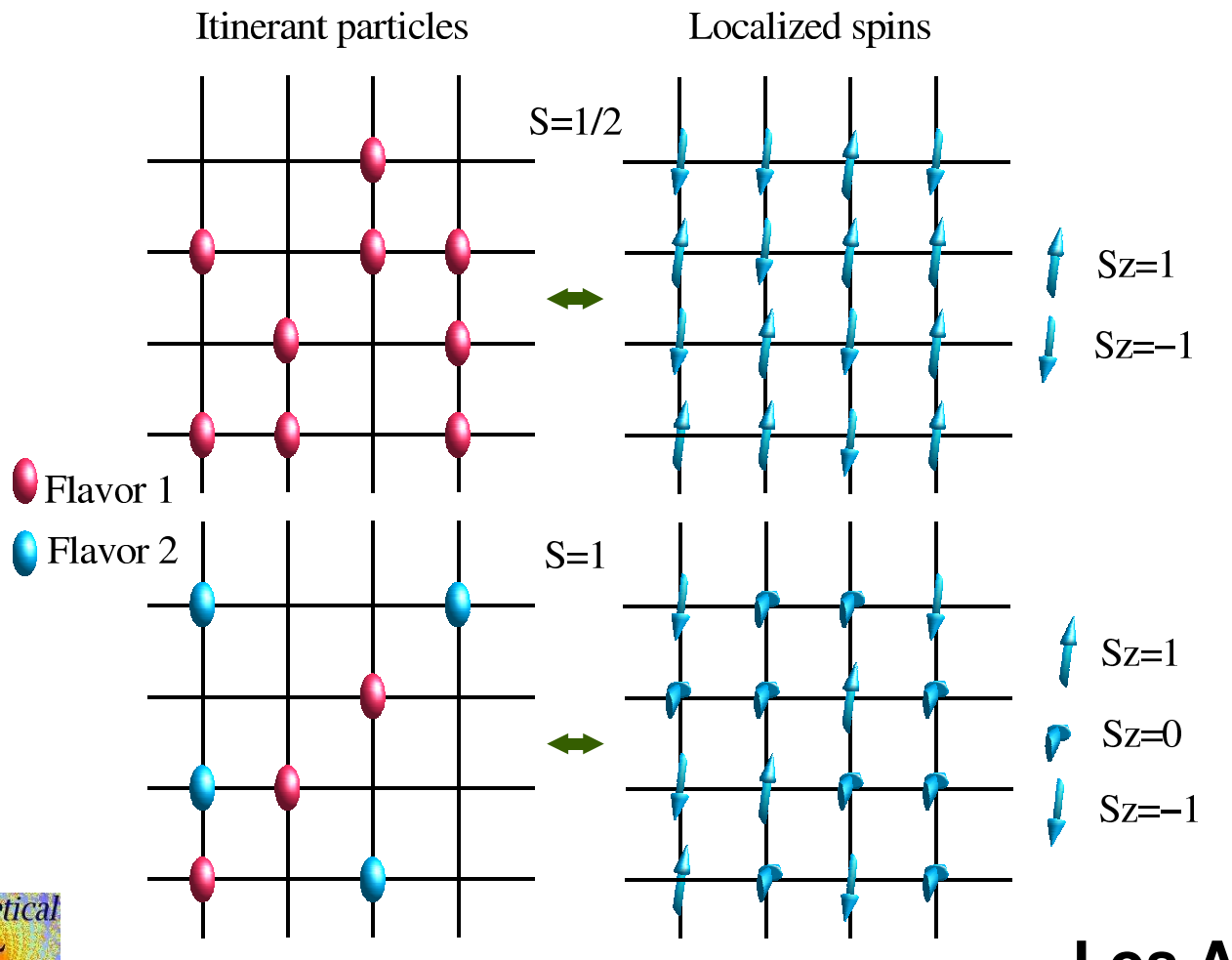
the following mapping of fermion operators results

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

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

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

Spin-Particle Connections



Theoretical Division

Los Alamos NATIONAL LABORATORY

Statistical Mechanics

Quantum Computing

Generalized Jordan-Wigner Transformations

Condensed Matter

Lattice Gauge Theories

Fermion Computation via the Standard Model

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

General Principle: 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.

One has to show that:

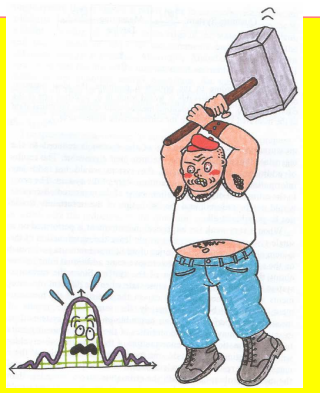
- **Evolution**
- **Preparation of Initial State**
- **Measurement**
- **Measurement Noise Control**

can be done with polynomial complexity

$$\Downarrow$$

Fermion(Phase) Problem is Solved

Defining a Quantum Algorithm



t=0

Preparation of Initial State Ψ_0

→

Evolution $e^{-iHt} = \prod_j U_j$

→

Quantum Measurement $\langle \mathcal{O} \rangle$

↓

Statistics $\sigma^2_{\mathcal{O}}$

Preparation of Initial State

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

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

where the integer N is a finite and small number

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

is a Slater determinant and

$$b_j^\dagger = \sum_{i=1}^{n} a_i^\dagger P_{ij}$$

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

$$e^{i\frac{\pi}{2}(b_m + b_m^\dagger)}|0\rangle \rightsquigarrow b_m^\dagger \ |0\rangle \ (\textbf{up to } e^{i\frac{\pi}{2}})$$

$$\Downarrow$$

Successive applications of $e^{i\frac{\pi}{2}(b_m + b_m^\dagger)} \rightsquigarrow |\Phi_\alpha\rangle$

$$\Downarrow$$

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

Evolution

Consider $H_c = a_1 a_j^\dagger + a_j a_1^\dagger$ **(**$j \in$ **odd)**

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

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** $\exp(-i\Delta t H_P/\hbar)$

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 $\sigma_z^1 \to \sigma_x^1$

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

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

$$\vdots$$

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

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

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

will bring the control operator to the desired one H_x

$$\Downarrow$$

The number of steps scales polynomially with the complexity

Measurement

Correlation function: $C_{AB}(t) = \langle A(t)B(0)\rangle = \langle e^{iHt}Ae^{-iHt}B\rangle$

Decompose:

$$A(0) = \sum_{i=1,m_A} A_i \text{ and } B(0) = \sum_{j=1,m_B} B_j$$

such that A_j **and** $B_j \in$ **unitary.**

Define:

$$U_i = e^{iHt}A_i^\dagger e^{-iHt} \text{ and } V_j = B_j$$

Measurement of $\langle U_i^\dagger V_j\rangle$ **and** $C_{AB}(t)$**: state** ρ

§1. Add an ancilla qubit a in the state $\frac{(|0\rangle+|1\rangle)}{\sqrt{2}}$ **with density matrix** $\rho_{\mathsf{a}} = \frac{(\mathbb{1}+\sigma_x^{\mathsf{a}})}{2}$

§2. Apply the conditional evolution $\bar{U} = |0\rangle\langle 0|\otimes U_i + |1\rangle\langle 1|\otimes V_j$

§3. Measure $2\sigma_+^{\mathsf{a}} = \sigma_x^{\mathsf{a}} + i\sigma_y^{\mathsf{a}} = 2|0\rangle\langle 1|$

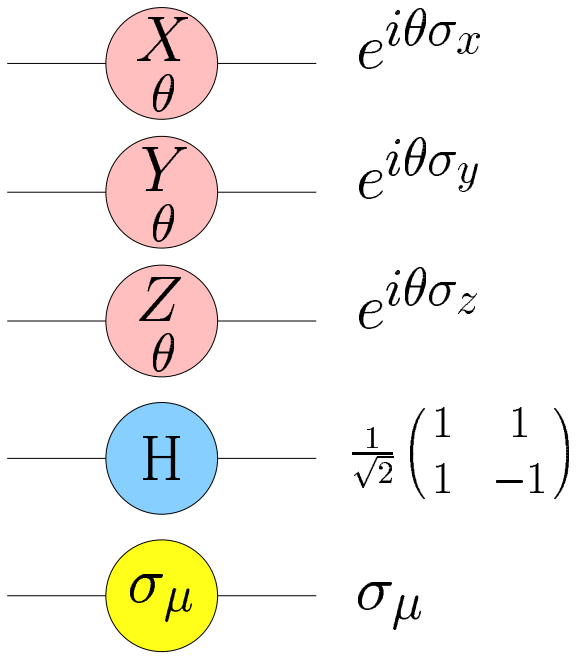
§4. $\langle\sigma_x^{\mathsf{a}} + i\sigma_y^{\mathsf{a}}\rangle_{\rho_{\mathsf{a}}\otimes\rho} = 2\mathrm{Tr}_{n+1}[\bar{U}^\dagger|0\rangle\langle 1|\bar{U}\rho_{\mathsf{a}}\otimes\rho] = \langle U_i^\dagger V_j\rangle_\rho = \mathrm{Tr}_n[U_i^\dagger V_j\rho]$

§5. Therefore, $C_{AB}(t) = \sum_{i,j}\langle U_i^\dagger V_j\rangle_\rho$

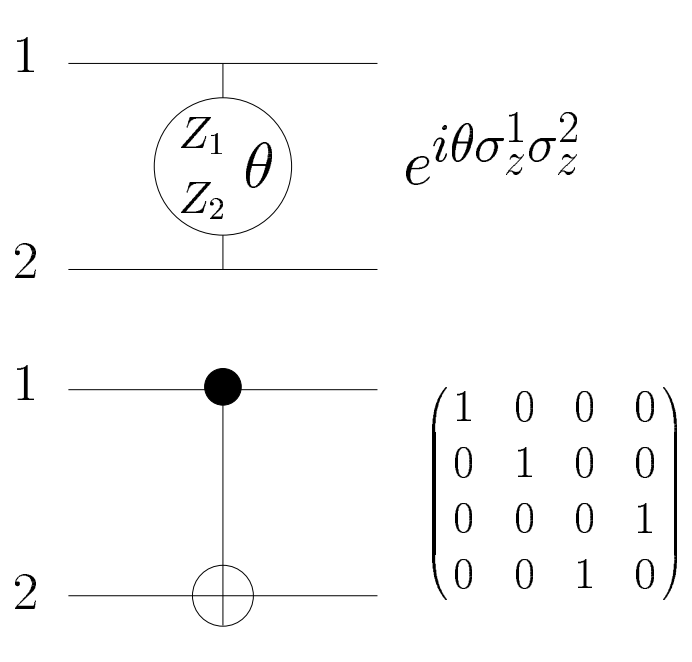
The statistical noise is determined by that of two binary random variables

The Language of Quantum Networks

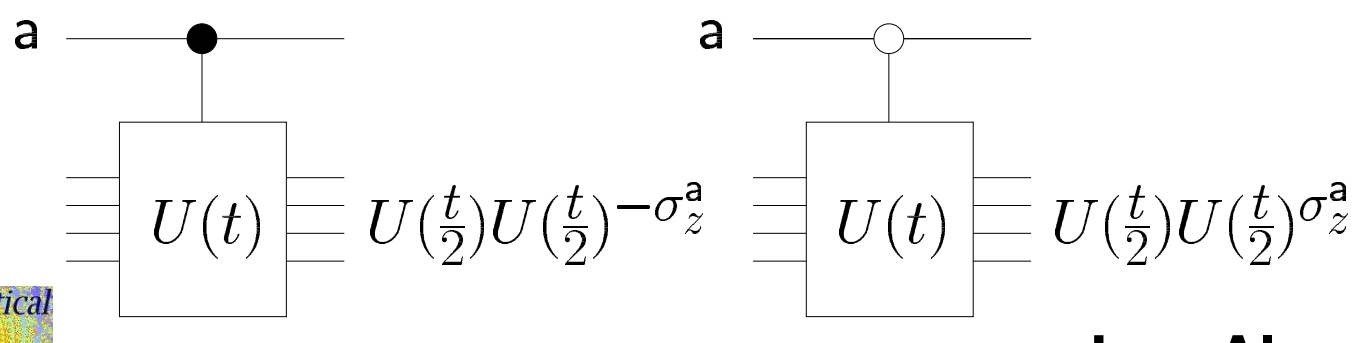
One qubit:



Two qubit:



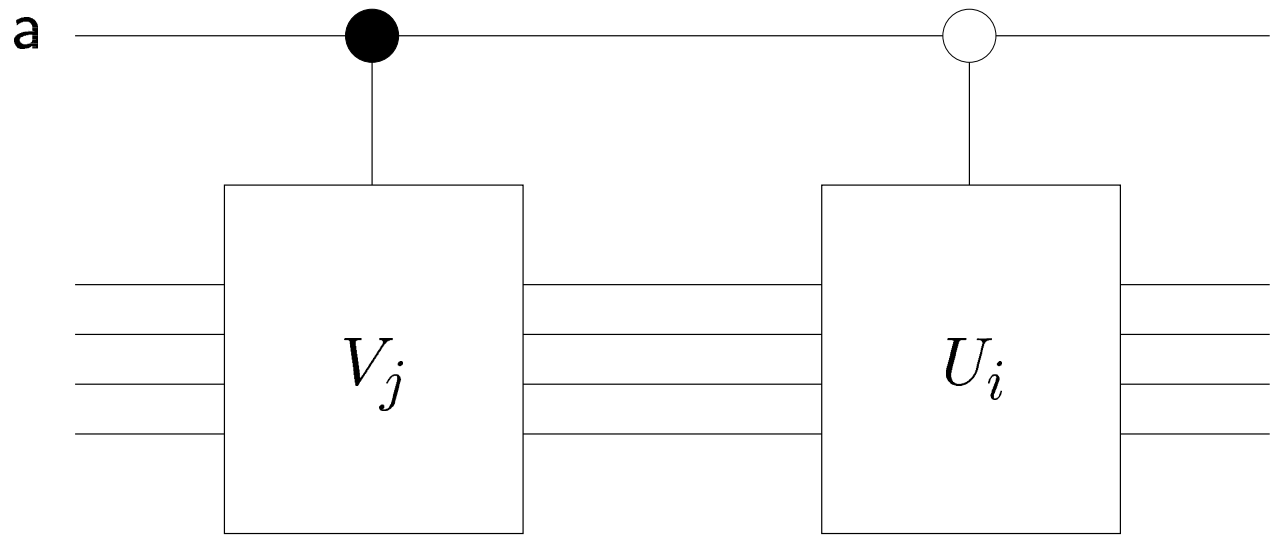
Controlled-U:



Theoretical Division

Los Alamos NATIONAL LABORATORY

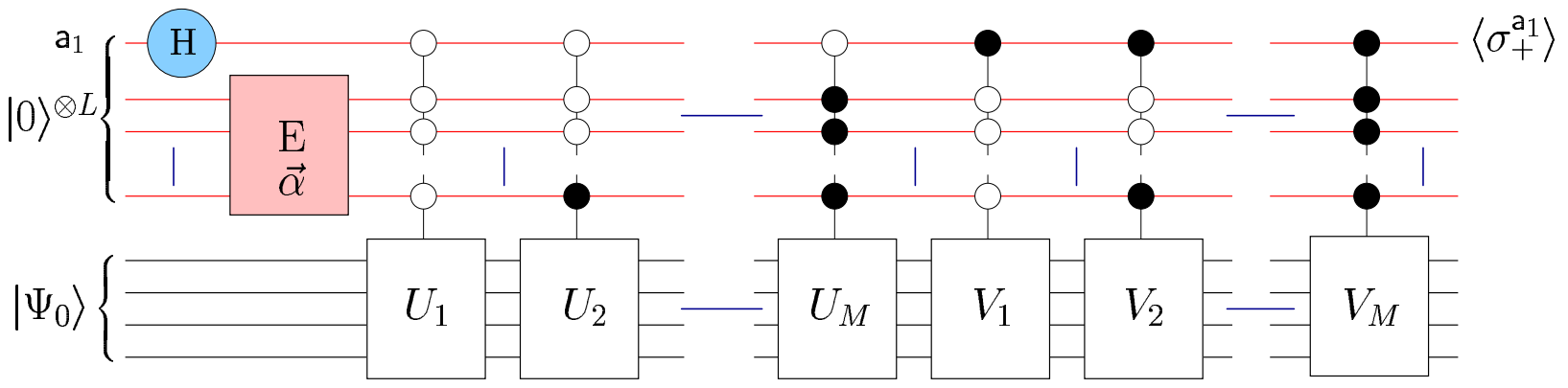
1-qubit Measurement: General Quantum Circuit



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

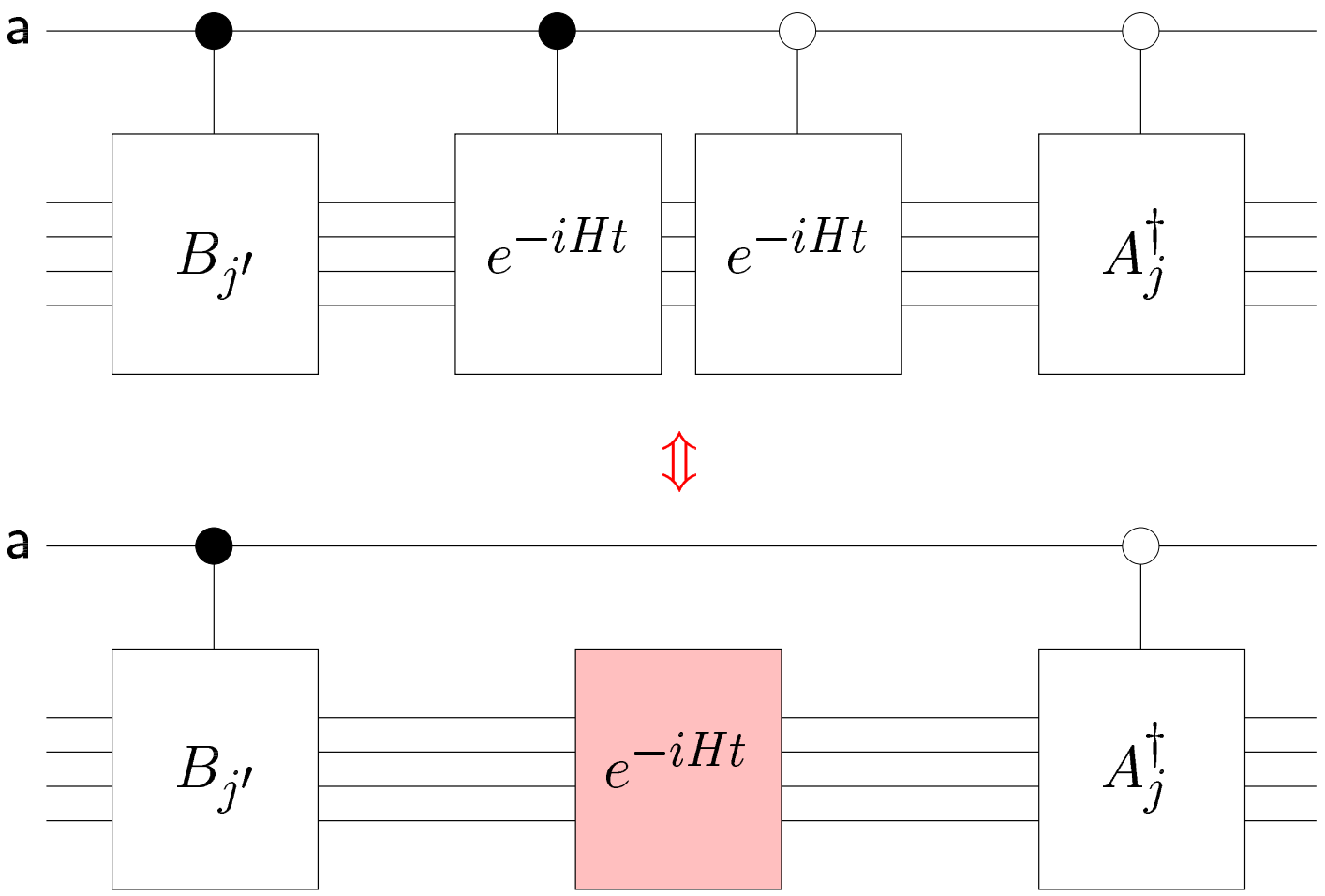
Step 2: $|0\rangle_{\mathsf{a}}\langle 0| \otimes U_i + |1\rangle_{\mathsf{a}}\langle 1| \otimes \mathbb{1}$

L-qubit Measurement: General Quantum Circuit



$$|\Psi(0)\rangle = |0\rangle^{\otimes L} \otimes |\Psi_0\rangle \rightarrow 2\langle\sigma_+^{a1}\rangle = \sum_{i=1}^{M=2^L} \alpha_i^2 \, \langle\Psi_0|U_i^\dagger V_i \Psi_0\rangle$$

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



Theoretical Division

Los Alamos NATIONAL LABORATORY

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)**

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

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

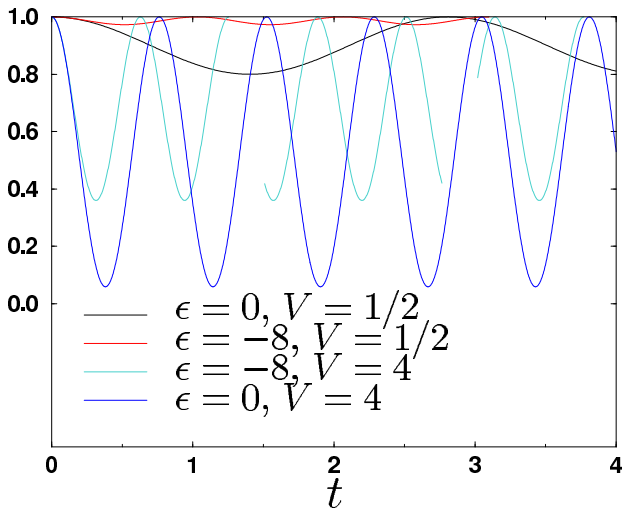
$$G(t) = \langle\Psi(0)|b(t)b^\dagger(0)|\Psi(0)\rangle\ ,\ b(t) = e^{iHt}\ b(0)\ e^{-iHt}\ .$$

C) Initial state: Fermi sea of $N_e \leq n$ fermions ($|0\rangle$:= vacuum)

$$|\Psi(0)\rangle = |FS\rangle = \prod_{i=0}^{N_e-1} c_{k_i}^\dagger|0\rangle\ ,\ c_{k_i}^\dagger = \frac{1}{\sqrt{n}}\sum_{j=1}^{n}\ e^{ik_iR_j}\ c_j^\dagger$$

$k_j = k_j = \frac{2\pi n_j}{L}$, **with n_j an integer** $(-\frac{\pi}{a} < k \leq \frac{\pi}{a})$

$|G(t)|^2$



Quantum Algorithm

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)

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

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

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

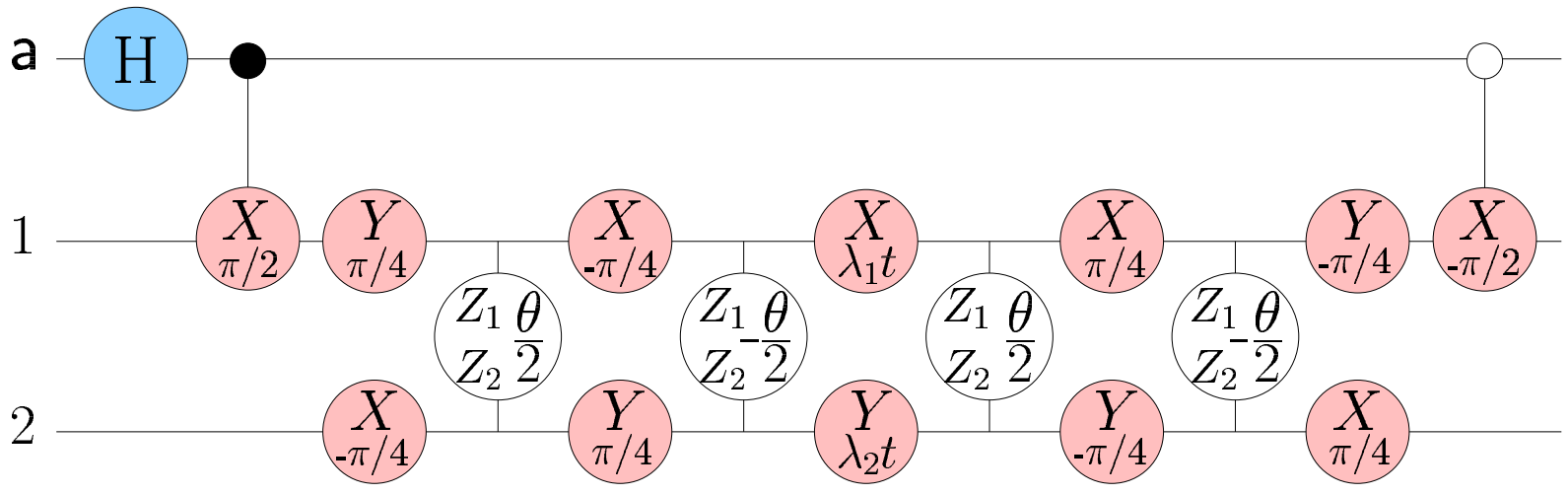
$$H_{P1} = \frac{1}{2}(E - \sqrt{\Delta^2+V^2})\sigma_z^1 + \frac{1}{2}(E + \sqrt{\Delta^2+V^2})\sigma_z^2 \ ,$$

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

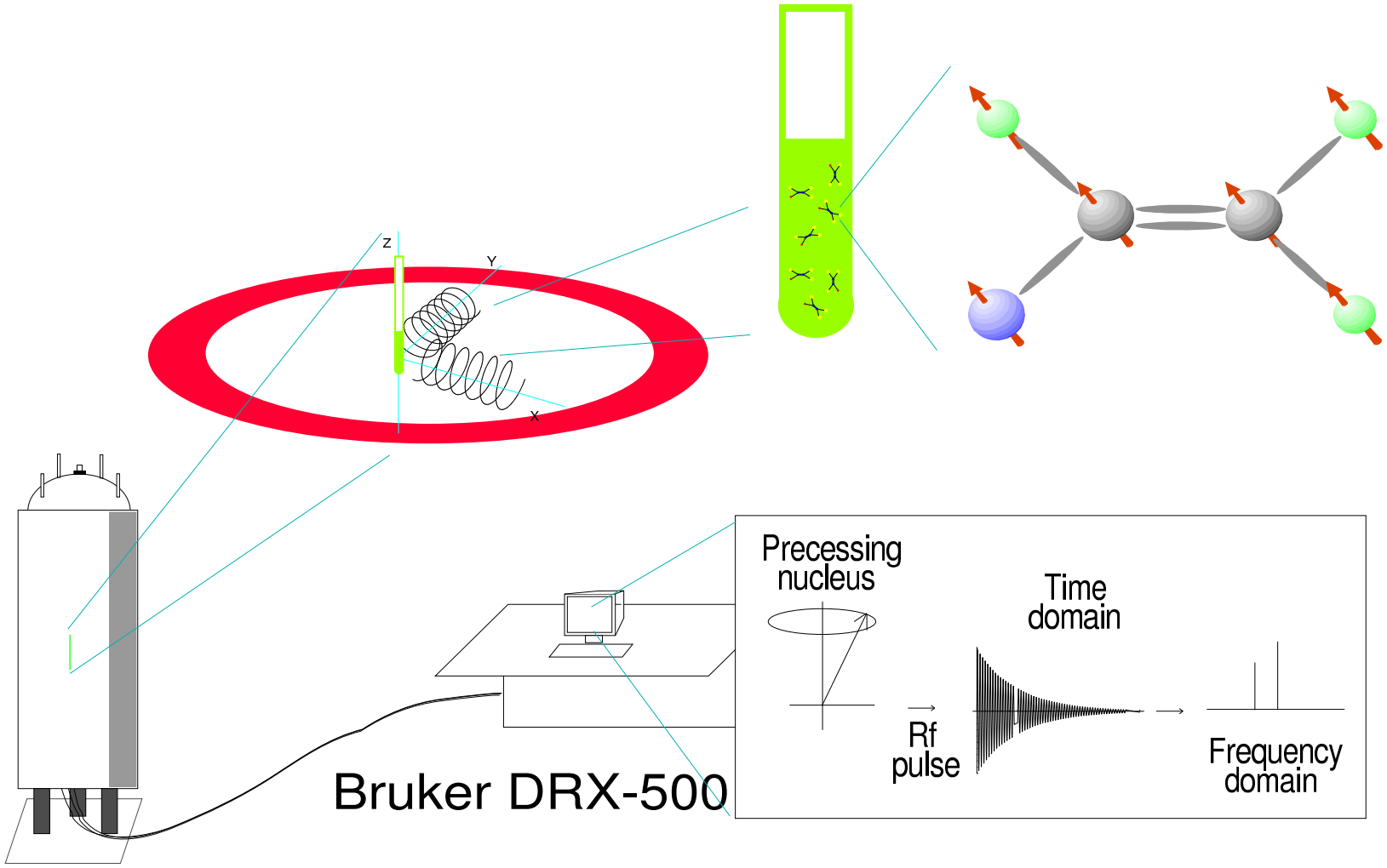
$$|\Psi(0)\rangle = |0\rangle_a \otimes |1\rangle_1 \otimes |0\rangle_2$$



Theoretical Division

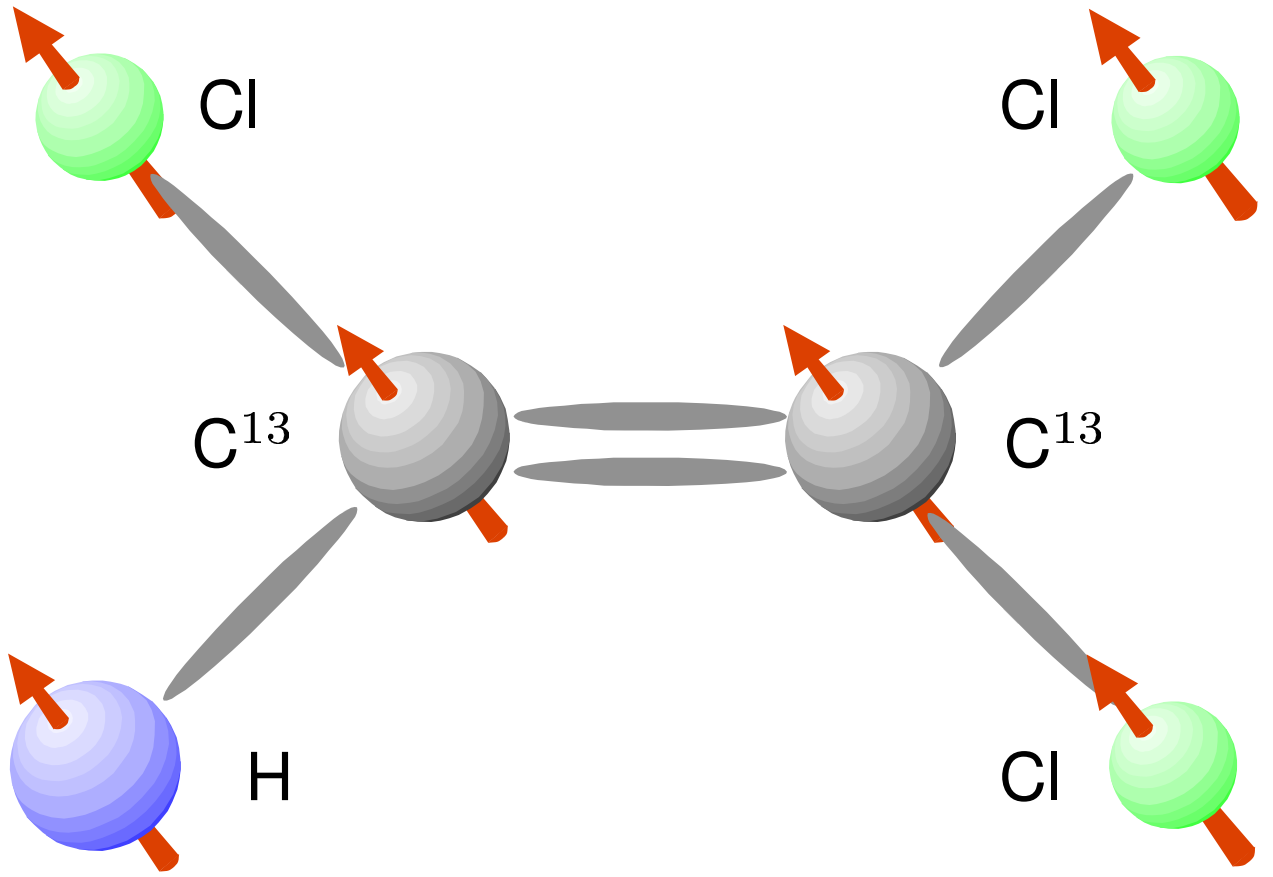
Los Alamos NATIONAL LABORATORY

NMR System Overview



Further Reading: Abragam[1], Ernst[4]

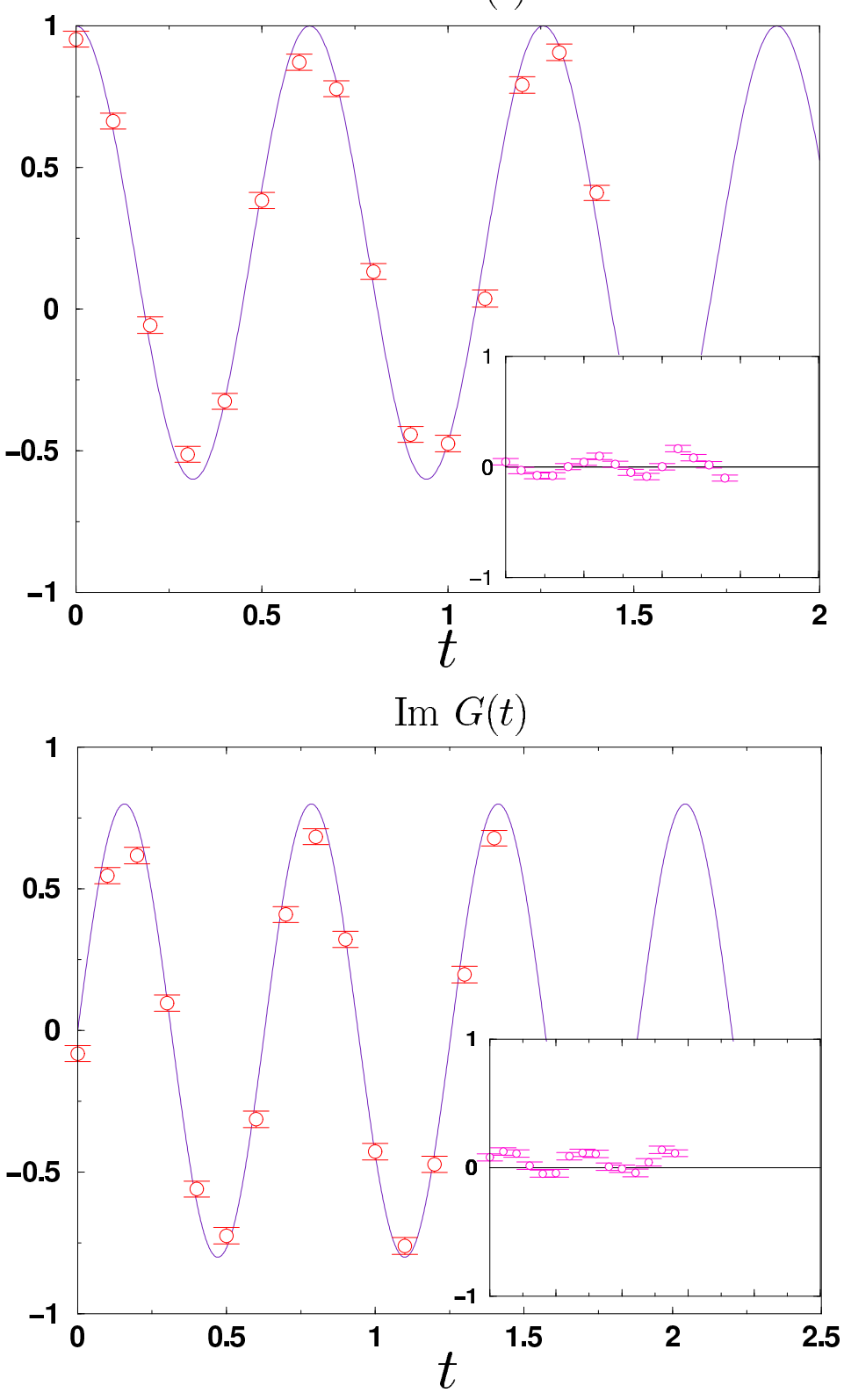
Labeled TCE†: A Three Qubit Register



† Trichloroethylene

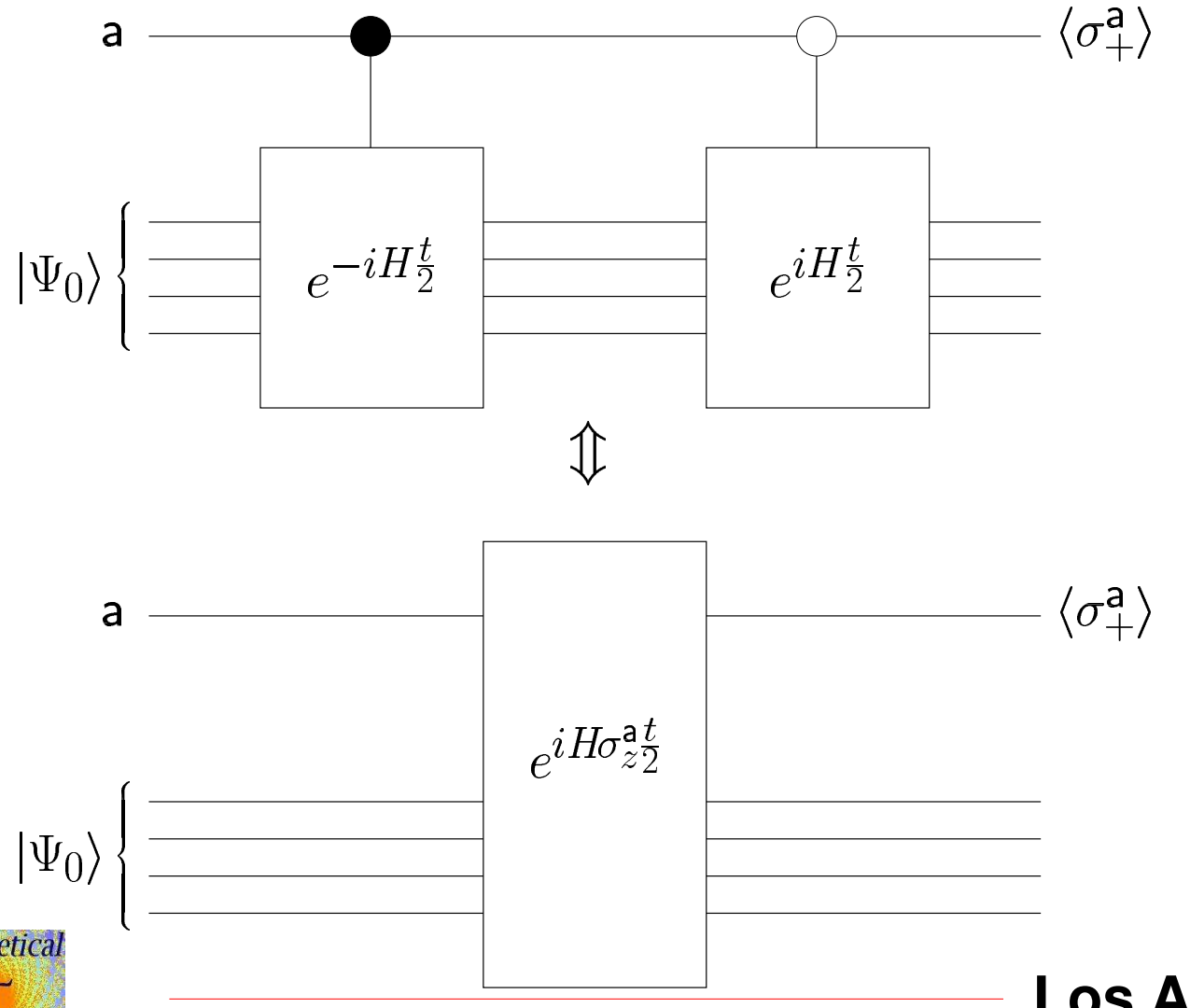
Liquid NMR: Resonant Impurity Scattering

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



Quantum Network for Determining the Spectrum of H

$$|\Psi(0)\rangle = |+\rangle_{\mathsf{a}} \otimes |\Psi_0\rangle \Longrightarrow \langle\sigma_+^{\mathsf{a}}\rangle = \langle\Psi_0|e^{-iHt}|\Psi_0\rangle$$



Theoretical Division

Los Alamos NATIONAL LABORATORY

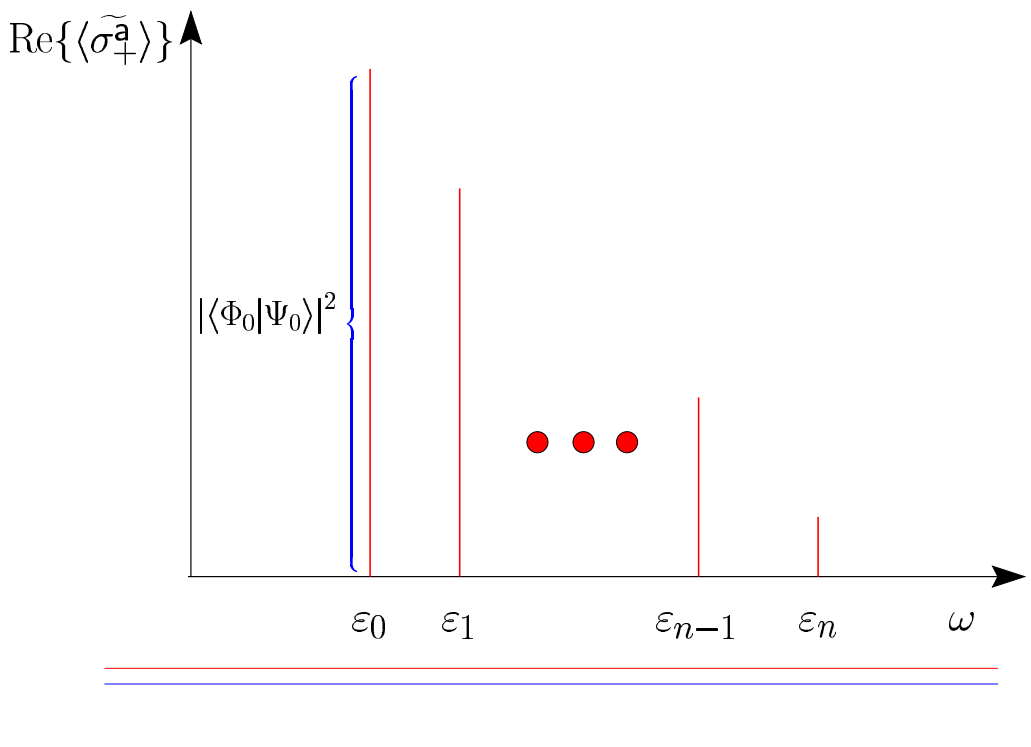
Quantum Network for Determining the Spectrum of H

$$H|\Phi_n\rangle = \varepsilon_n|\Phi_n\rangle$$

$$\Downarrow$$

$$\langle\sigma_+^{\mathsf{a}}\rangle = \langle\Psi_0|e^{-iHt}|\Psi_0\rangle = \sum_n |\langle\Phi_n|\Psi_0\rangle|^2 \, e^{-i\varepsilon_n t}$$

Fourier Transform $\langle\sigma_+^{\mathsf{a}}\rangle$



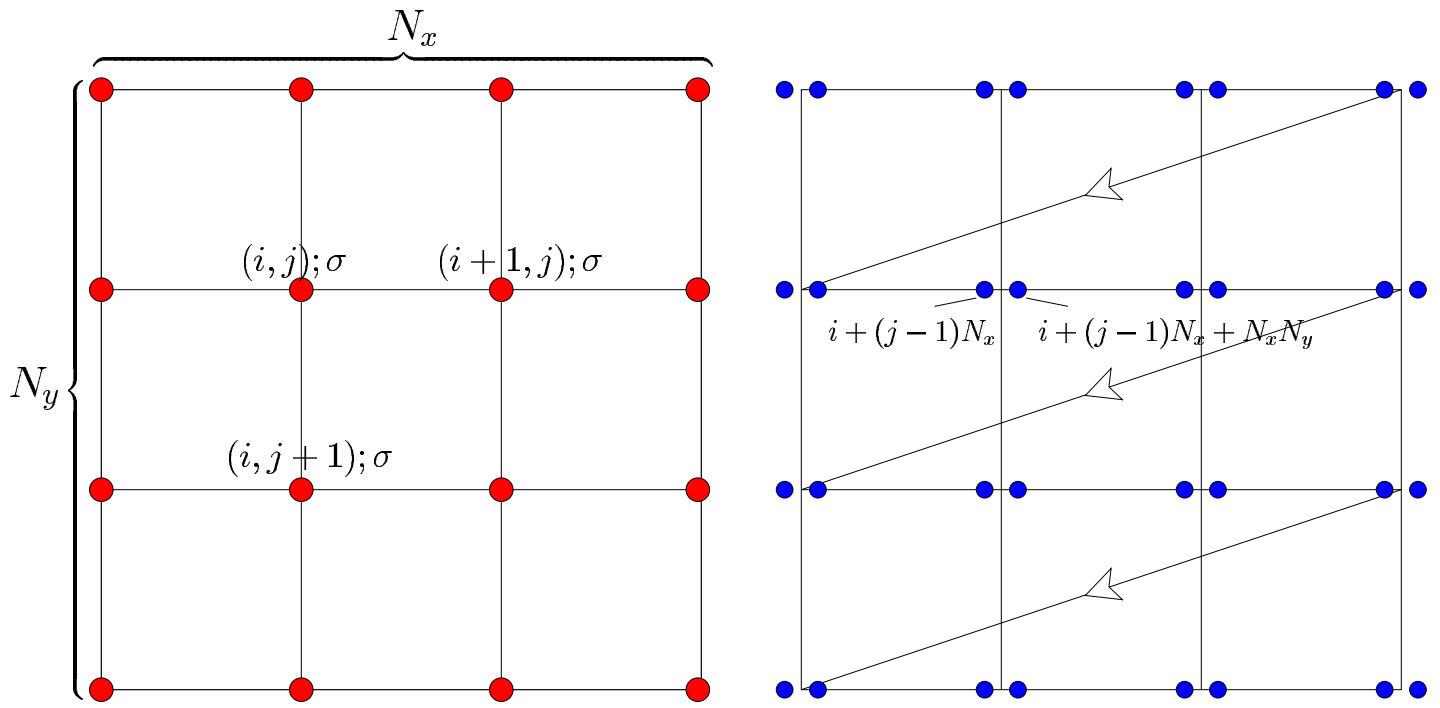
Theoretical Division

Los Alamos NATIONAL LABORATORY

Hubbard Model

$$H = -T \sum (a^{\dagger}_{\mathbf{r},\sigma} a_{\mathbf{r}+\delta,\sigma} + \text{H.c.}) + U \sum n_{\mathbf{r},\uparrow} n_{\mathbf{r},\downarrow}$$

$\mathbf{r},\delta,\sigma$ $\qquad\qquad$ $\mathbf{r}$



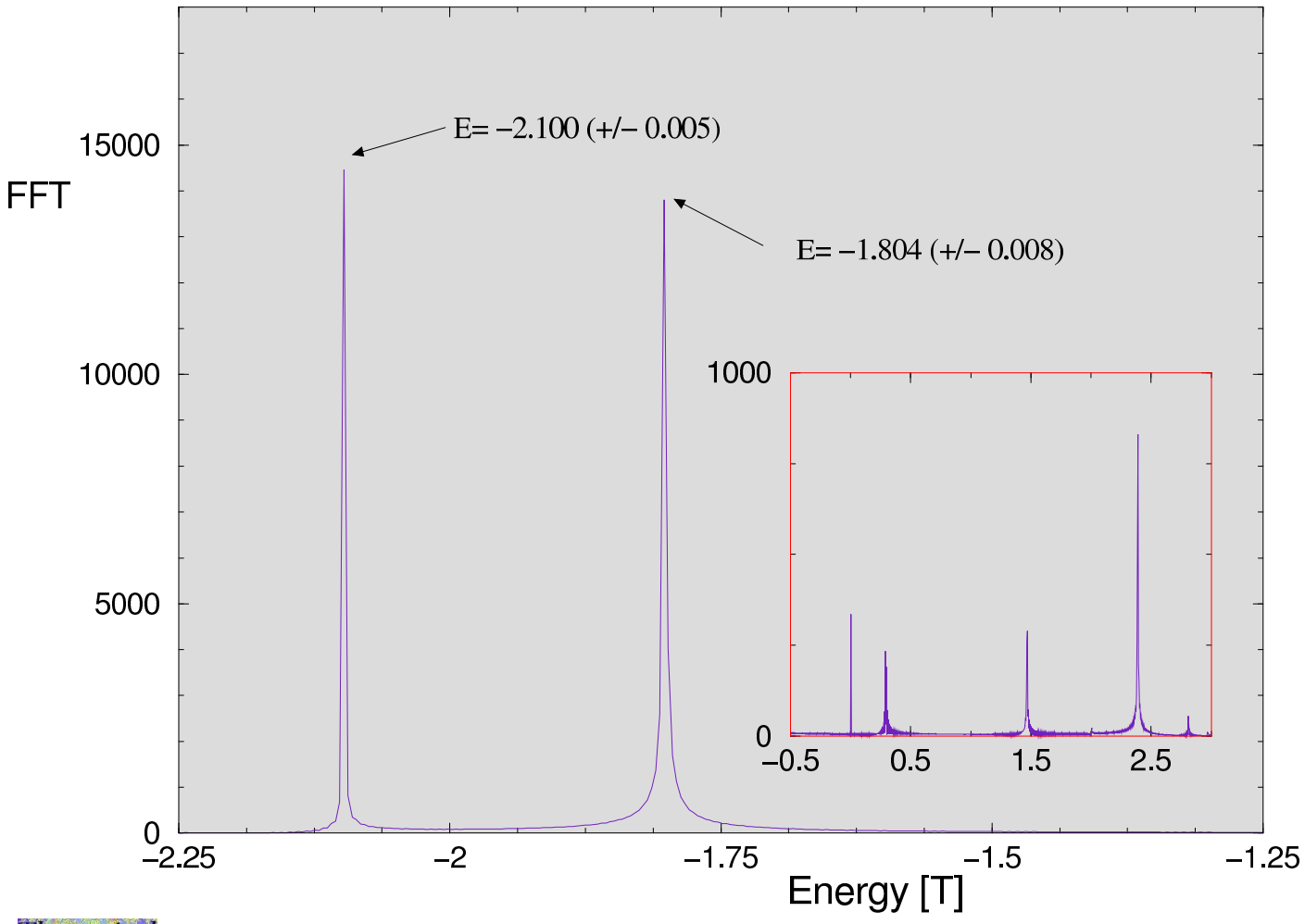
$$a_{(1,1);\uparrow} \to \tilde{a}_1 \quad \cdots \quad a_{(i,j);\uparrow} \to \tilde{a}_{[i+(j-1)N_x]} \quad \cdots \quad a_{(N_x,N_y);\uparrow} \to \tilde{a}_{N_xN_y}$$

$$a_{(1,1);\downarrow} \to \tilde{a}_{[1+N_xN_y]} \quad \cdots \quad a_{(i,j);\downarrow} \to \tilde{a}_{[i+(j-1)N_x+N_xN_y]} \quad \cdots \quad a_{(N_x,N_y);\downarrow} \to \tilde{a}_{2N_xN_y}$$

Theoretical $\mathcal{T}$ Division

Los Alamos
NATIONAL LABORATORY

Spectrum of the Hubbard Model (2×2, U=4, $N_e = 4$)



Theoretical Division

Los Alamos NATIONAL LABORATORY

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)

§2. Can we really efficiently simulate a QFT with a discrete quantum computer?

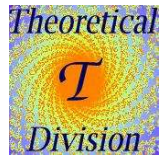
§3. What computational resources are required to answer interesting questions?

— Confinement, etc. in QCD ?

— $N > 12$ nuclei ?

— ...

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



Main Messages

Equivalence of 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 a closed 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 (Fermion simulations).

Quantum Networks and Physical Phenomena:

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

Conclusions + Next Steps

§1. We have shown how quantum computers avoid some sign(phase) problems present in probabilistic classical simulations.

$$\Downarrow$$

Exponential complexity $\mapsto$ Polynomial complexity

§2. Essential to the simulation of quantum phenomena is the spin-particle connection.

§3. The spin-particle connection allows one to define $*$-algebra isomorphisms to the algebra of operators of the standard model.

$$\Downarrow$$

Models of quantum computation $\Longleftrightarrow$ Algebra of operators

§4. There is nothing special about "Fermionic Computation." The key point is the physical realization of the Grassmann Chip. We propose "Hard-core Boson Computation" which admits, in principle, a realization in terms of He^4.

§5. Next steps:

— Ground state properties: Gell-Mann-Low theorem ?

— Simulation of models of physical interest: Hubbard, Anderson, Hofstadter-like, etc.