

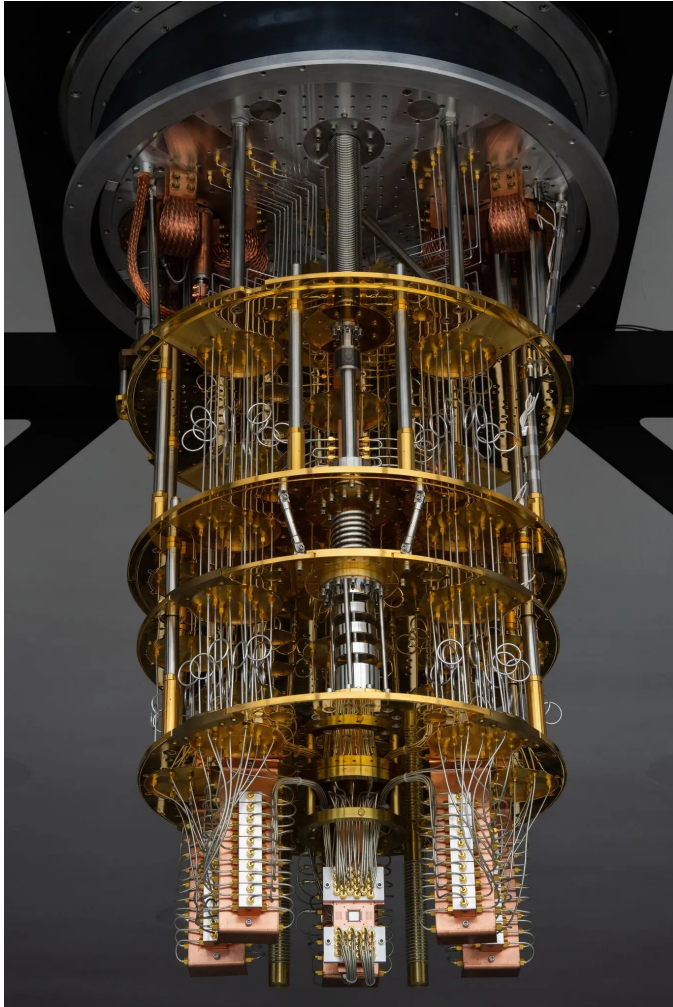
Quantum Computing for Plasma Physics: State of the Art and Potential Opportunities

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3rd International Fusion and Plasma Conference
Seoul Olympic Parktel, Seoul



- Introduction to quantum computing
 - History
 - Current specs
 - Basic concepts
- Quantum algorithms for plasma physics
 - Linear solvers
 - Nonlinear solvers
- Final thoughts & summary

Part I: Introduction to quantum computing



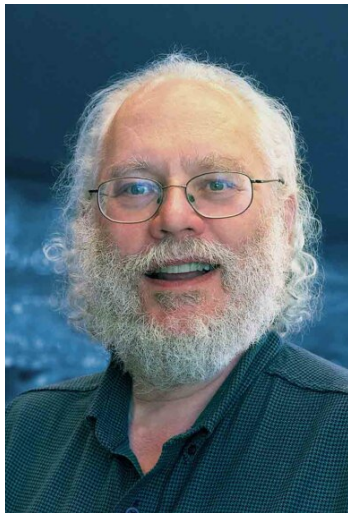
Yury Manin



Richard Feynman



David Deutsch



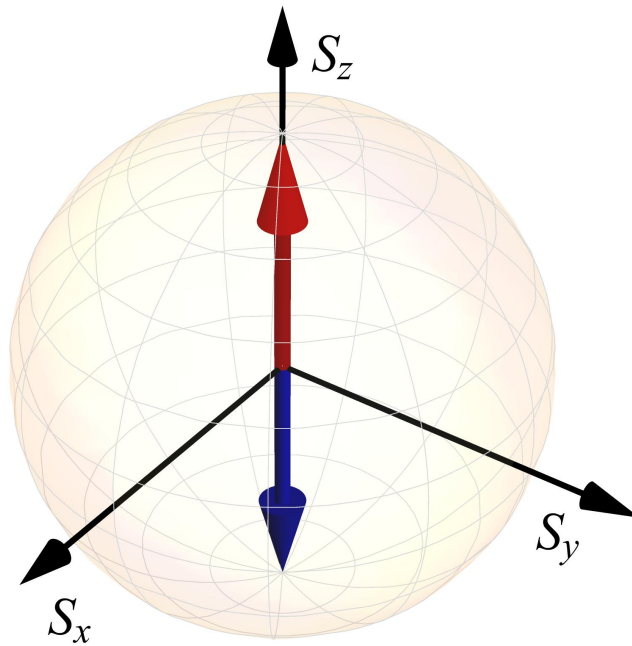
Peter Shor

- Inception of the idea in the early 80s: Manin, Feynman
- Feynman, in “Simulating Physics with Computers” ('81):

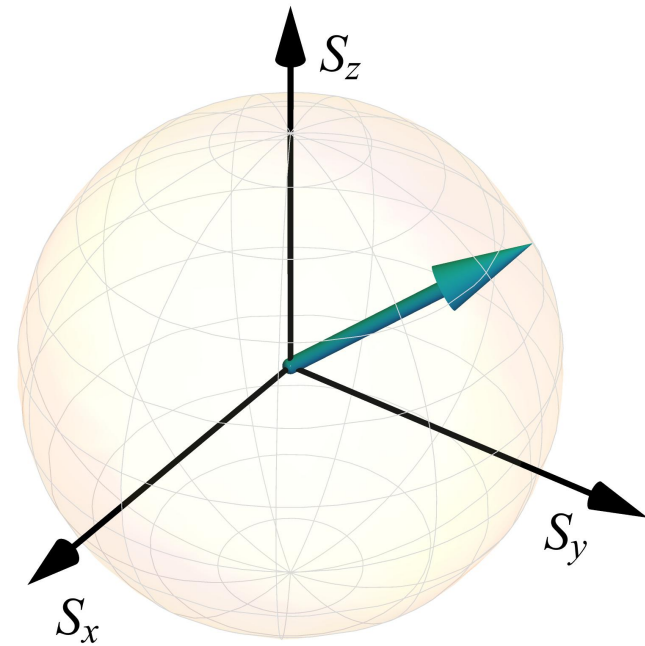
“...nature isn't classical, dammit, and if you want to make a simulation of Nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem...”

- Formalized notion of a quantum computer, question about applications beyond QM: Deutsch ('85)
- Applied algorithms: Shor's algorithm for factoring integers ('94). . .

Elementary memory cells: classical bit vs. qubit



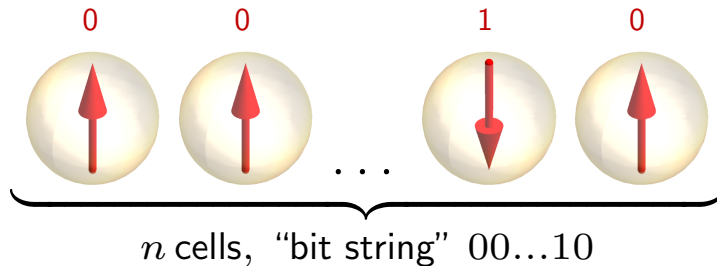
vs.



$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |0\rangle, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |1\rangle$$

- Memory cell = two-level system characterized by a state vector ψ or $\mathbf{S}_a \sim \psi^\dagger \boldsymbol{\sigma}_a \psi$.
- A classical memory cell (bit) can be only in one of the pure states: $|0\rangle$ or $|1\rangle$. A quantum cell (qubit) can be in any state $\alpha |0\rangle + \beta |1\rangle$ with $|\alpha|^2 + |\beta|^2 = 1$.
- Bits are flipped using $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Qubits: can use any unitaries, e.g. $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$.

Quantum parallelism



- A classical register with n cells allows one to encode **one integer** $a \in [1, N]$, $N = 2^n$:

$$|\psi\rangle = 0|b_1\rangle + 0|b_2\rangle + \dots + \mathbf{1}|b_a\rangle + \dots 0|b_N\rangle$$

operations = shifts of the unit coefficient

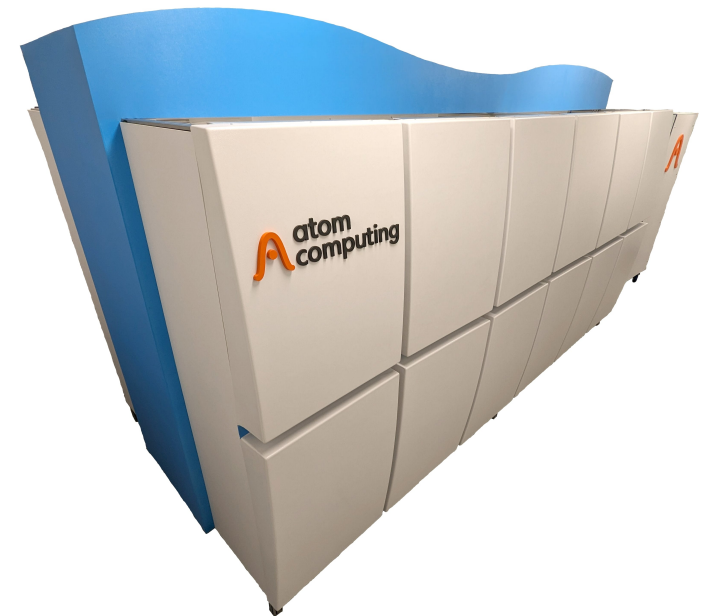
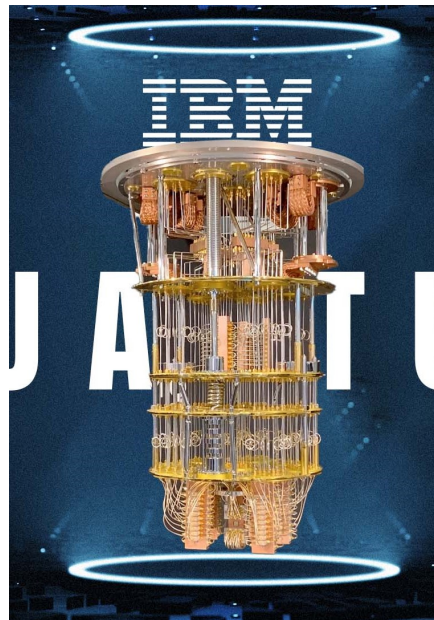
- A quantum register with n cells allows one to encode **$N = 2^n$ complex numbers** ψ_k :

$$|\psi\rangle = \sum_{k=1}^N \psi_k |b_k\rangle, \quad \sum_{k=1}^N |\psi_k|^2 = 1$$

operations = any unitary transformations
(single-qubit and multi-qubit gates)

- A quantum computer can perform parallel processing of exponentially many complex numbers (e.g. field amplitudes on a grid).

- D-Wave Advantage: 5000+ qubits, but it does only quantum annealing.
- Atom's chip: 1125 qubits. IBM's Condor chip: 1121 qubits. But IBM's latest System Two uses Heron chips with only 133 qubits (5x smaller error rates).
- Typical are NISQ* computers: $< 10^3$ qubits, error rate $\sim 1\%$.





- In 2019, Google claimed “quantum supremacy” on a 53-qubit machine:

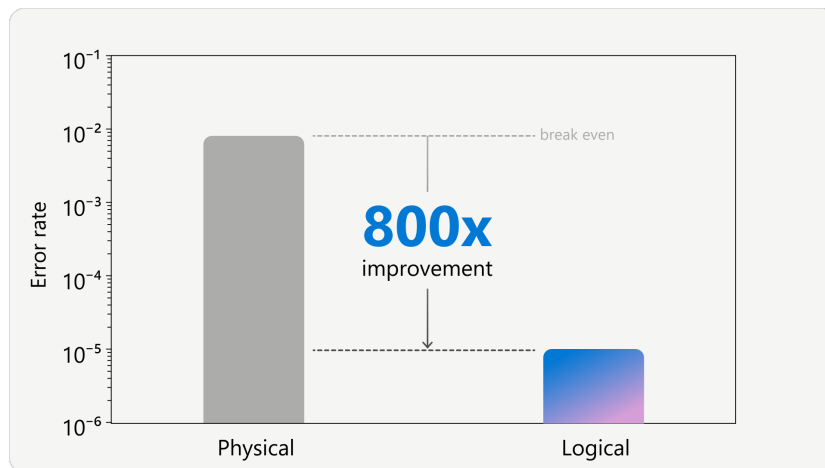
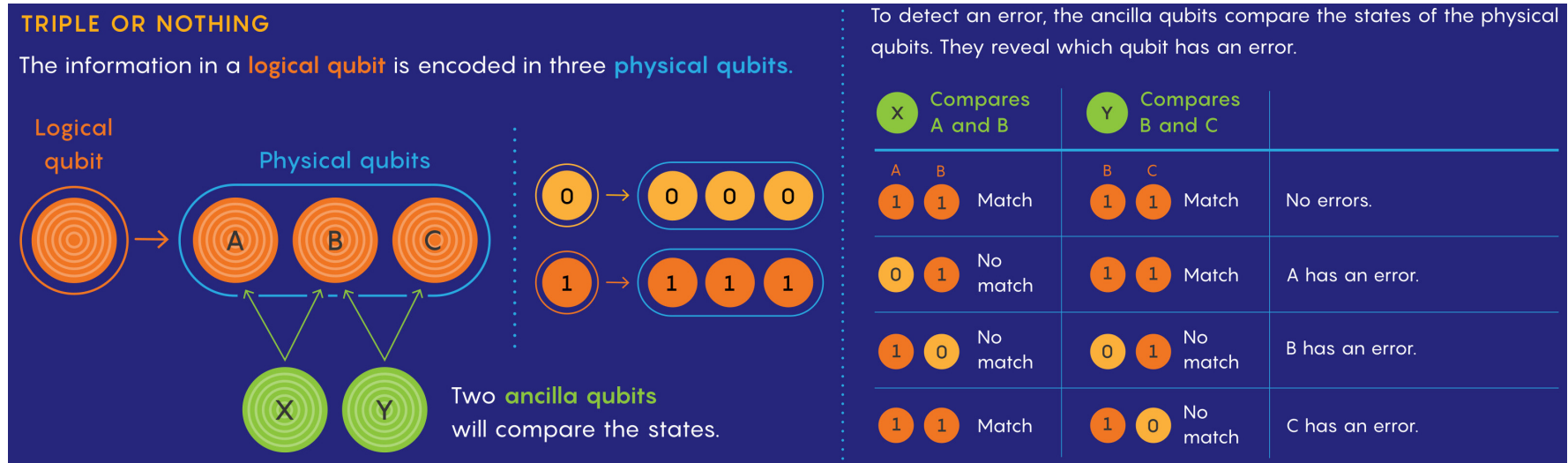
circuit depth ~ 20
number of gates $\sim 1.5k$
fidelity $\sim 0.2\%$
equiv classical simulation $\sim 10^4$ yrs

- But:
 - later debunked: classical computers can do the same within days and with much higher accuracy;
 - not a useful problem anyway.

- As of now, classical computers outperform quantum computers for all real-world applications. We need more qubits, and we need qubits to be more reliable.

Quantum error correction

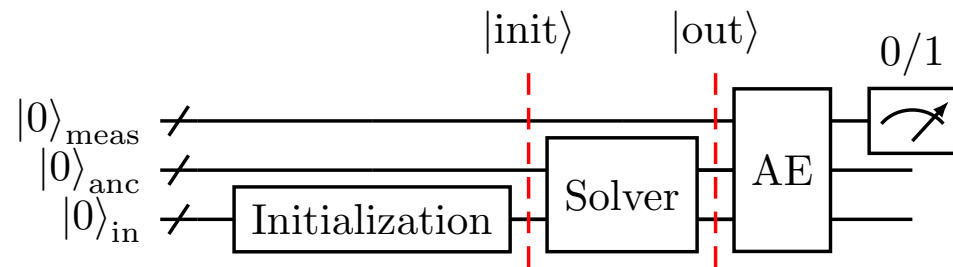
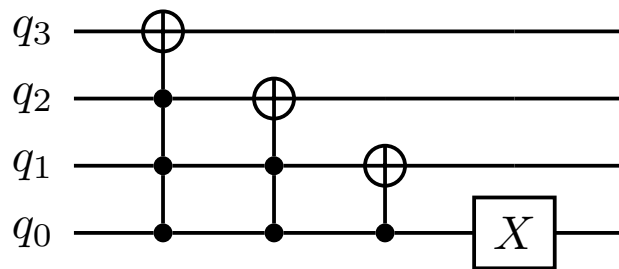
- A set of physical qubits can operate as a fault-tolerant logical qubit:



- Record by Microsoft (April 2024):
 - error rate reduced by 800x, to 10^{-5}
 - 4 stable logical qubits made out of 30 physical (ion-trap) qubits
- Let's assume we have enough logical qubits. . .

Quantum program is a circuit.

- Quantum computation = sequence of unitary operations on qubits. An immediate bottleneck (one of many): hardware implementation of multi-controlled gates.



- Generic circuit: initialization → solver → amplitude estimation (AE) → measurement.
 - Initialization:** only certain states can be created efficiently – bottleneck.
 - Solver:** involves ancilla qubits for intermediate calculations and returns

$$|\text{out}\rangle = |\mathbf{0}\rangle_{\text{anc}} \sum_k \psi_k^{\text{out}} |s_k\rangle_{\text{in}} + |\neq \mathbf{0}\rangle_{\text{anc}} |\dots\rangle$$

- Measurement:** run N_{run} times, $|\psi_k^{\text{out}}|^2 = N_k/N_{\text{run}} + \mathcal{O}(N_{\text{run}}^{-1/2})$. With AE, a measurement returns $|\psi_k^{\text{out}}|^2$ with probability close to one and error $\mathcal{O}(N_{\text{run}}^{-1})$.

Part II: Quantum algorithms for plasma physics

	initial-value problems	boundary-value problems*
linear	$\partial_t \psi = -i\hat{H}\psi$	$A\psi = b$
nonlinear	$\partial_t u = g(u)$	$F(u) = 0$

* These also include non-differential equations and optimization problems.
Not discussing eigenvalue problems here, but see, e.g. Parker & Joseph (2020).

Quantum Hamiltonian simulations (QHS)

- Quantum computers are naturally fit for *quantum Hamiltonian simulations*. For a Hermitian \hat{H} , a quantum circuit can directly implement unitary $\hat{U} = \exp(-i\hat{H}t)$.

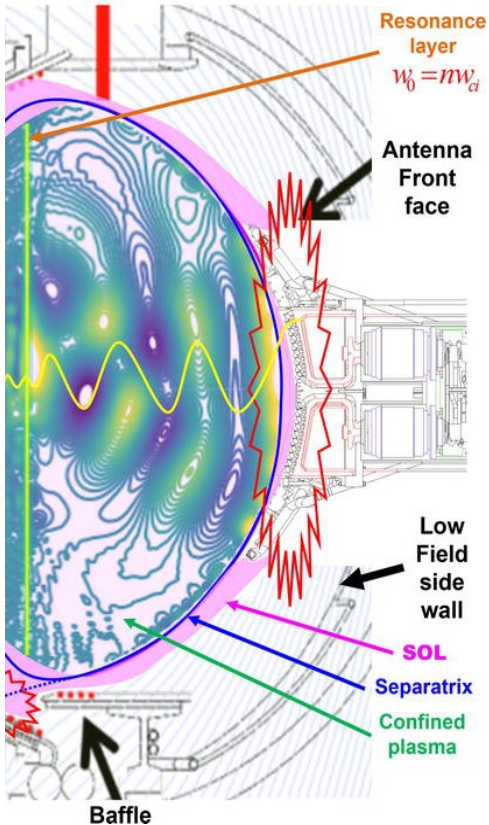
$$\partial_t \psi = -i\hat{H}\psi, \quad \psi(t) = \exp(-i\hat{H}t)\psi_0$$

- Example: cold-plasma waves, $\psi \sim (g_1 \mathbf{v}_1, g_2 \mathbf{v}_2, \dots, \tilde{\mathbf{E}}, \tilde{\mathbf{B}})^\top$

$$\begin{aligned} \partial_t \tilde{\mathbf{v}}_s &= e_s \tilde{\mathbf{E}}/m_s + \tilde{\mathbf{v}}_s \times \boldsymbol{\Omega}_s \\ \partial_t \tilde{\mathbf{E}} &= c \nabla \times \tilde{\mathbf{B}} - 4\pi \sum_s e_s n_{0s} \tilde{\mathbf{v}}_s \\ \partial_t \tilde{\mathbf{B}} &= -c \nabla \times \tilde{\mathbf{E}} \end{aligned}$$

$$\hat{H} = \begin{pmatrix} -\boldsymbol{\alpha} \cdot \boldsymbol{\Omega}_1(\mathbf{x}) & 0 & \dots & 0 & i\omega_{p1}(\mathbf{x}) & 0 \\ 0 & -\boldsymbol{\alpha} \cdot \boldsymbol{\Omega}_2(\mathbf{x}) & \dots & 0 & i\omega_{p2}(\mathbf{x}) & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & -\boldsymbol{\alpha} \cdot \boldsymbol{\Omega}_q(\mathbf{x}) & i\omega_{pq}(\mathbf{x}) & 0 \\ -i\omega_{p1}(\mathbf{x}) & -i\omega_{p2}(\mathbf{x}) & \dots & -i\omega_{pq}(\mathbf{x}) & 0 & c\boldsymbol{\alpha} \cdot \nabla \\ 0 & 0 & \dots & 0 & -c\boldsymbol{\alpha} \cdot \nabla & 0 \end{pmatrix}$$

$$\alpha_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \alpha_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad \alpha_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

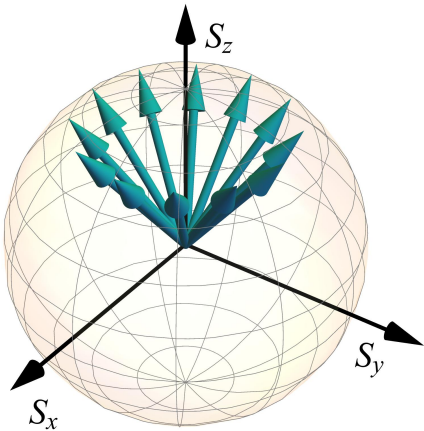


There are various ways to construct $\hat{U} = \exp(-i\hat{H}t)$.

- **Suzuki–Trotter expansion:** (i) decompose $\hat{H} = \sum_j \hat{H}_j$, where \hat{H}_j are rotation gates; (ii) divide t into $m \gg 1$ intervals $\Delta t = t/m$, so $[\hat{H}_i \Delta t, \hat{H}_j \Delta t] = \mathcal{O}(m^{-2})$.

$$\hat{U} = \left[\exp \left(- \sum_j \hat{H}_j \Delta t \right) \right]^m \approx \left[\prod_j \underbrace{\exp(-i\hat{H}_j \Delta t)}_{\text{implementable w/elementary gates}} \right]^m$$

- Quantum Signal Processing (QSP)/Quantum Singular Value Transformation (QSVT):
 - Allow to calculate **polynomials of given matrices** for many applications.
 - Based on the idea of rotating unitaries. For example, by properly choosing r angles ϕ_k , one can construct an r th-order polynomial $P_r(a)$ of a scalar a :



$$U(a) = \begin{pmatrix} a & \sqrt{1-a^2} \\ \sqrt{1-a^2} & -a \end{pmatrix}, \quad R(\phi) = \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix}$$

$$R(\phi_0) \underbrace{U(a) R(\phi_2) \dots R(\phi_{r-1}) U(a)}_{r \text{ powers of } U} R(\phi_r) = \begin{pmatrix} P_r(a) & * \\ * & * \end{pmatrix}$$

Block encoding and application to Hamiltonian simulations

- To obtain a polynomial of a matrix, encode A as a block of a unitary U_A , then rotate:

$$U_A = \begin{pmatrix} A & * \\ * & * \end{pmatrix}, \quad R(\phi) = \begin{pmatrix} e^{i\phi} 1 & 0 \\ 0 & e^{-i\phi} 1 \end{pmatrix}, \quad A \rightarrow \frac{A/\|A\|}{\text{sparsity}}$$

$$\underbrace{R(\phi_0) U_A R(\phi_2) U_A^\dagger \dots U_A^\dagger R(\phi_{r-1}) U_A R(\phi_r)}_{\text{same } \phi_k \text{ as for scalars; finding them for large } r \text{ is a bottleneck}} = \begin{pmatrix} P_r(A) & * \\ * & * \end{pmatrix}$$

- QSP for Hamiltonian simulations:** express $e^{-i\hat{H}t}$ through Chebyshev polynomials $T_k(\hat{H})$ defined via $T_k(\cos \theta) = \cos(k\theta)$; calculate $T_k(\hat{H})$ using the appropriate ϕ_k .

$$e^{-i\hat{H}t} = J_0(t) + 2 \sum_{\text{even } k>0}^{\infty} (-1)^{k/2} J_k(t) \mathbf{T}_k(\hat{H}) + 2i \sum_{\text{odd } k>0}^{\infty} (-1)^{(k-1)/2} J_k(t) \mathbf{T}_k(\hat{H})$$

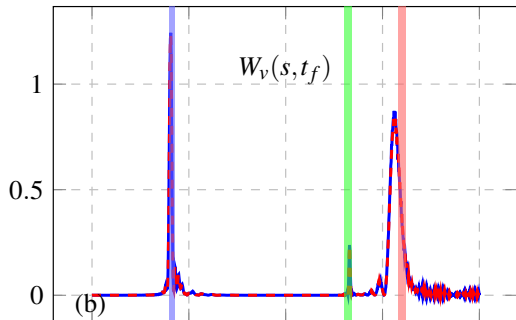
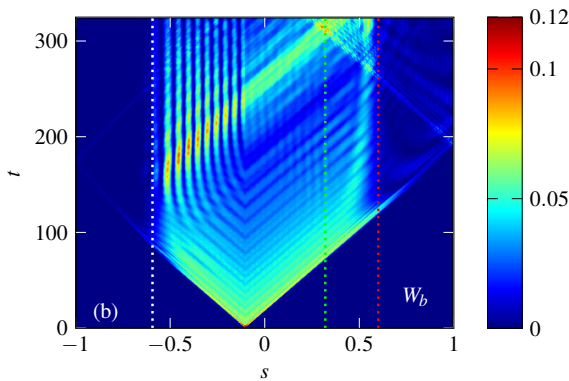
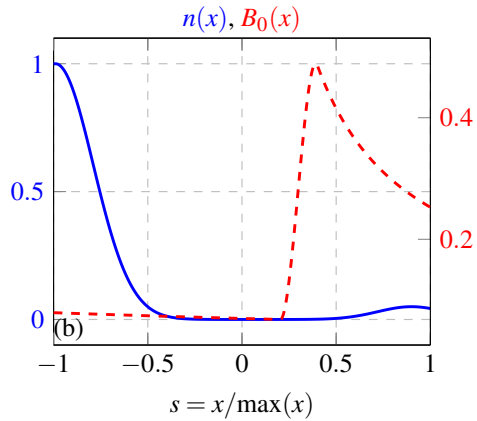
Near-optimal dependence of the number of calls to \hat{H} on time and error:

$$e^{-i\hat{H}t} = \sum_{k=0}^q (\dots) + \underbrace{\mathcal{O}((et/q)^q)}_{\epsilon} \Rightarrow q = \mathcal{O}(t + \log(1/\epsilon))$$

Example: exponential speedup of full-wave simulations for cold plasma

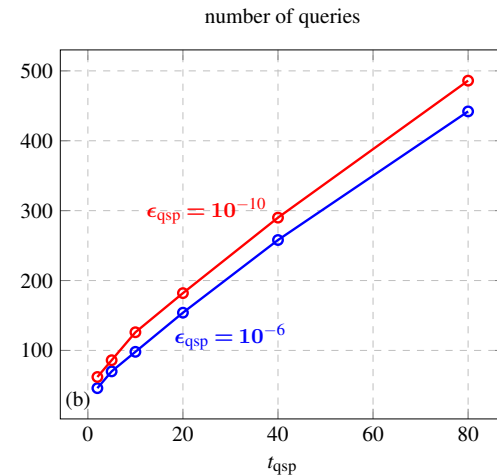
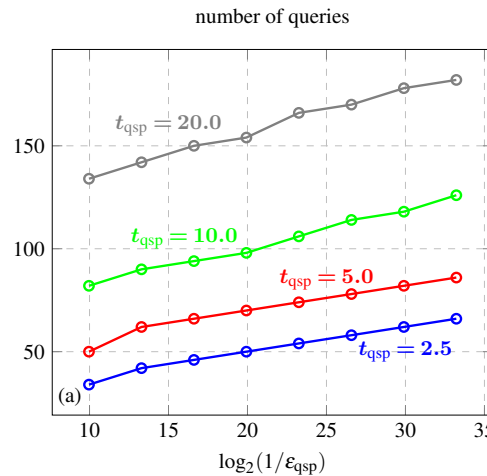
$$\mathcal{O}\left(\underbrace{\text{poly}(\log_2 N_x)}_{\text{oracle}} \underbrace{(t + \log_2(1/\delta))}_{\text{QSP circuit}} \underbrace{\delta^{-1}}_{\text{measurements}}\right)$$

- X wave propagation in 1-D electron plasma; antenna = oscillator. Efficient initialization and measurements.



$$|\psi|^2 = n_0 m_e \tilde{v}_e^2 / 2 + (\tilde{E}^2 + \tilde{B}^2) / 8\pi$$

$$\langle \psi | \text{window operator} | \psi \rangle = \text{energy}$$

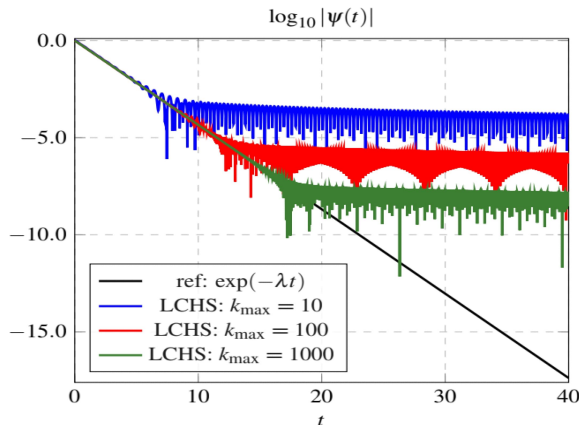


- QHS are applicable to linear kinetic waves in *homogeneous isotropic plasma*. The general linearized Vlasov–Maxwell dynamics is not always Hermitian (instabilities).

$$\begin{aligned}
 i\partial_t \mathbf{E} &= c(\boldsymbol{\alpha} \cdot \nabla) \mathbf{B} + \sum_{s,p} R_s \mathbf{v}_s g_s \\
 i\partial_t \mathbf{B} &= -c(\boldsymbol{\alpha} \cdot \nabla) \mathbf{E} \\
 i\partial_t g_s &= \hat{h}_s g_s + R_s \mathbf{E} \cdot \mathbf{v}_s, \quad g_s \propto \tilde{f}_s
 \end{aligned}
 \quad \left| \quad
 \underbrace{i\partial_t \begin{pmatrix} \tilde{\mathbf{E}} \\ \tilde{\mathbf{B}} \\ \mathbf{g} \end{pmatrix}}_{\psi} = \underbrace{\begin{pmatrix} 0 & c(\boldsymbol{\alpha} \cdot \nabla) & R\mathbf{v} \\ -c(\boldsymbol{\alpha} \cdot \nabla) & 0 & 0 \\ R\mathbf{v} & 0 & \hat{h} \end{pmatrix}}_{\hat{H}=\hat{H}^\dagger \text{ when } R_s \propto (f'_{0s})^{1/2} \text{ is real}} \begin{pmatrix} \tilde{\mathbf{E}} \\ \tilde{\mathbf{B}} \\ \mathbf{g} \end{pmatrix}$$

- QHS w/non-Hermitian \hat{H} : Linear Combination of Hamiltonian Simulations (LCHS)

$$e^{-i\hat{H}t} = \frac{1}{\pi} \int \frac{1}{1+k^2} \underbrace{\exp\left(-i\hat{H}_H t + ik\hat{H}_A t\right)}_{\text{unitary}} dk \approx \sum_k (\dots)_k \Delta k$$



However, truncation and discretization cause errors, so one needs *many* terms in the sum.

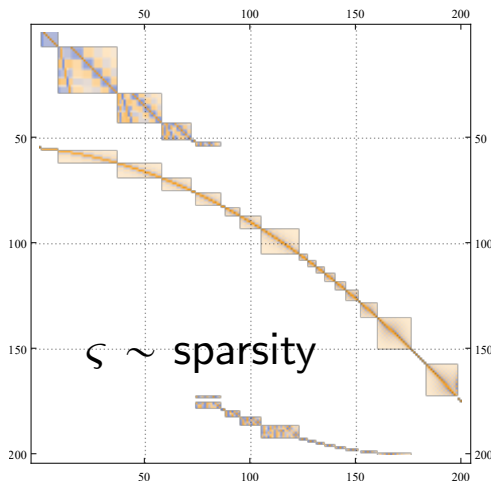
- Also, in practice, linear-wave problems are usually boundary-value, so let's consider those. . .

Linear boundary-value problems using QSVT

- A typical RF problem: $\partial_t = -i\omega$, so $\hat{\epsilon}$ is a *spatial* operator with ω as a parameter.

$$c^2 \nabla \times \nabla \times \tilde{\mathbf{E}} - \omega^2 \hat{\epsilon}(\omega) \tilde{\mathbf{E}} = \underbrace{4\pi i \omega J_{\text{ext}}}_{\text{antenna}} \Rightarrow A\psi = b, \quad \psi = A^{-1}b$$

- **QHS-based:** Harrow–Hassidim–Lloyd (HHL) algorithm and its later variations
 - Exponential speedup for sparse and well-conditioned A , $\kappa \equiv \lambda_{\text{max}}/\lambda_{\text{min}} \sim 1$.
 - Pre-exponential factors can be prohibitively large: quantum advantage would take $N \sim 10^8$, 340 qubits, depth $\sim 10^{25-29}$, runtime 10^{8-12} yrs (2-D scattering).



- **QSVT-based:** polynomial approximation to A^{-1}
 - FEM matrices, $N = N_x^D$: $\kappa = \mathcal{O}(N^{2/D}) = \mathcal{O}(N_x^2)$
 $\mathcal{O}(\kappa^2 \zeta \ln(N) \ln(\kappa/\epsilon)) \rightarrow \mathcal{O}(N_x^4 \zeta \ln(N_x) \ln(N_x^2/\epsilon))$
 - best classical methods have $\mathcal{O}(\zeta N_x^{D+2} \ln(1/\epsilon))$, so quantum advantage is possible at $D \geq 3$

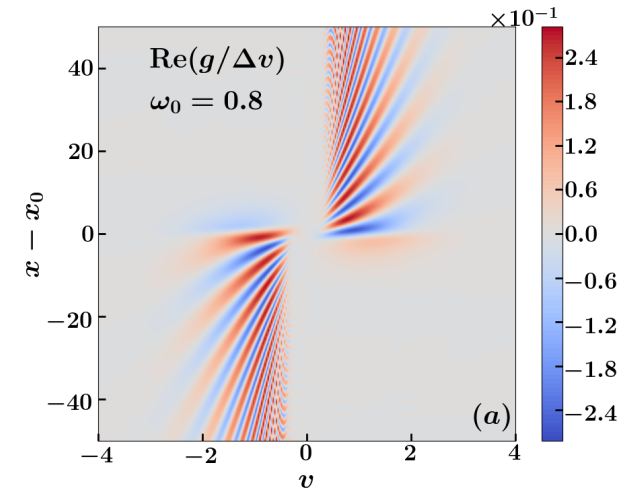
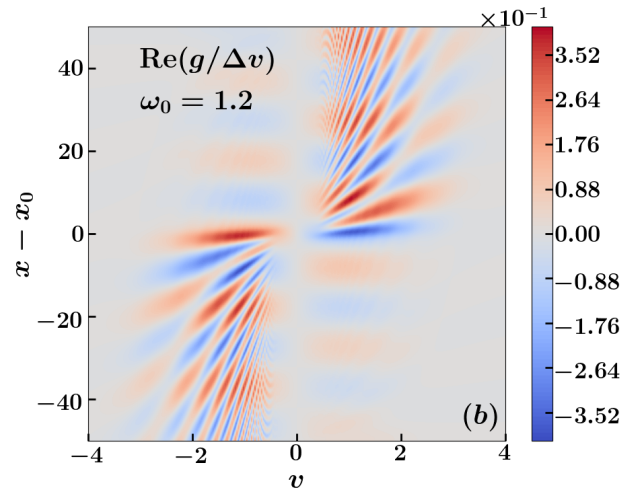
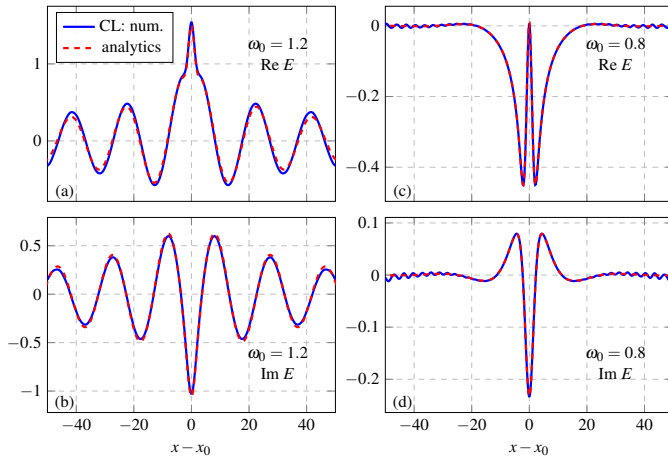
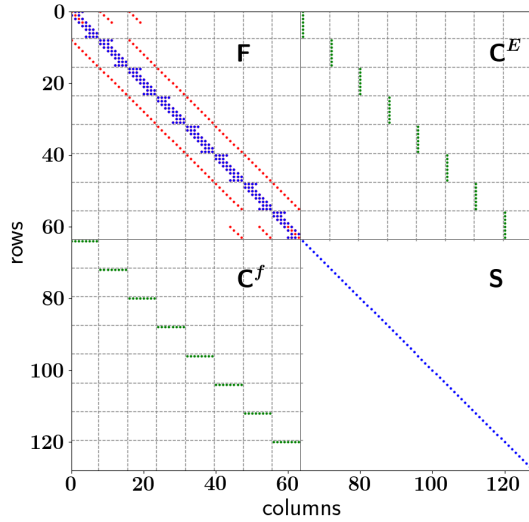
Example: boundary-value problem for kinetic waves

- Linearized Vlasov–Ampere system: 1-D electron plasma, $f(t, x, v) = F(x, v) + g(t, x, v)$, $\partial_t = -i\omega$:

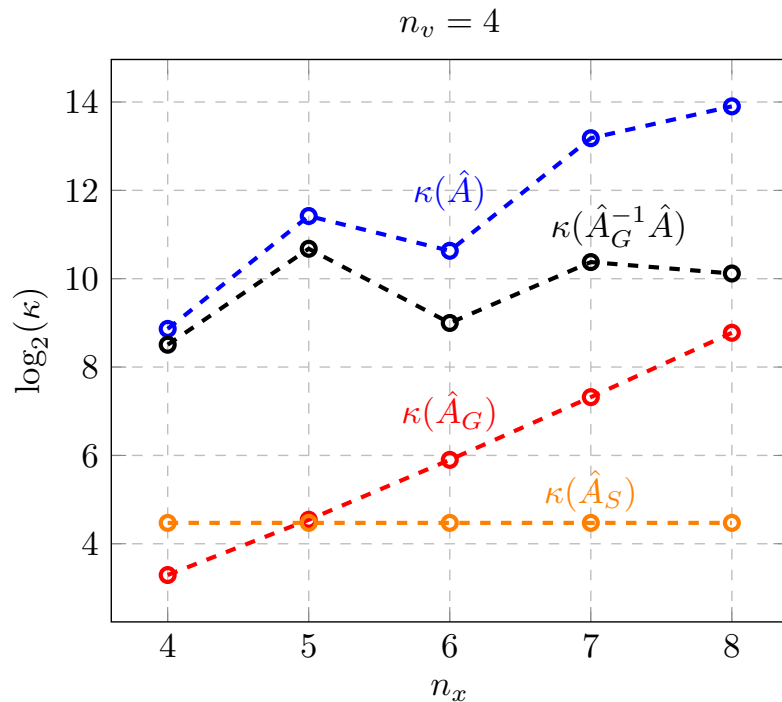
$$-i\omega g + v\partial_x g - E\partial_v F = 0$$

$$-i\omega E - \int v g dv = -j_{\text{ext}}$$

- Solve $A\psi = b$ for $\psi = (g, E)^\top$ and $b \sim (0, j_{\text{ext}})^\top$



- Since the QSVT scaling, $\mathcal{O}(\kappa^2 \varsigma \ln(N_x) \ln(\kappa/\epsilon))$, involves strong dependence on the condition number $\kappa \sim N_x^2$, preconditioning is likely necessary at large N_x .



- A matrix P can serve as a preconditioner for A if PA has a condition number $\kappa(PA) \ll \kappa(A)$.

$$A\psi = b \quad \Rightarrow \quad PA\psi = Pb$$

$$\psi = (PA)^{-1} Pb$$

- Since $\kappa(PA) \ll \kappa(A)$, the matrix $(PA)^{-1}$ is easier to calculate than A^{-1} .

- For example, an approximation to A_G^{-1} can serve as a preconditioner for our A .

$$A = A_G + A_S, \quad A_G = \begin{pmatrix} F & 0 \\ 0 & S \end{pmatrix} - \alpha I, \quad A_S = \begin{pmatrix} 0 & C^E \\ C^f & 0 \end{pmatrix} + \alpha I$$

The challenge of nonlinear simulations

- **No-cloning theorem:** it is impossible to create a copy of an unknown quantum state. So one can't, for example, calculate ψ^2 like this:

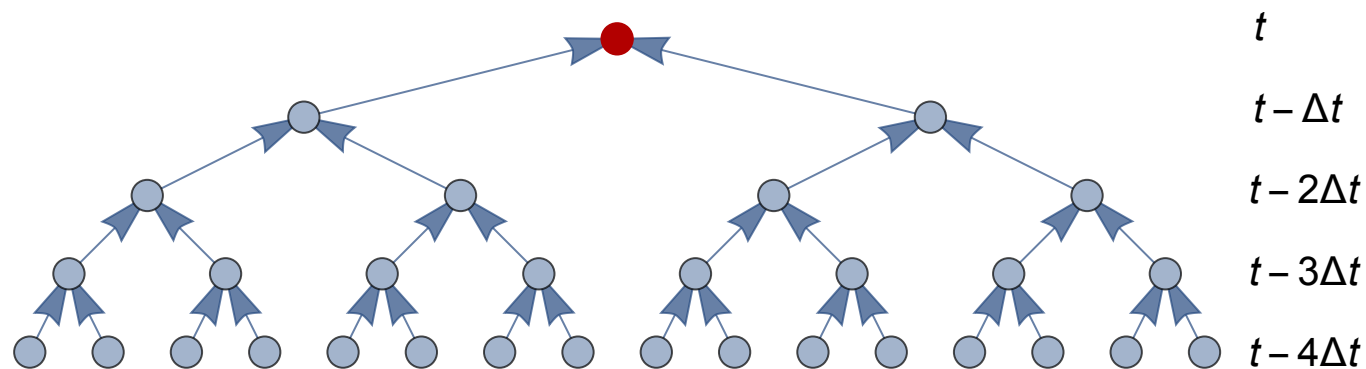
$$|\psi\rangle \not\mapsto \sum_{jk} A_{ijk} \psi_j \psi_k |i\rangle$$

- One *can* make ψ^2 out of two copies of ψ prepared independently (w/post-selection):

$$|\psi\rangle |\psi\rangle |0\rangle_a \longrightarrow |\psi\rangle |\psi\rangle |0\rangle_a + \sum_{jk} A_{ijk} \psi_j \psi_k |i\rangle |0\rangle |1\rangle_a$$

$$\langle 1|_a (\dots) = \sum_{jk} A_{ijk} \psi_j \psi_k |i\rangle |0\rangle$$

- But then, at integrating, say, $\partial_t \psi_i = \sum_{jk} A_{ijk} \psi_j \psi_k$, r steps require **2^r** copies of ψ :



- **Theorem** (kind of): any nonlinear system can be made *exactly* linear using a sufficiently large phase-space extension.
- For example, Hamiltonian systems can be *quantized*.
 - **Example 1:** single-particle motion in prescribed fields

$$\frac{dx}{dt} = \frac{p}{m}, \quad \frac{dp}{dt} = -\frac{\partial V}{\partial x} \quad \Rightarrow \quad i \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2 \nabla^2}{2m} + V \right) \psi$$

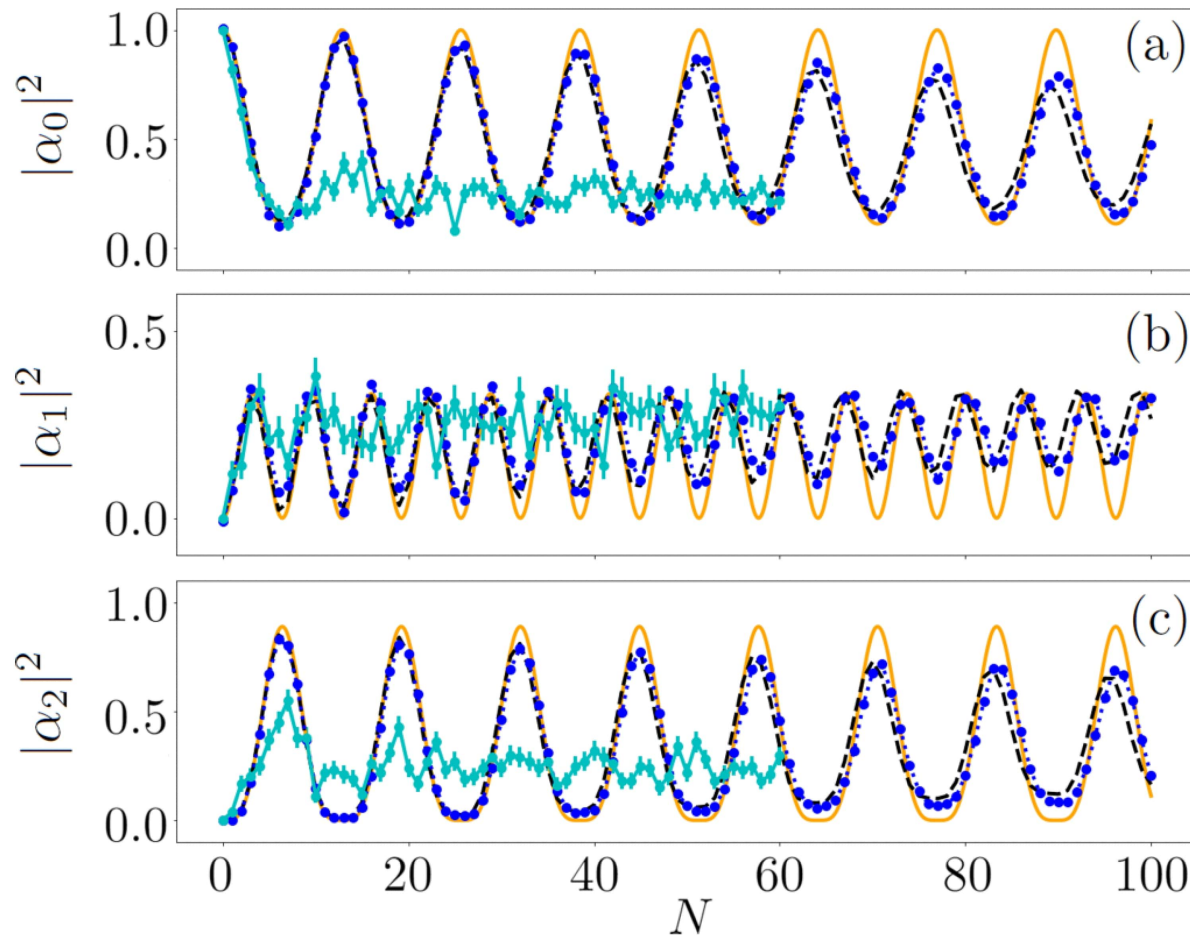
- **Example 2:** three-wave interaction. Use $A_i \rightarrow \hat{A}_i$ and $A_i^* \rightarrow \hat{A}_i^\dagger$. Due to $n_1 + n_2 = \text{const}$ and $n_1 + n_3 = \text{const}$, the accessible Fock space is finite-D.

$$\dot{\hat{A}}_1 = g \hat{A}_2 \hat{A}_3, \quad \dot{\hat{A}}_2 = -g^* \hat{A}_1 \hat{A}_3^*, \quad \dot{\hat{A}}_3 = -g^* \hat{A}_1 \hat{A}_2^*$$

$$h = \begin{pmatrix} 0 & g\sqrt{2(s-1)} & 0 \\ g^*\sqrt{2(s-1)} & 0 & g\sqrt{2s} \\ 0 & g^*\sqrt{2s} & 0 \end{pmatrix}$$

Quantum simulations of three-wave interaction: an experiment

- LLNL experiment on Aspen-4-2Q-A of Rigetti Computing, 2 qubits. $\hat{U} = e^{-i\hat{H}t}$ is converted to ~ 20 native gates. N is the number of times \hat{U} is applied.



Ad hoc linear embeddings are generally unstable.

- Example:** Carleman embedding (1932)

$$\dot{u} = g(u) = \underbrace{g(u_0)}_{a_0} + \sum_{k=1}^{\infty} \underbrace{\frac{g^{(k)}(u_0)}{k!}}_{a_k} \underbrace{u^k}_{y_k}$$

$$\dot{y}_1 = a_0 + a_1 y_1 + a_2 y_2 + \dots$$

$$\begin{aligned} \dot{y}_2 &= 2u\dot{u} \\ &= 2u(a_0 + a_1 u + a_2 u^2 + \dots) \\ &= 2a_0 y_1 + 2a_1 y_2 + 2a_2 y_3 + \dots \end{aligned}$$

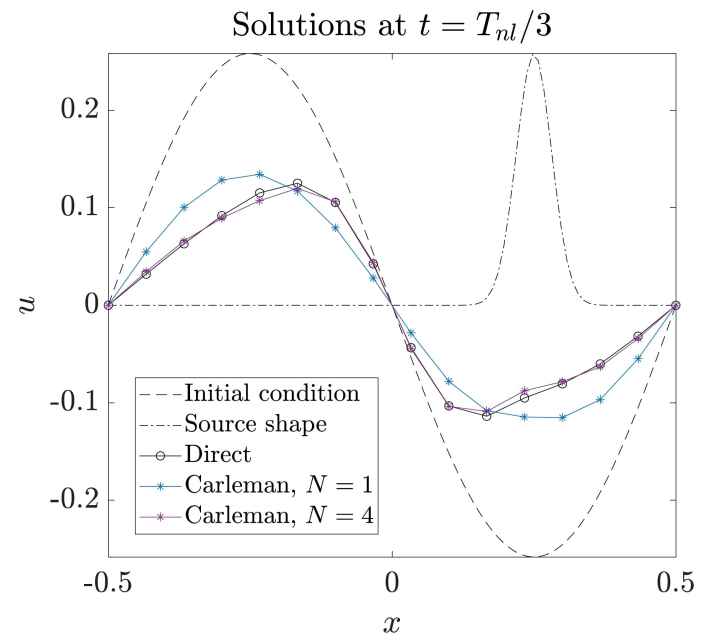
$$\dot{y}_3 = 3a_0 y_2 + 3a_1 y_3 + 3a_2 y_4 + \dots$$

$$\dot{\mathbf{y}} = \mathbf{A}\mathbf{y} + \mathbf{b}, \quad \mathbf{y} = (y_1, y_2, \dots)^T$$

- Works *only* for stable dynamics. Figure: 1-D driven Burgers' eqn at small enough Re.

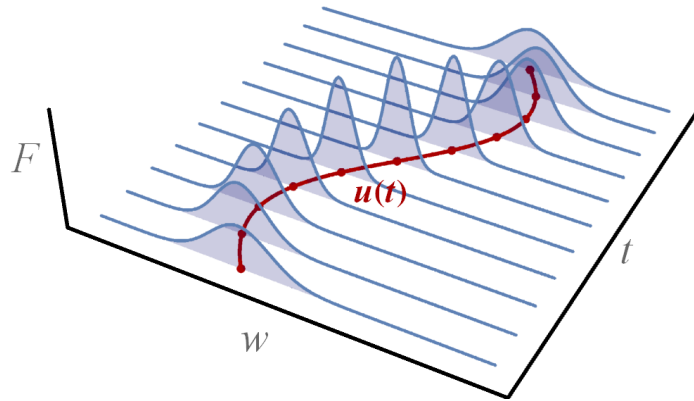


Torsten Carleman



- Instead of u , consider the probability distribution $F(t, w) = \delta(w - u(t))$:

$$\dot{u} = g(u) \quad \Rightarrow \quad \underbrace{\partial_t F + \partial_w [g(t, w) F]}_{\text{Liouville equation}} = 0$$



- $\psi = \sqrt{F}$ satisfies $i\partial_t \psi = \hat{H} \psi$ with $\hat{H} = \hat{H}^\dagger$:

$$\hat{H} = 1/2(g\hat{\rho} + \hat{\rho}g), \quad \hat{\rho} = -i\partial_w$$
- Variational representation $\delta \langle \psi | i\partial_t - \hat{H} | \psi \rangle = 0$
→ structure-preserving truncations possible.

- A finite-dimensional representation is obtained by substituting a truncated expansion $|\psi\rangle = \sum_{i=1}^r \psi_i |e_i\rangle$ in a suitable basis $|e_i\rangle$ into the variational principle:

$$i\partial_t \begin{pmatrix} \psi_1 \\ \dots \\ \psi_r \end{pmatrix} = \hat{H} \begin{pmatrix} \psi_1 \\ \dots \\ \psi_r \end{pmatrix}, \quad \hat{H}_{jk} = \langle e_j | \hat{H} | e_k \rangle = \hat{H}_{kj}^*$$

- Maybe $\dim \psi$ does not have to be very large if one chooses the right basis?..

Koopman–von Neumann embedding for the Vlasov–Poisson system

- Vlasov equation does not feature individual particles, but one can emulate Vlasov dynamics using N macroparticles. The N -particle distribution equation is **linear**:

$$\frac{\partial \Psi}{\partial t} = - \sum_{i=1}^N v_i \frac{\partial \Psi}{\partial x_i} + \sum_{i=1}^N \left(\frac{\partial V_{\text{ext}}}{\partial x_i} + \sum_{j=1, j \neq i}^N \frac{\partial V_{ij}}{\partial x_i} \right) \frac{\partial \Psi}{\partial p_i} \equiv -i \hat{\mathcal{H}} \Psi$$

Here, V_{ext} is the external potential and $V_{ij} = V(|x_i - x_j|)$ is the interaction (Coulomb) potential, which is a fixed known function.

- No need to simulate macroparticles as highly localized objects. Use expansion in global modes (e.g. Gauss–Hermite) → **finite-D conservative linear system**:

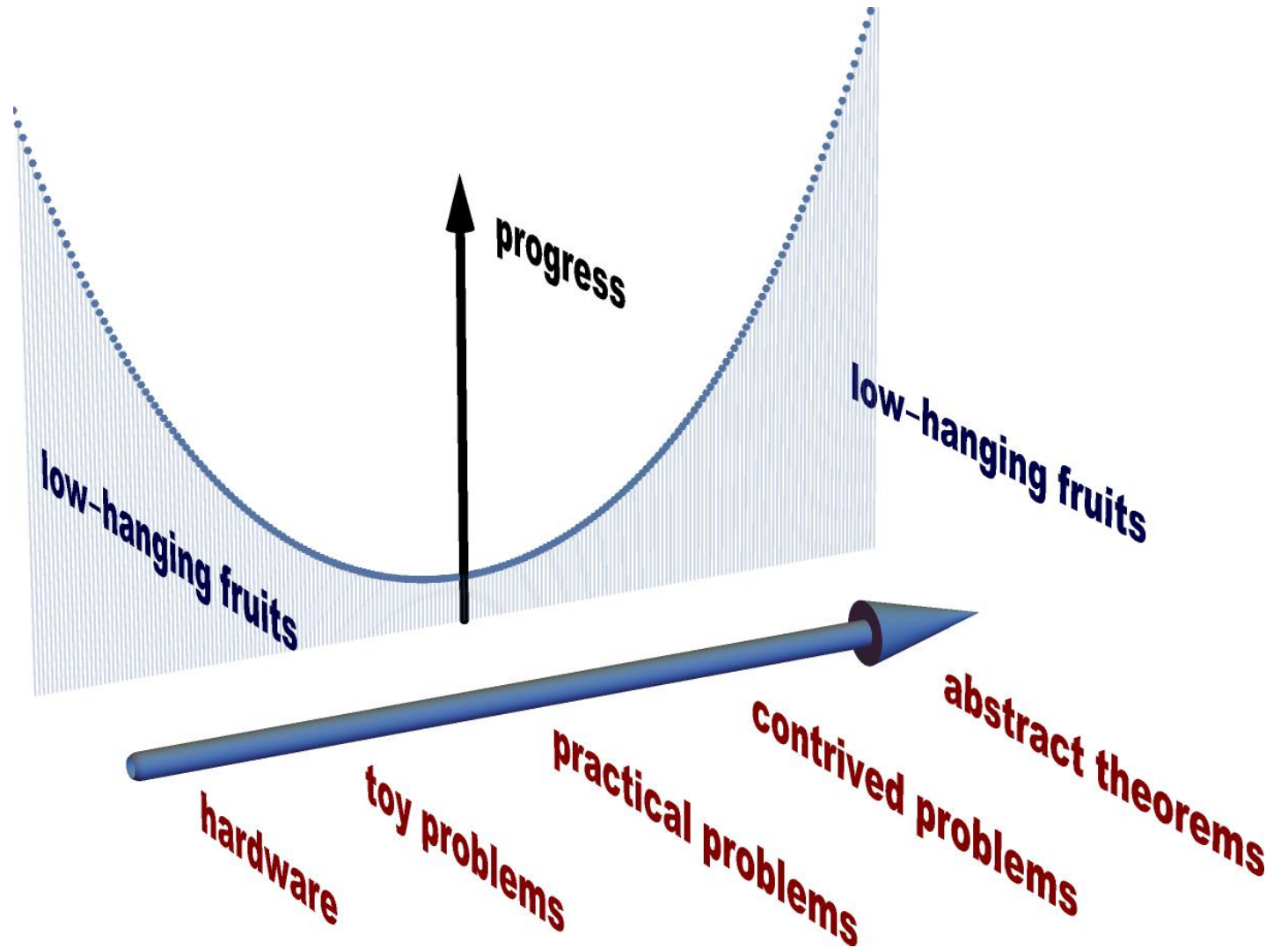
$$i \partial_t \begin{pmatrix} \psi_1 \\ \dots \\ \psi_r \end{pmatrix} = \hat{H} \begin{pmatrix} \psi_1 \\ \dots \\ \psi_r \end{pmatrix}, \quad \hat{H}_{jk} = \langle e_j | \hat{\mathcal{H}} | e_k \rangle = \hat{H}_{kj}^*$$

- Can this provide quantum advantage in practice? This remains to be seen.

Part III: Final thoughts. Where are we?



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Summary (and the obligatory comic strip)



- The hype aside, quantum computing remains a **legitimate physics problem**.
- Possibly promising directions of research for plasma applications:
 - algorithms: **physics-based linear embeddings, hybrid computing**;
 - circuit engineering: automation of circuit development (ML/AI);
 - hardware: specialized gates for classical problems, e.g. multi-controlled gates.
- Little is done in the area of **practical algorithms** – may be a land of opportunity.
- Will it ever work? We'll never know unless we try hard, *and we have not yet*.

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