

and Twitter cats

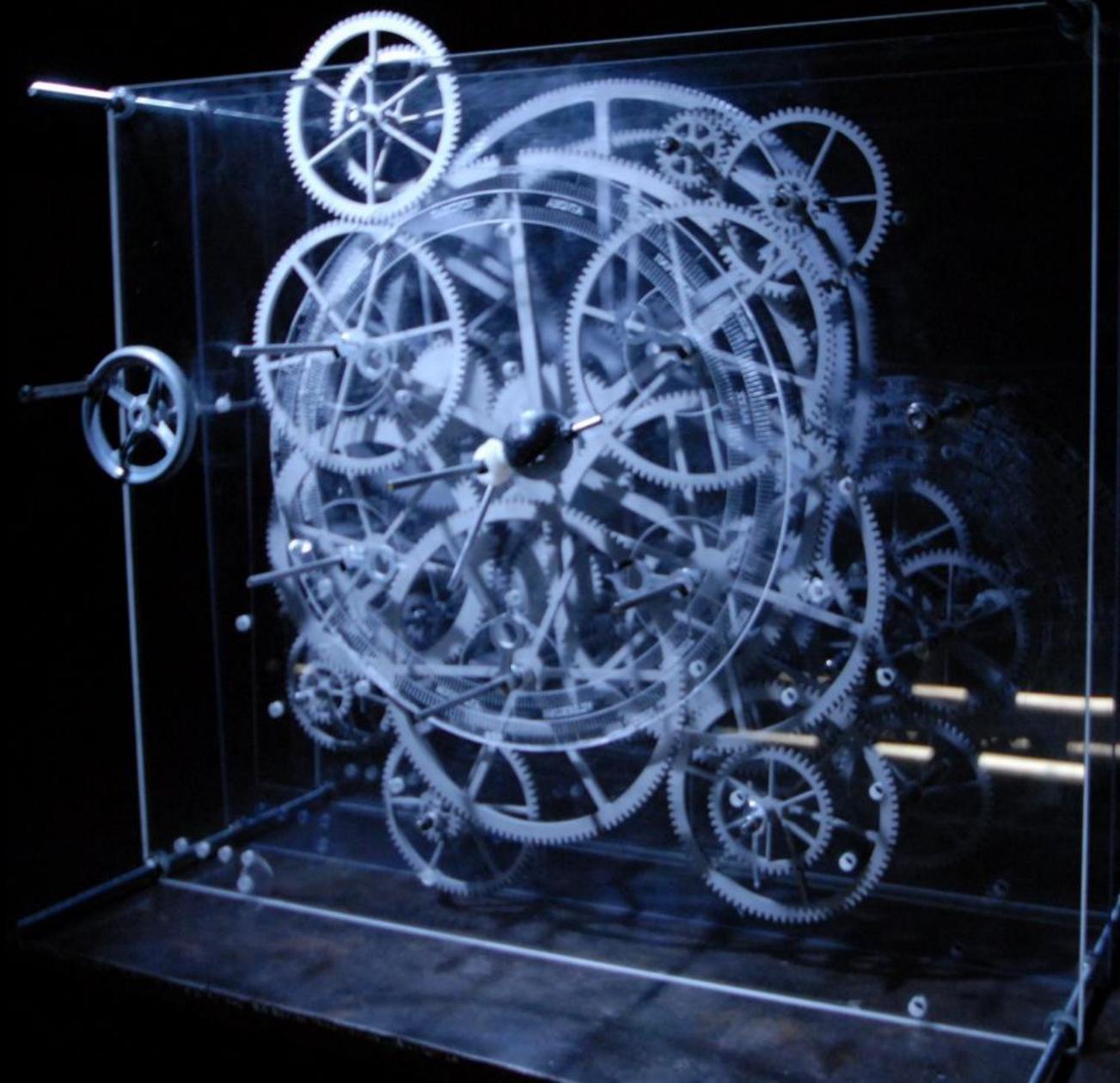
Applied mathematics with a quantum computer

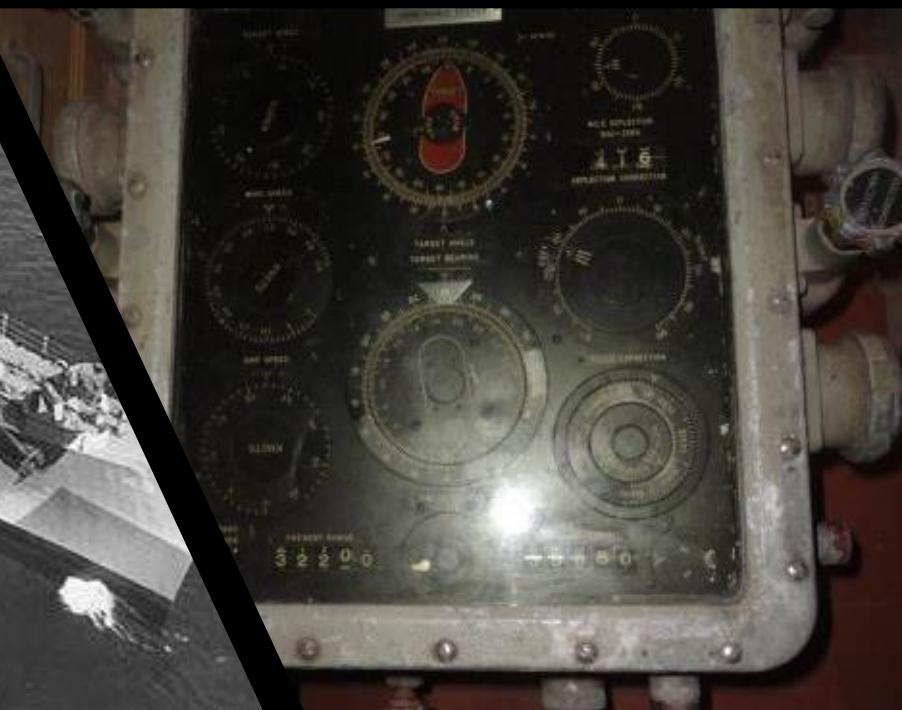
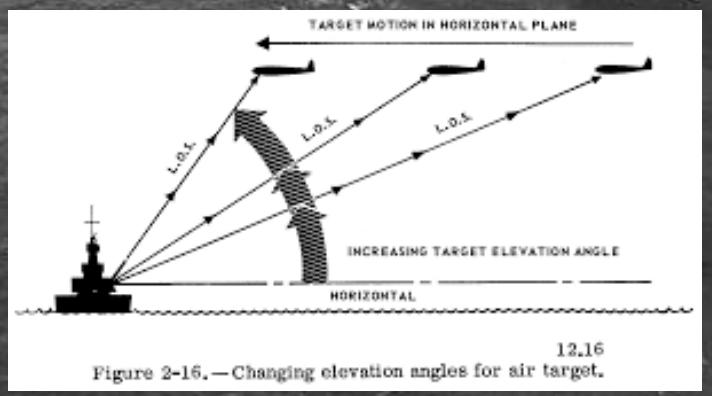
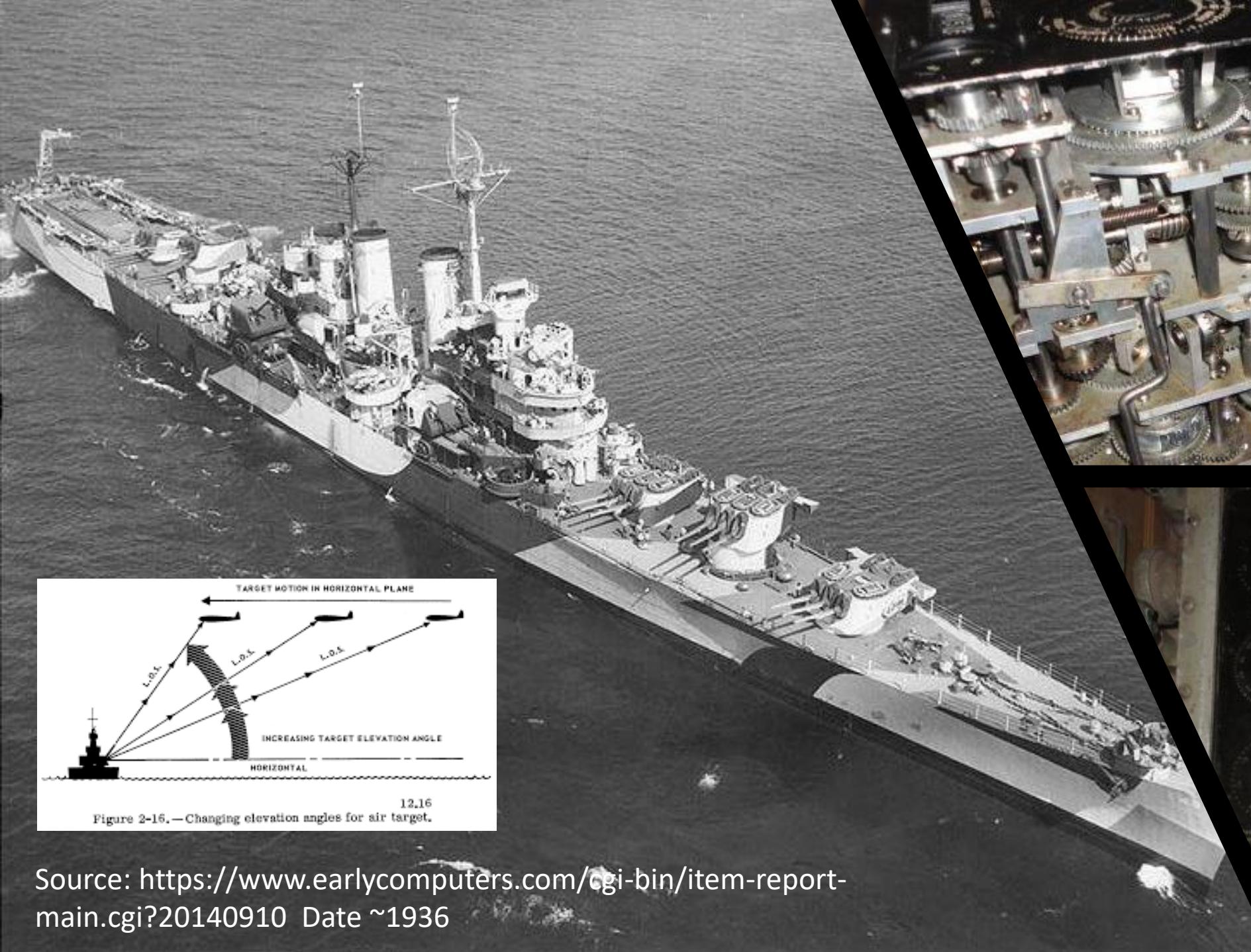
Juan José García Ripoll (IFF-CSIC, Spain)





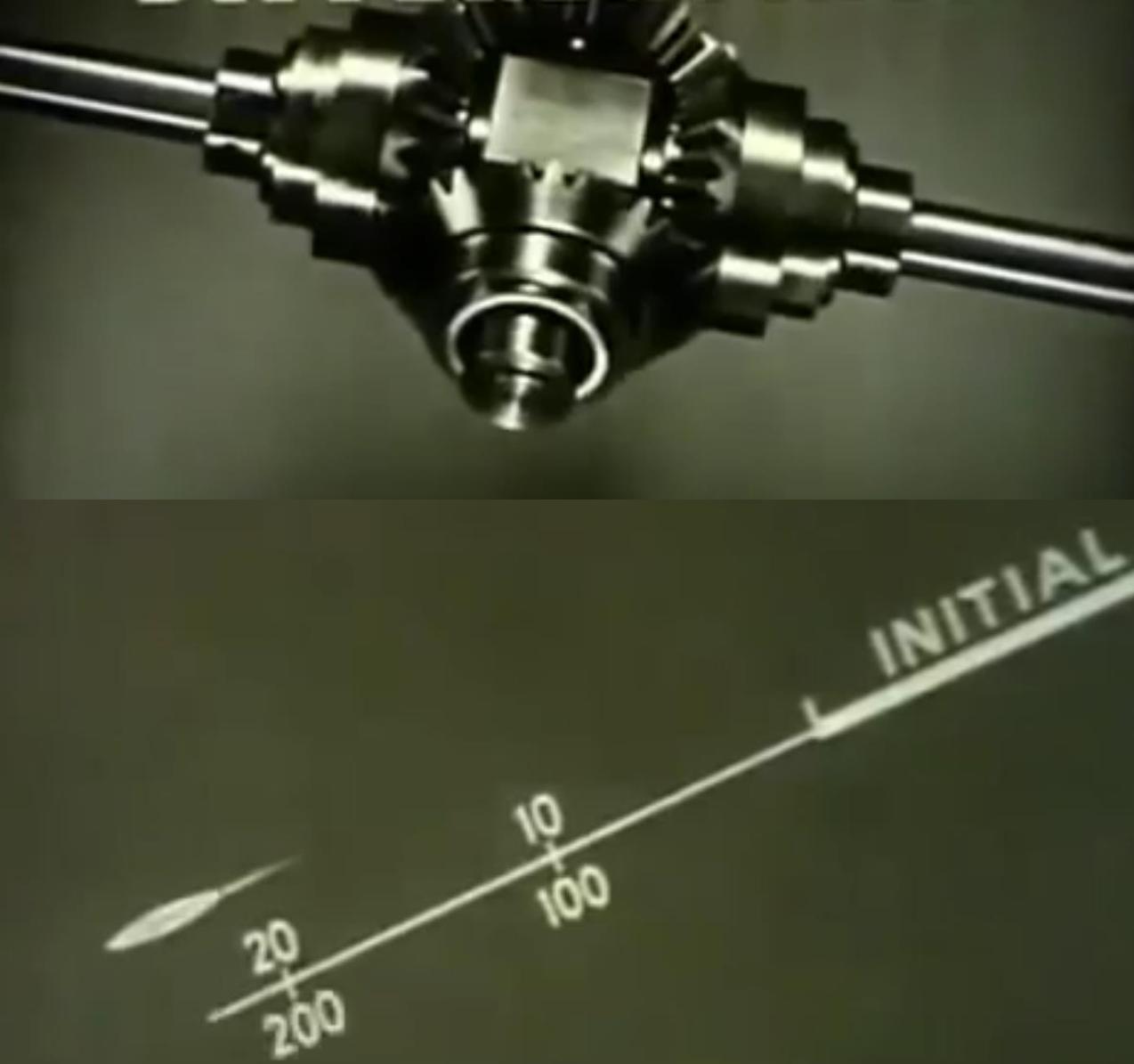
Antikythera Mechanism
200-100 BC





Source: <https://www.earlycomputers.com/cgi-bin/item-report-main.cgi?20140910> Date ~1936

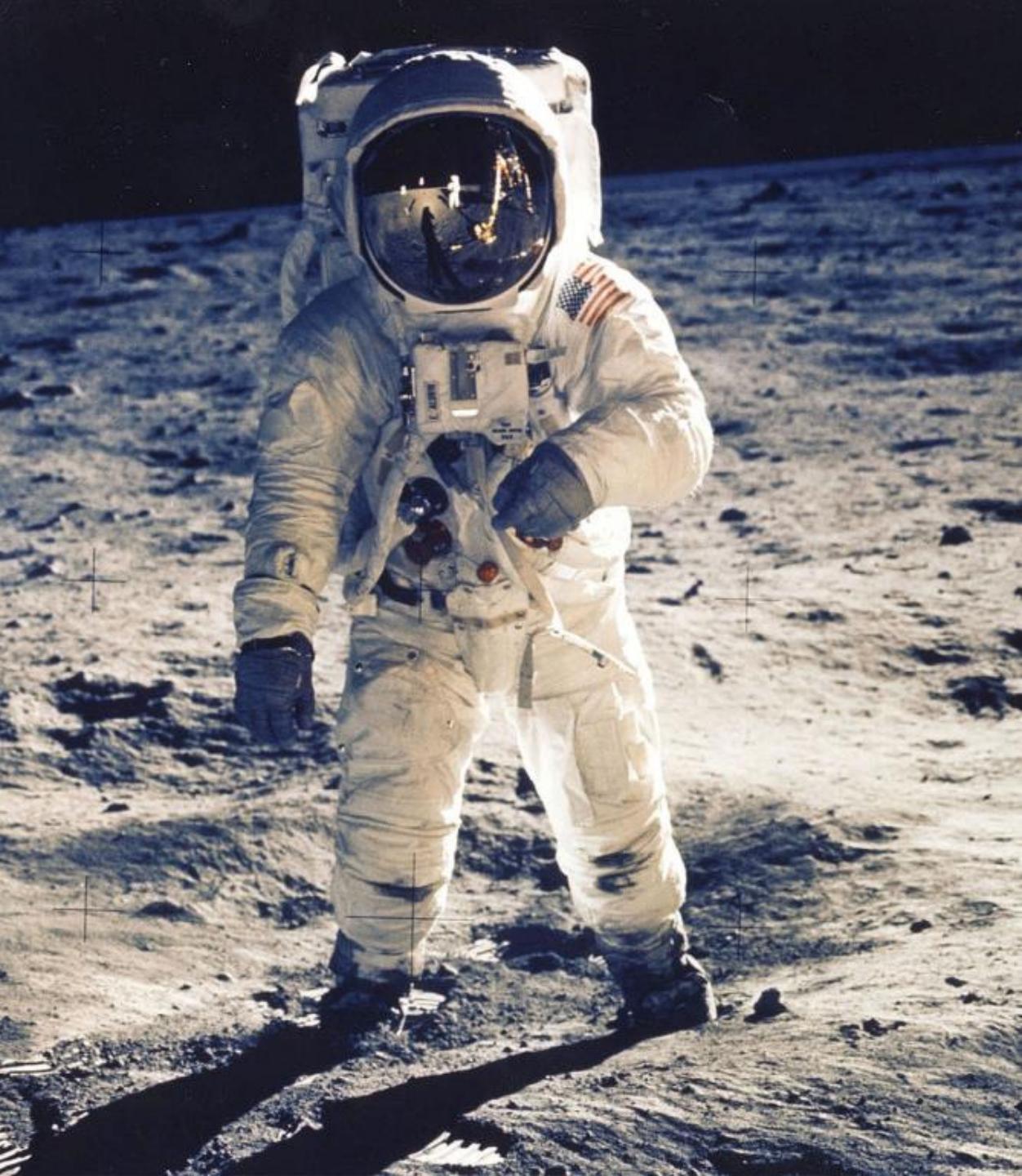
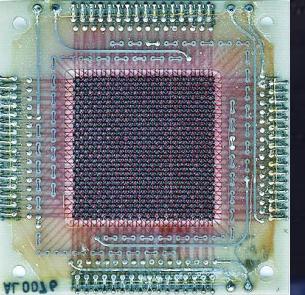
DIFFERENTIALS



INTEGRATORS

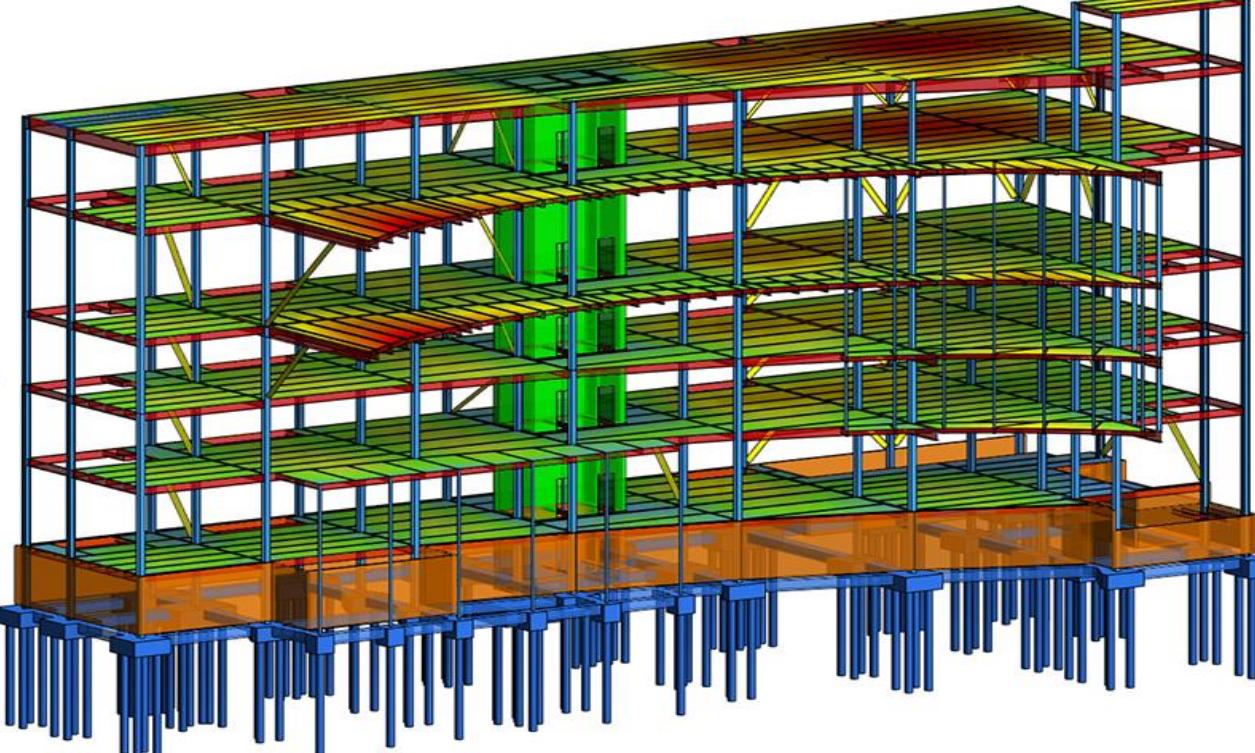
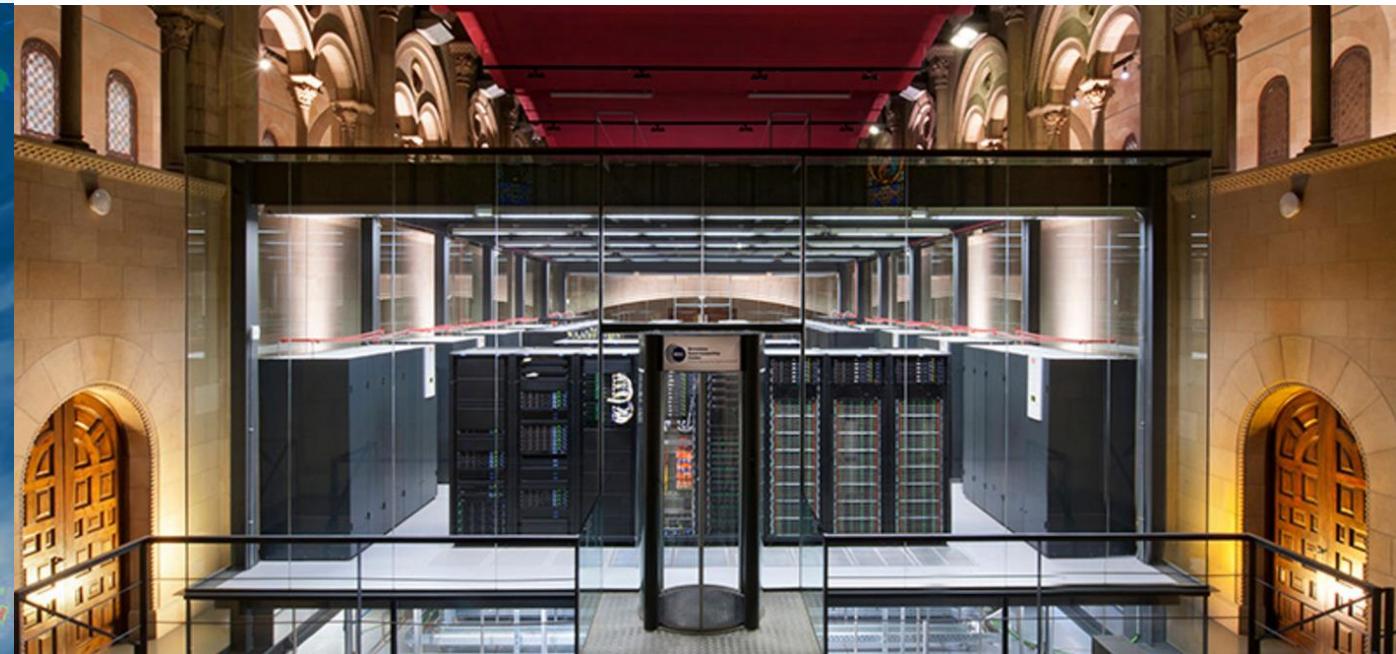
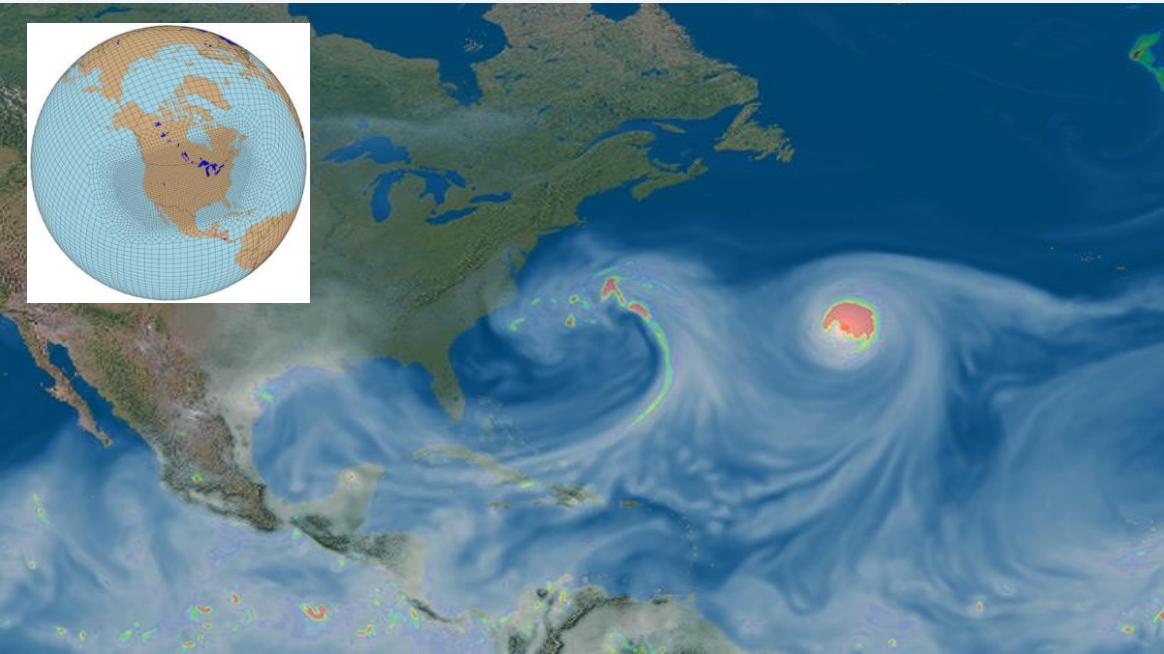
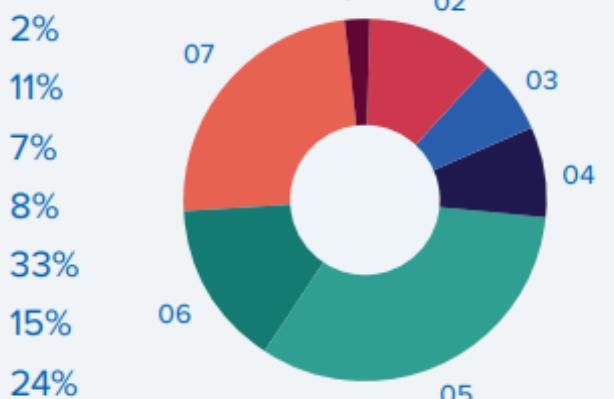






220M

- 01 Biological Sciences
- 02 Chemistry
- 03 Earth Science
- 04 Energy Technologies
- 05 Engineering
- 06 Materials Science
- 07 Physics



IBM Q™



Google AI
Quantum



Many interesting
problems to
address...

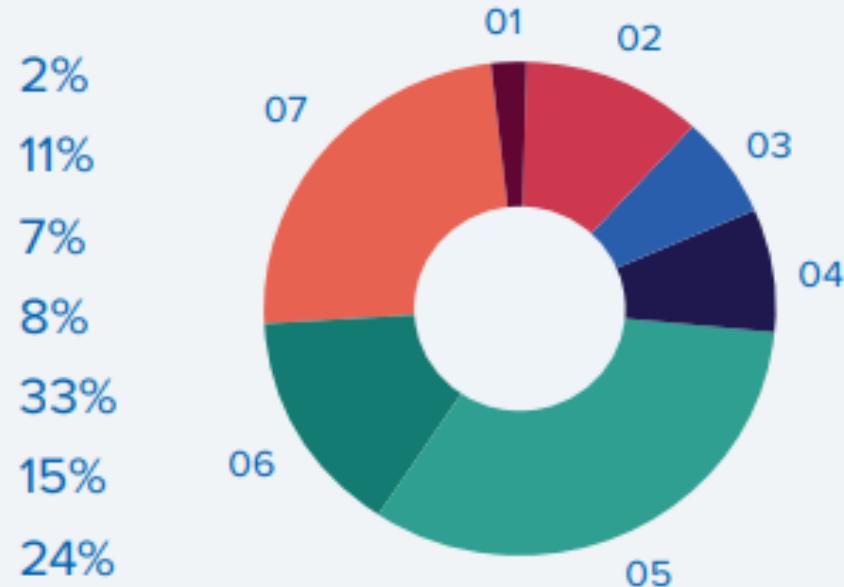
Quantum
advantage?

2019 INCITE
Million Node-Hours

- 01 Biological Sciences
- 02 Chemistry
- 03 Earth Science
- 04 Energy Technologies
- 05 Engineering
- 06 Materials Science
- 07 Physics

MIRA

220M





Problem domain: numerical analysis

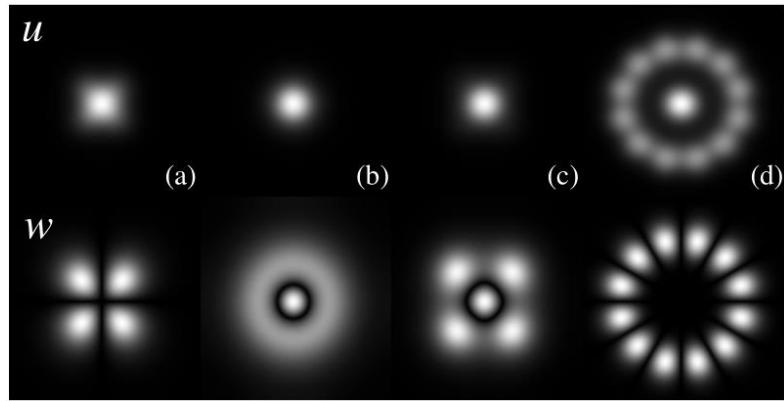
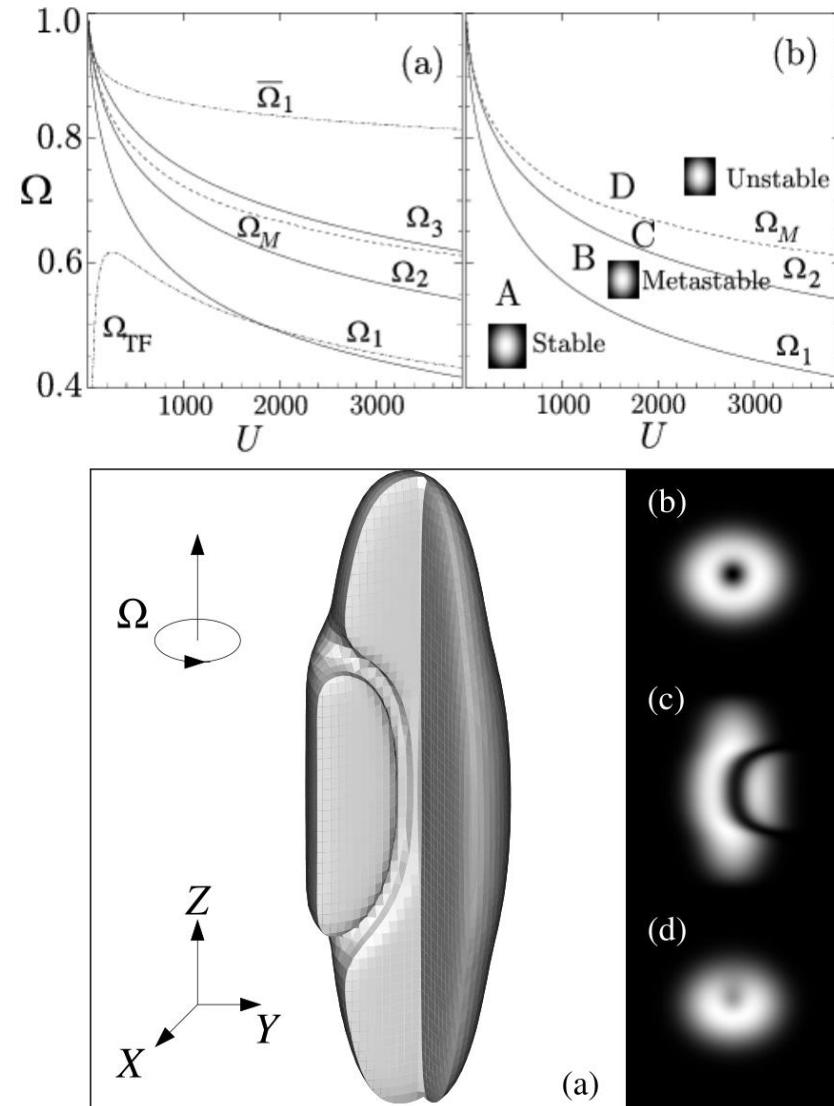


FIG. 5.3. Different unstable multi-solitonic configurations arising from Eq. (5.14) with a change of the initial conditions for fixed $\mu_u = -1, \mu_w = -0.3, \kappa = 0.5$.

JJGR & Pérez-García, V.M., SIAM J. Sci. Comp. (2001)

$$\frac{\partial \psi}{\partial t} = \left[-\frac{1}{2} \Delta + V(x) + U|\psi|^2 - i\hbar\partial_\theta \right] \psi(x, t)$$

Nonlinear Schrödinger equations, applications,
mathematical properties, new numerical
techniques, etc.

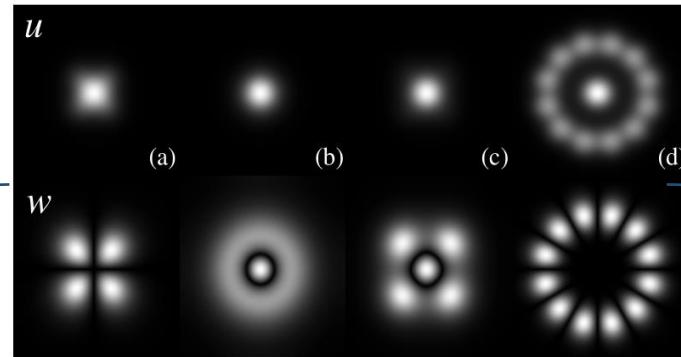
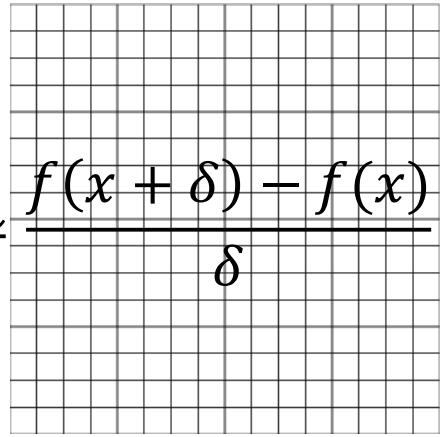


JJGR & Pérez-García, V.M., PRA (1999)

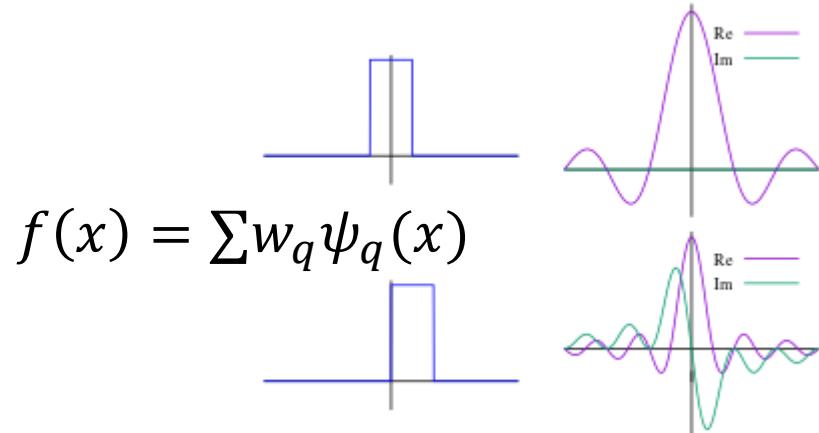
Many classical encodings

Finite differences

$$\frac{df}{dx} \simeq \frac{f(x + \delta) - f(x)}{\delta}$$

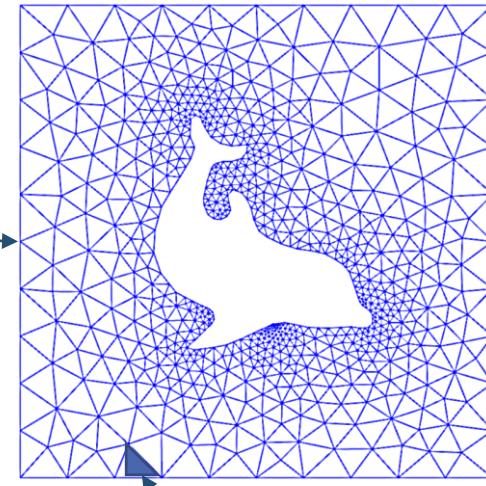


Spectral method

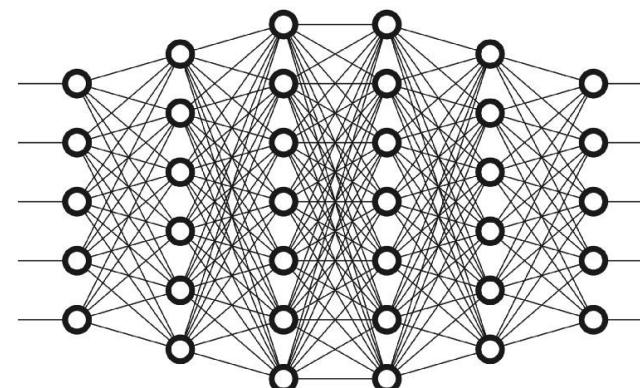


$$f(x) = \sum w_q \psi_q(x)$$

Finite element



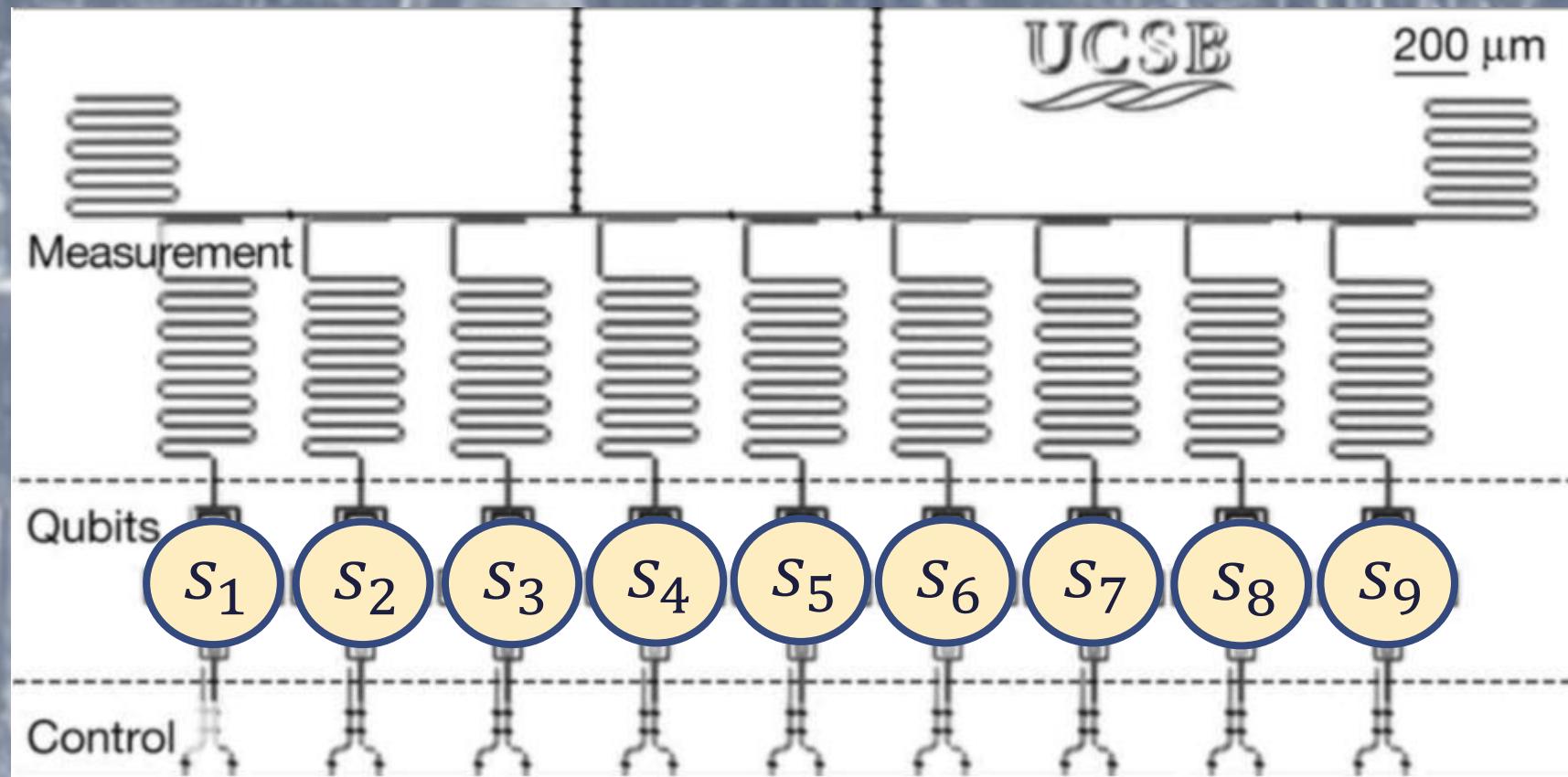
Variational methods



$$f(x)_m \simeq \sum_n c_n^m x^n$$

$$f(x_1, x_2, \dots)$$

Quantum register



Quantum register

Exponential capacity

$$|\psi\rangle = \sum_s \psi(s_1, s_2, \dots) |s_1, s_2, \dots\rangle$$

Quantum superposition

$$2^9 = 512$$

$$2^4 = 16$$

$$\{0,1\} \times \{0,1\} \times \{0,1\}$$

$$s_1 \quad s_2 \quad s_3 \quad s_4 \quad s_5 \quad s_6 \quad s_7 \quad s_8 \quad s_9$$

Quantum algorithms

$$|\psi\rangle = \sum_s \psi(s_1, s_2, \dots) |s_1, s_2, \dots\rangle$$

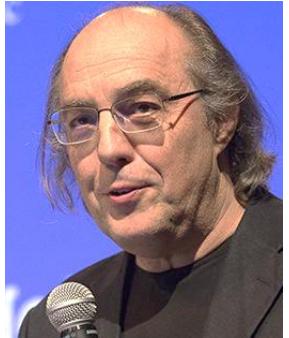
$$|\psi\rangle = \psi(s_1^{opt}, s_2^{opt}, \dots) |s_1^{opt}, s_2^{opt}, \dots\rangle$$

$$\langle O_1 \rangle, \langle O_1 O_2 \rangle, \dots$$

Construction of complex
wavefunctions that solve or
encode problems.

Interrogating those
wavefunctions for properties
or features.

Quantum image processing



*Image compression
and entanglement,*
J. I. Latorre
[quant-ph/0510031](#)



Quantum image processing



B&W image encoded in pure intensity,
with an integer between 0 and 255

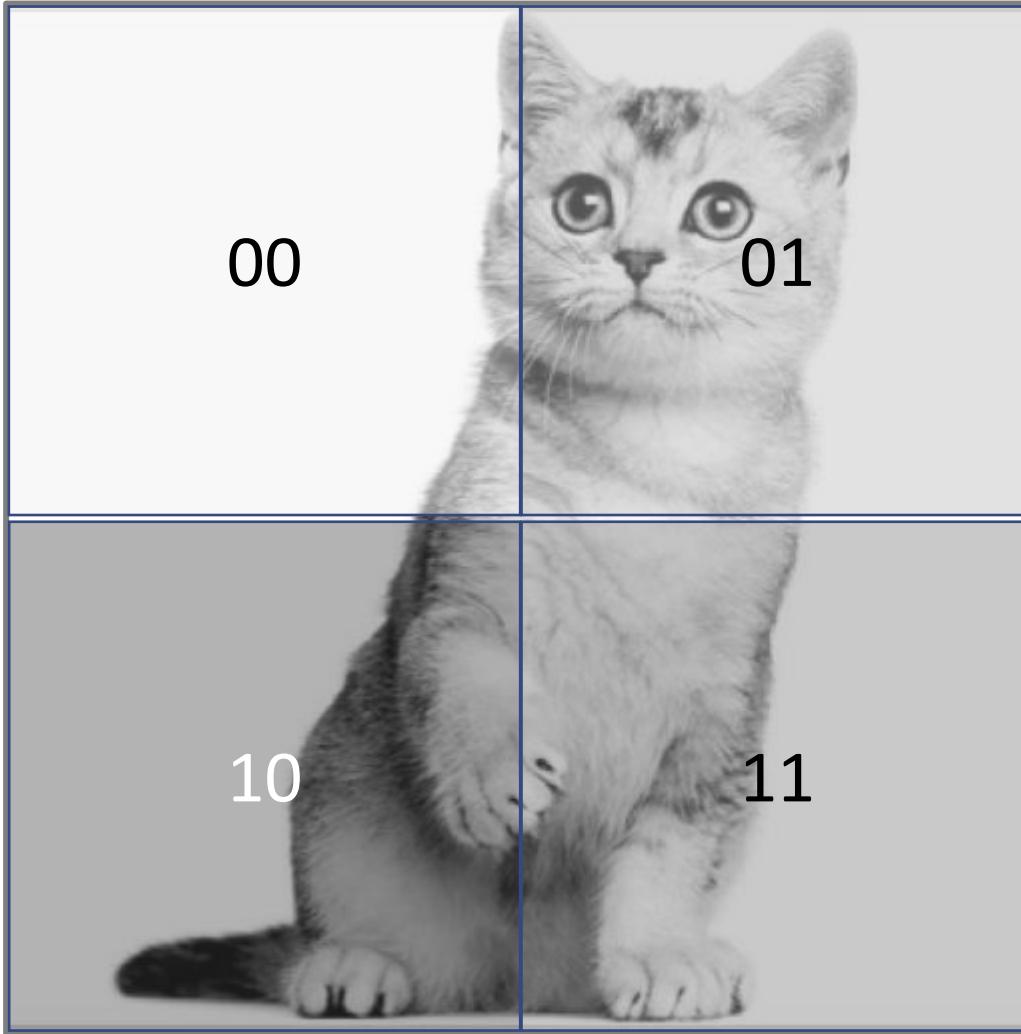
$$\begin{aligned} I(0) &= 213 \\ I(1) &= 213 \\ I(2) &= 213 \\ \dots \\ I(100) &= 213 \\ \dots \\ I(1300) &= 214 \\ \dots \\ I(2600) &= 254 \\ \dots \\ I(2700) &= 254 \\ \dots \\ I(4530) &= 253 \\ \dots \end{aligned}$$

**512 x 512 pixels
= 262144 values
= 9 + 9 qubits**

Image encoding

$s_2 \sim x$ coordinate

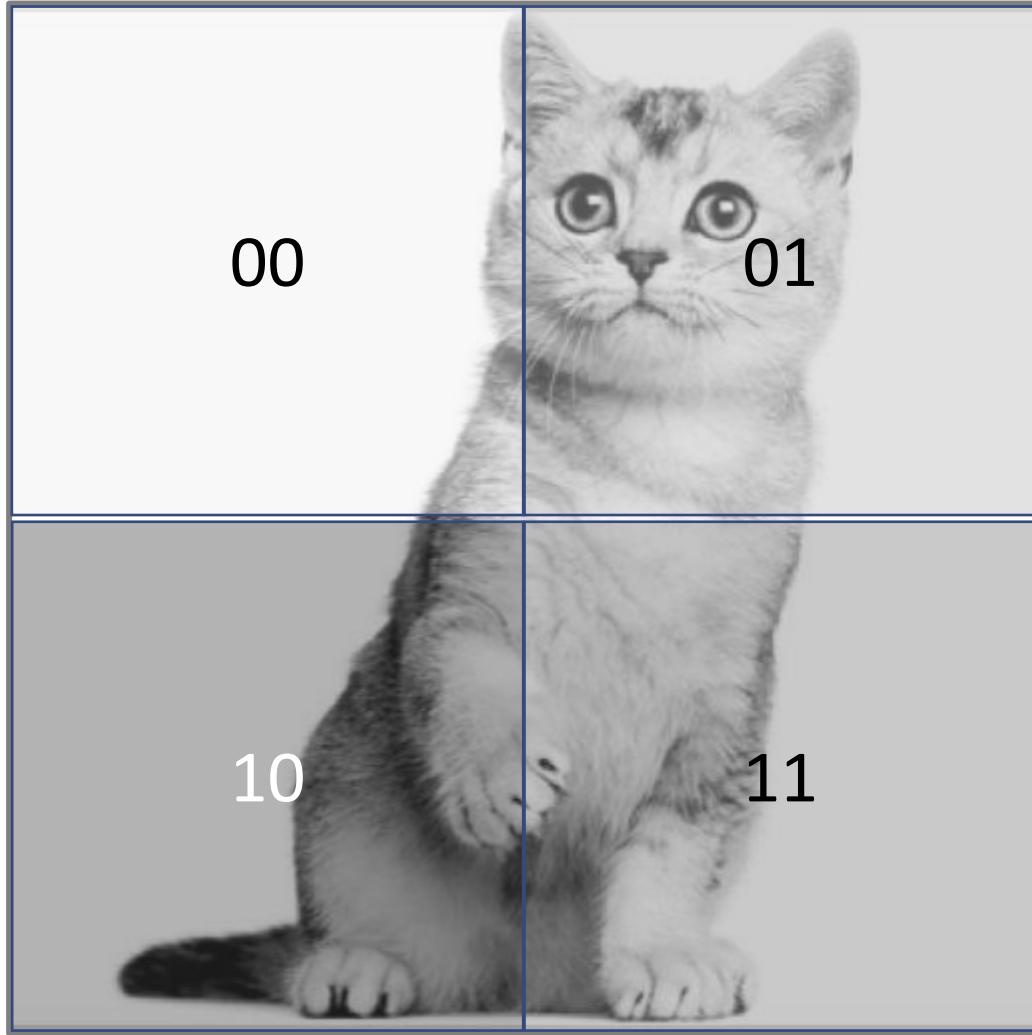
$s_1 \sim y$ coordinate



For instance, using 2x2 pixels, 4 values

$$I(s_1, s_2) \sim I(00), I(01), I(10), I(11)$$

Image encoding



For instance, using 2×2 pixels, 4 values

$$I(s_1, s_2) \sim I(00), I(01), I(10), I(11)$$

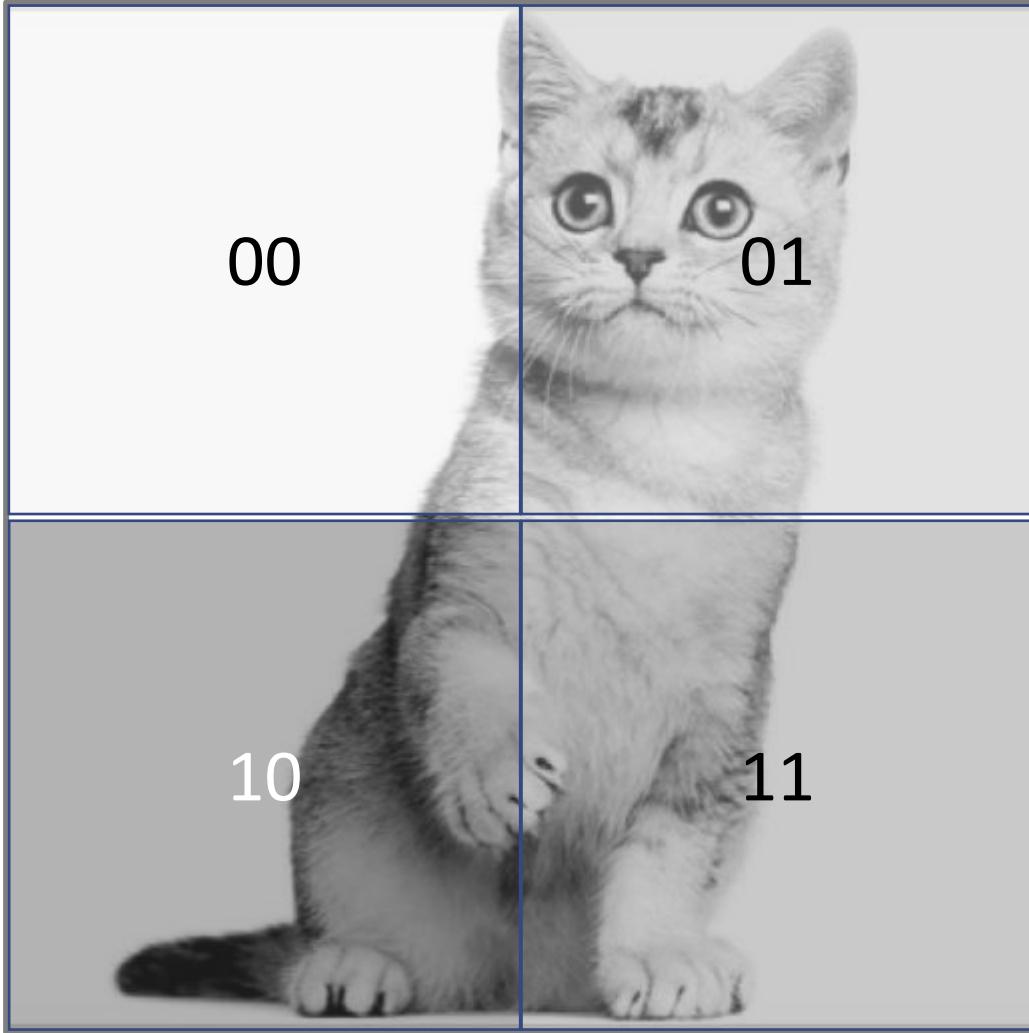
We identify “I” with the probability of finding the quantum register in a given state

$$|\psi\rangle \sim \sum_{\vec{s}_2} \sqrt{I(s_1, s_2)} |s_1, s_2\rangle$$

Explicitely

$$|\psi\rangle \sim \sqrt{I(0,0)} |0,0\rangle + \sqrt{I(0,1)} |0,1\rangle + \sqrt{I(1,0)} |1,0\rangle + \sqrt{I(1,1)} |1,1\rangle$$

Normalization



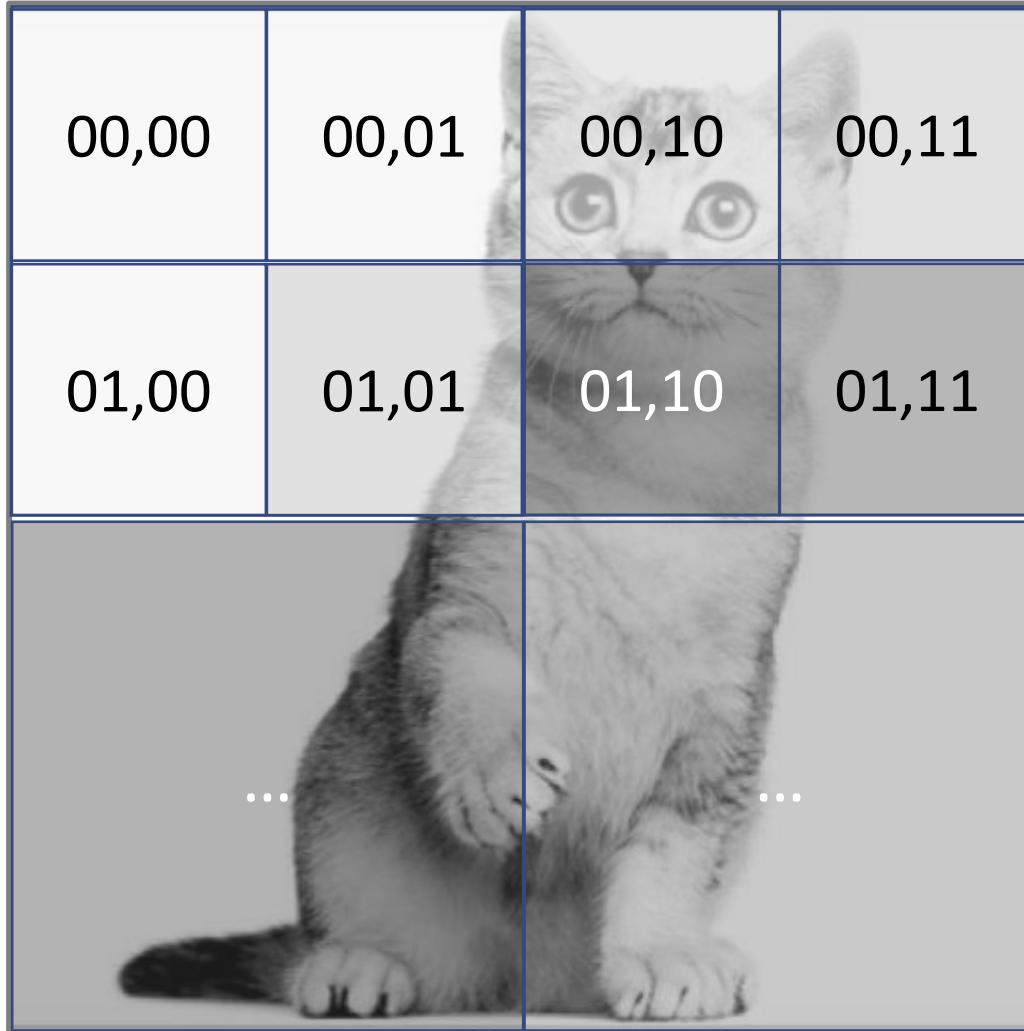
Original and encoding do not perfectly match:

$$|\psi\rangle = \sum_{\vec{s}_2} \sqrt{\frac{I(s_1, s_2)}{I_T}} |s_1, s_2\rangle$$

Probability is normalized with respect to total intensity

$$I_T = \sum_{\vec{s}_2} I(s_1, s_2)$$

+1 qubit = double resolution



1 qubits x 1 qubits

4 pixels

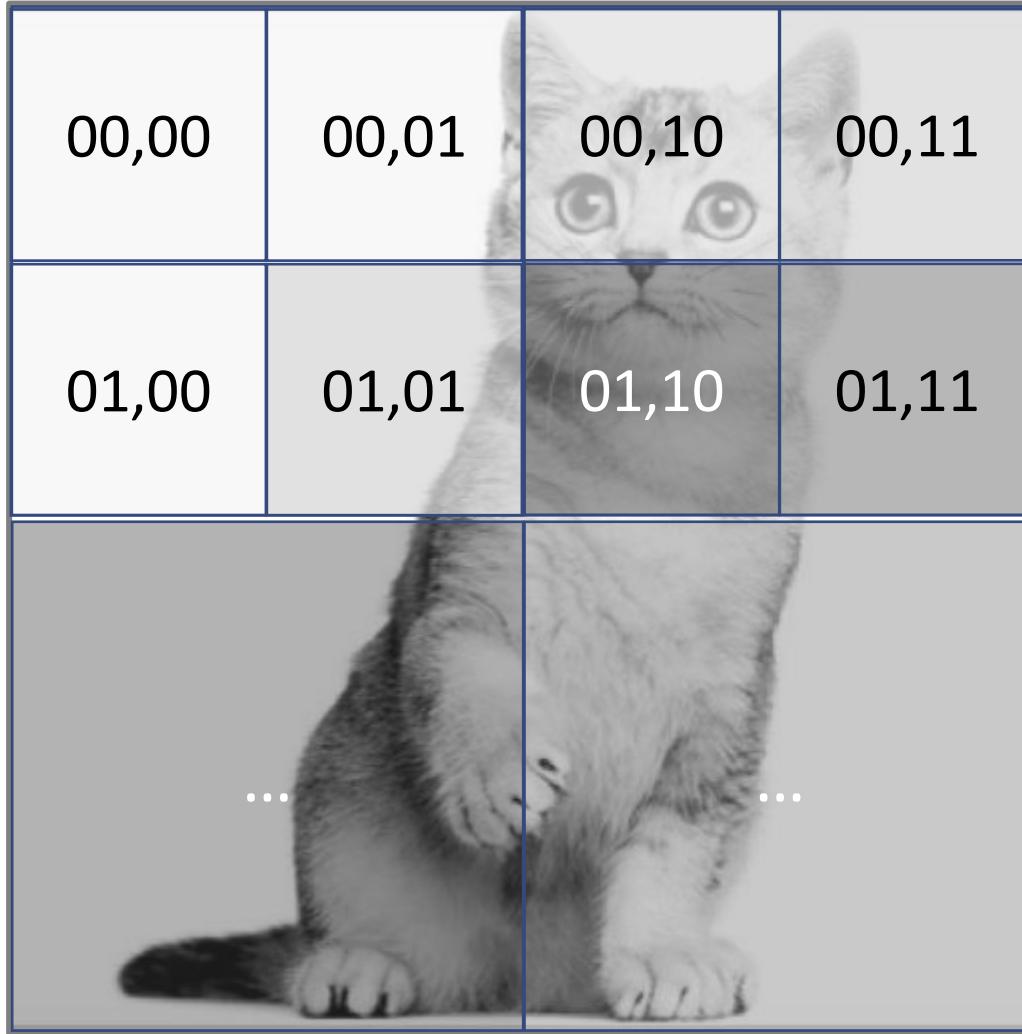


2 qubits x 2 qubits



16 pixels

Quantum register ordering

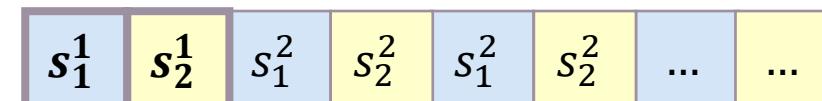


Different orders: coordinate first



(A)

Precision first



(B)

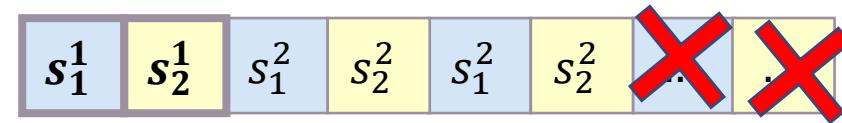
Implicit renormalization.

Most important length scales appear first,
correlated details at the end.

“Forgetting” information

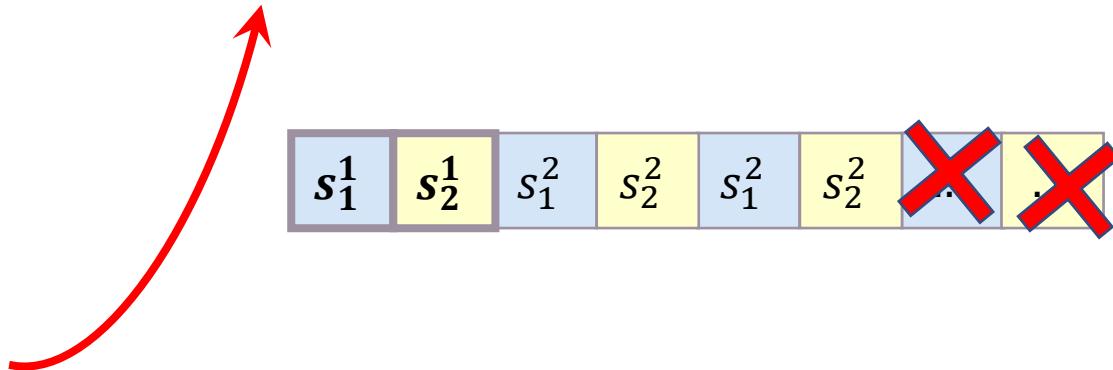


What happens when qubits disappear?





8+8



9 qubits + 9 qubits

$$|\psi\rangle = \sum \psi(\vec{s}) |s_1 \dots s_{18}\rangle$$



9 qubits + 9 qubits

$$|\psi\rangle = \sum \psi(\vec{s}) |s_1 \dots s_{18}\rangle$$



8+8

Original state:

$$|\psi\rangle = \sum \psi(\vec{s}) |s_1 \dots s_{18}\rangle$$

Separate bits that we ignore:

$$|\psi\rangle = \sum \psi(\vec{s}_{16}, \vec{r}_2) |\vec{s}_{16}\rangle |\vec{r}\rangle$$

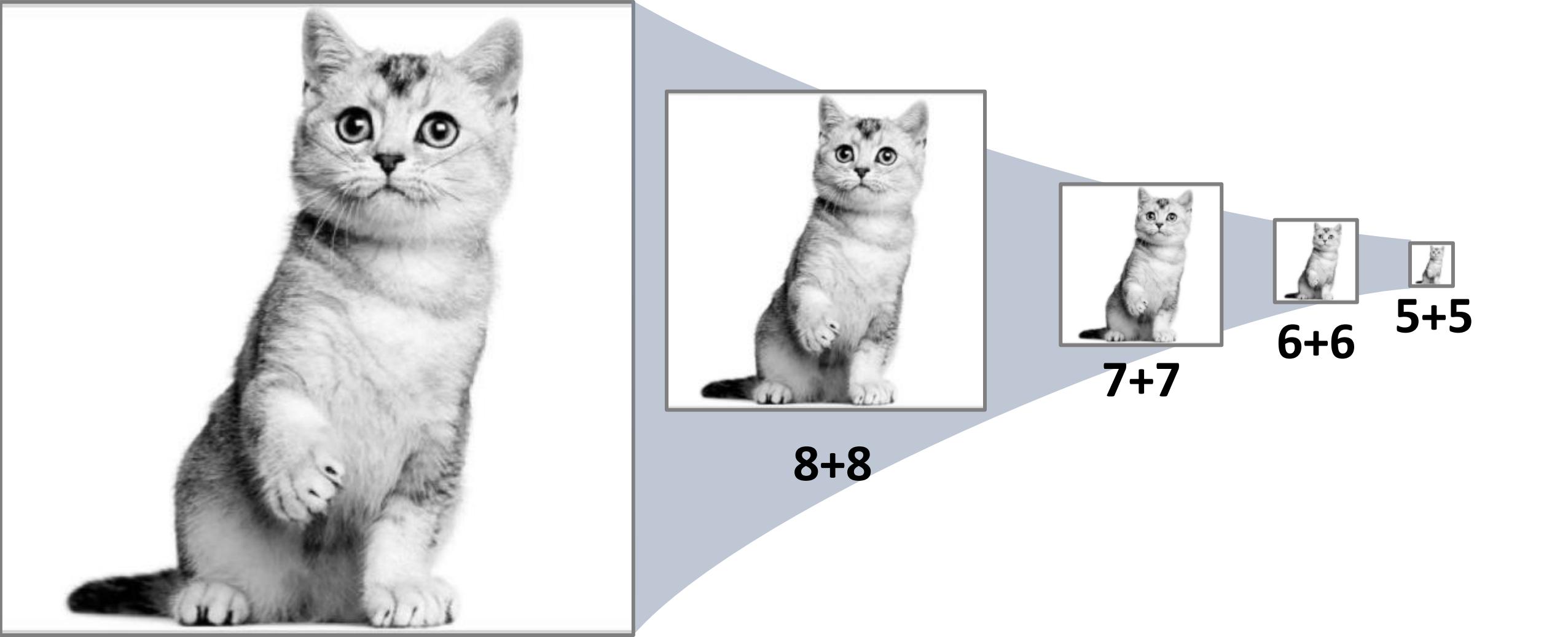
Image is the probability of a state:

$$\rho(\vec{s}_{16}, \vec{s}'_{16}) = \sum_{\vec{r}_2} \psi(\vec{s}_{16}, \vec{r}_2) \psi^*(\vec{s}_{16}, \vec{r}_2)$$

$$I(\vec{s}_{16}) = \rho(\vec{s}_{16}, \vec{s}_{16})$$

This is related to the density matrix of remaining qubits:

$$\rho = \sum \rho(\vec{s}_{16}, \vec{s}'_{16}) |\vec{s}_{16}\rangle \langle \vec{s}'_{16}|$$



9 qubits + 9 qubits

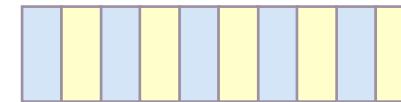
Resampling



9 qubits + 9 qubits

We bring in fresh qubits with no information
about details (all zero)

5+5



$|I_{10}\rangle$

4+4



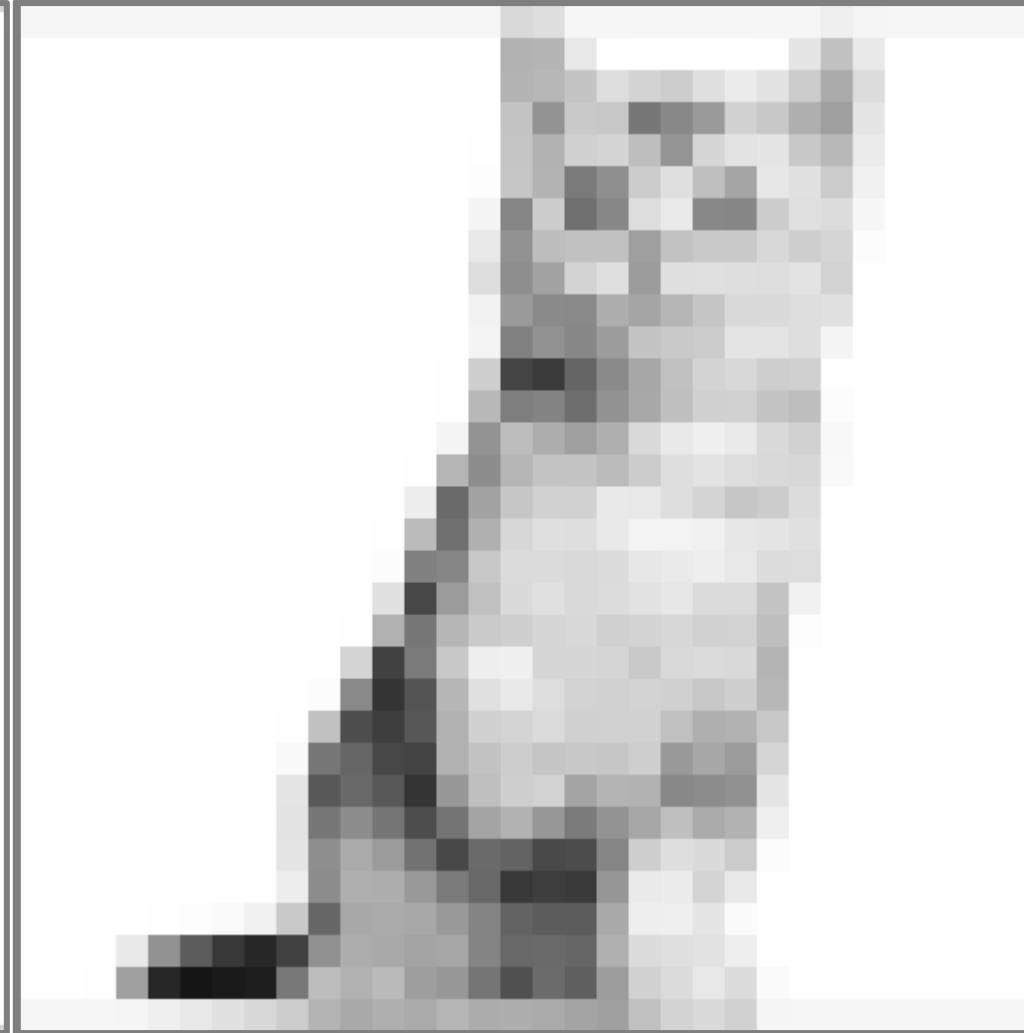
$|0,0,\dots,0\rangle$

\otimes

Upscaling



9 qubits + 9 qubits



5+5

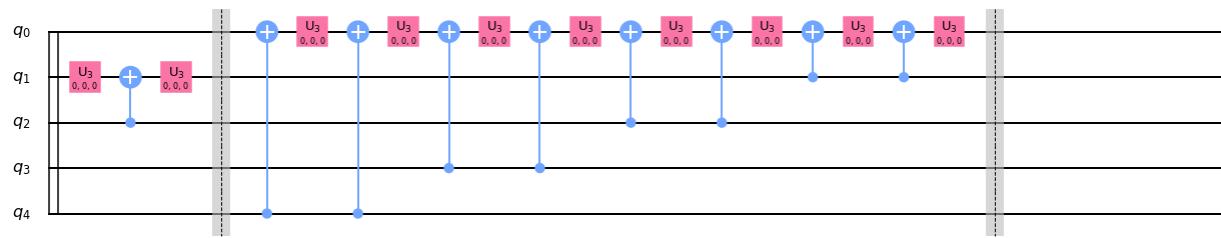
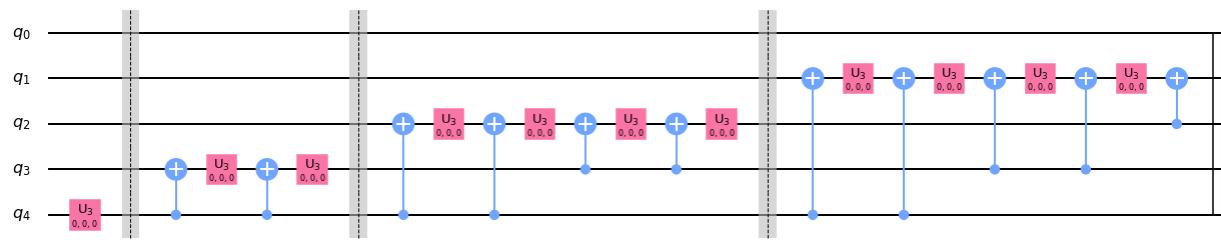
Resampling

A word of caution!



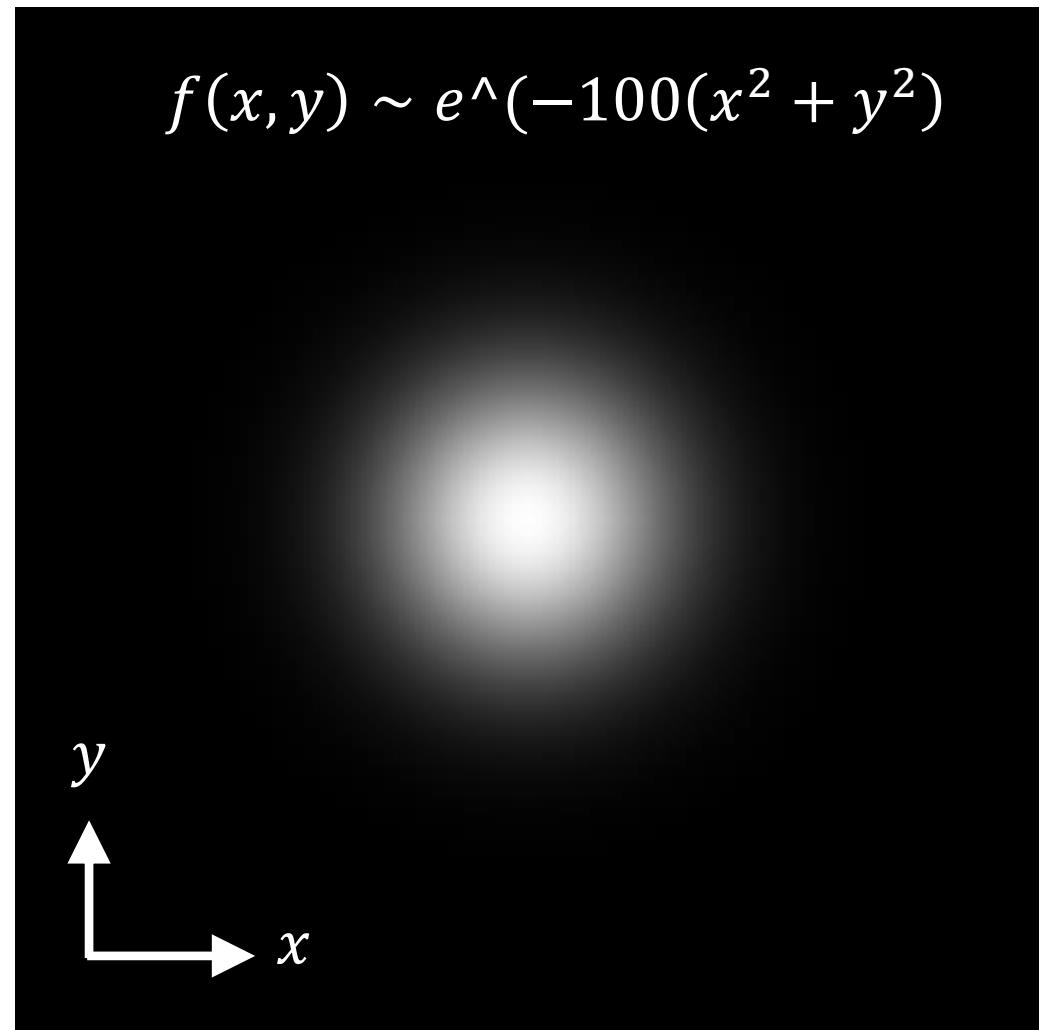
A lot of information!
Cost of reading+writing?

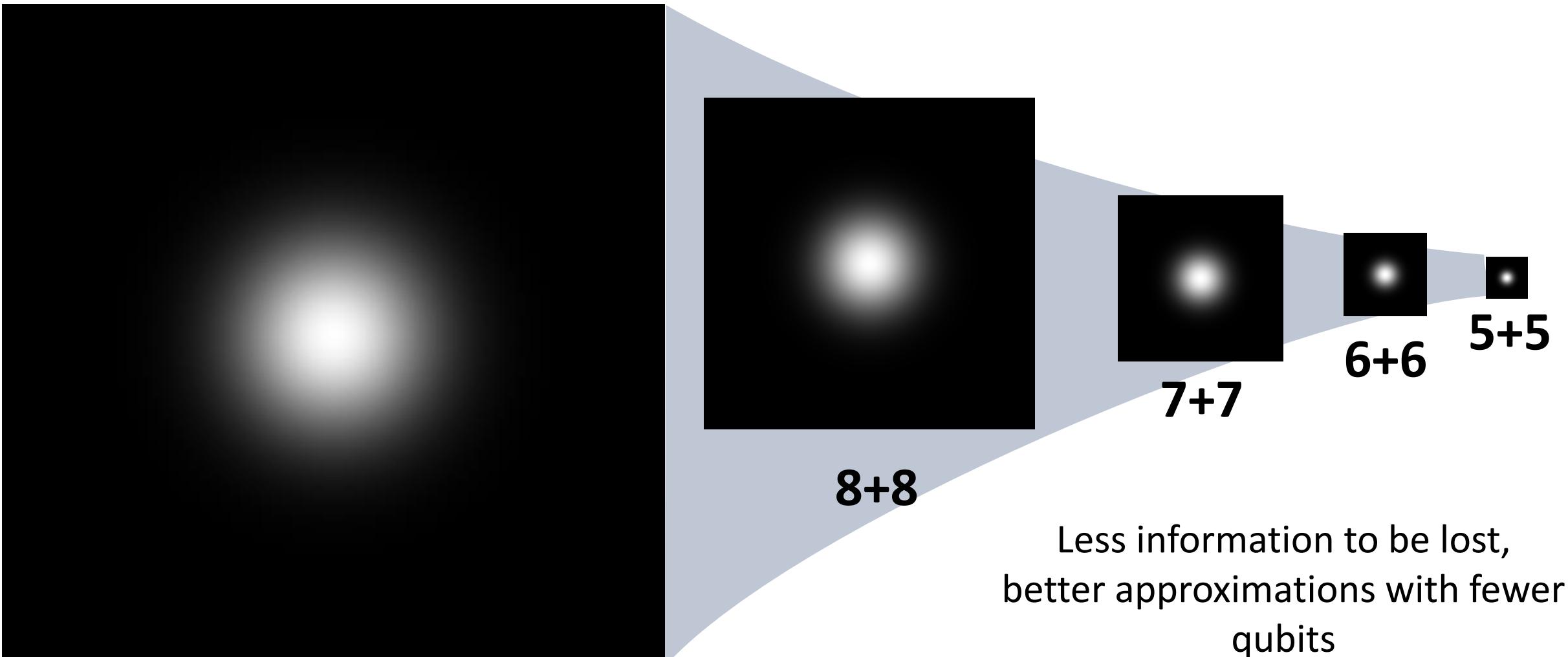
- Can not write wavefunction
- Need to find a quantum circuit



Unclear advantage!!!

Generic functions



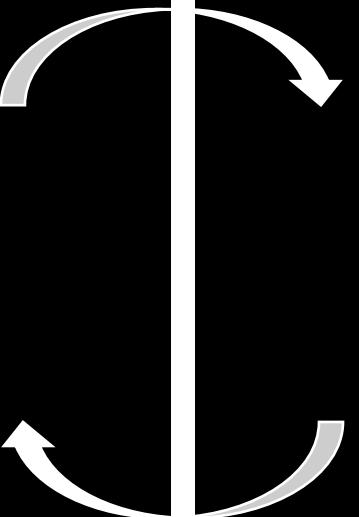


9 qubits + 9 qubits

Downsampling

Less information to be lost,
better approximations with fewer
qubits

Resampling



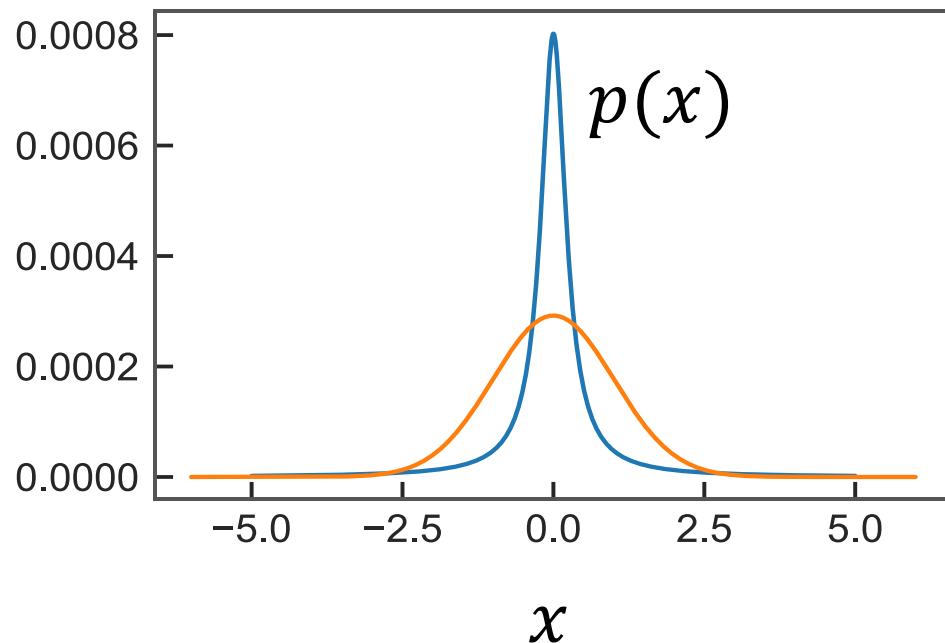
**Upscaling
(also interpolating!)**

9 qubits + 9 qubits

5+5

Downsampling

Quantum register encoding



Discretize space

$$x = a + (b - a)s$$

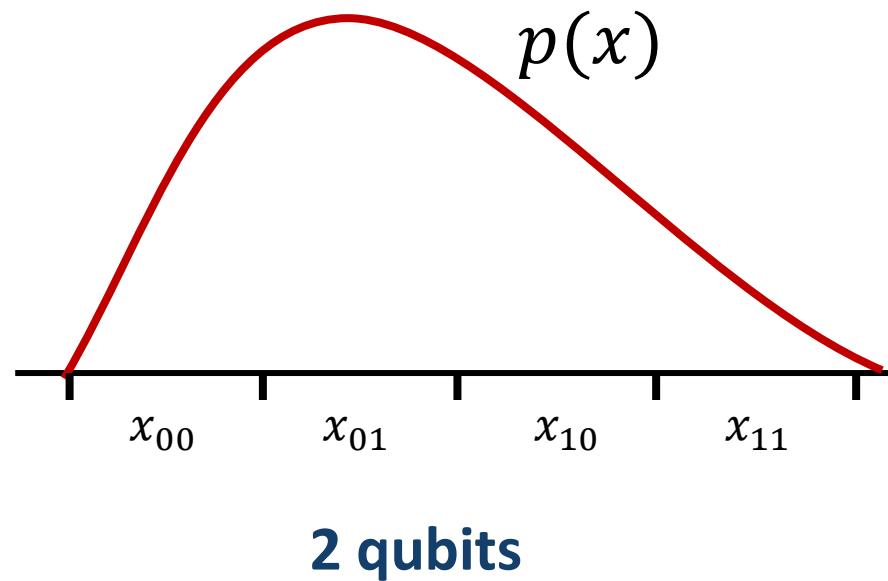
with integer labels

$$s = \sum_{k=1} \frac{s_1^k}{2^k}$$

Encode probability as register amplitude

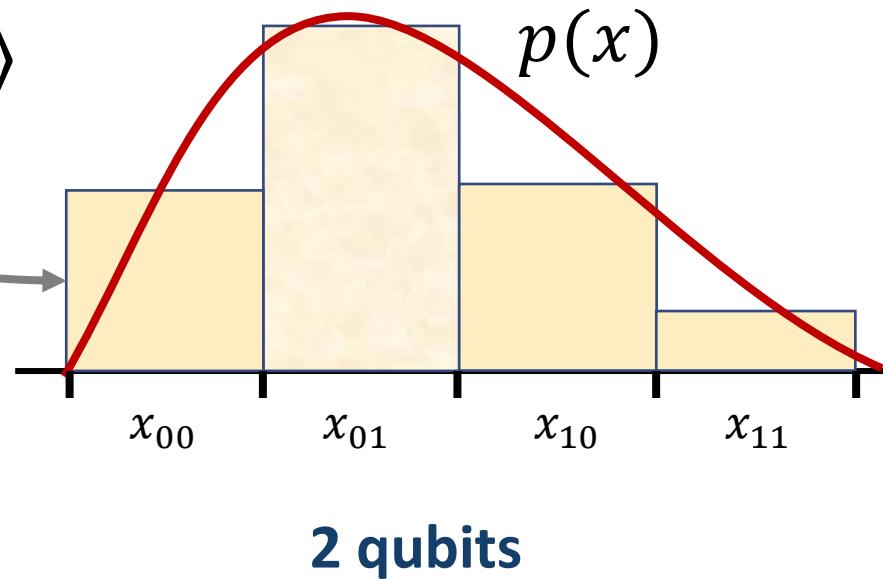
$$|\psi\rangle = \sum_{\{s_1, s_2, \dots\}} \sqrt{p(x_s)} |s_1, s_2, \dots\rangle$$

Discretized functions

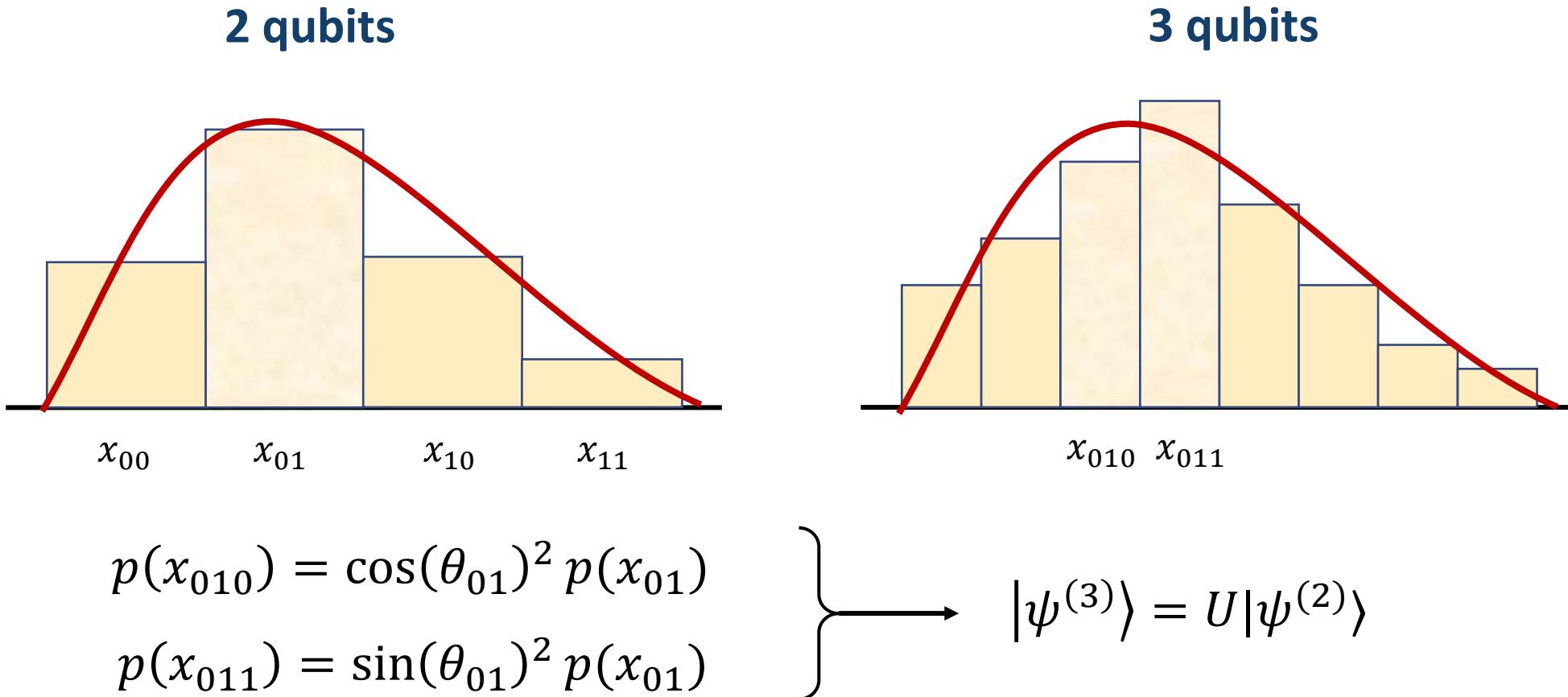


Wavefunction encoding

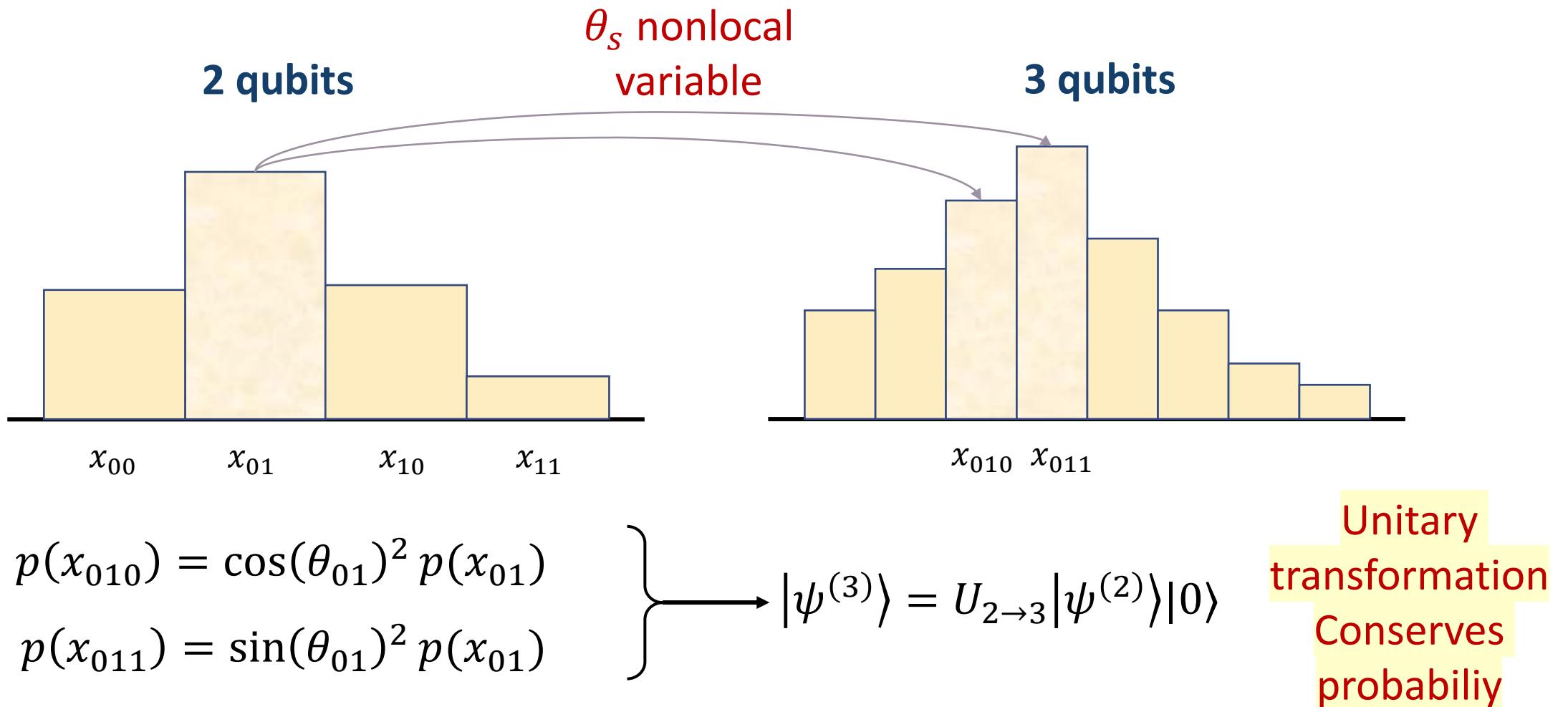
$$|\psi\rangle = \psi_{00}|00\rangle + \psi_{01}|01\rangle \\ + \psi_{10}|10\rangle + \psi_{11}|11\rangle$$



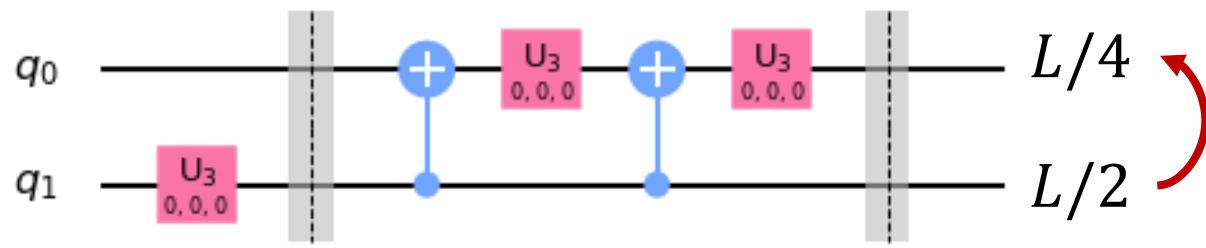
Probability state creation



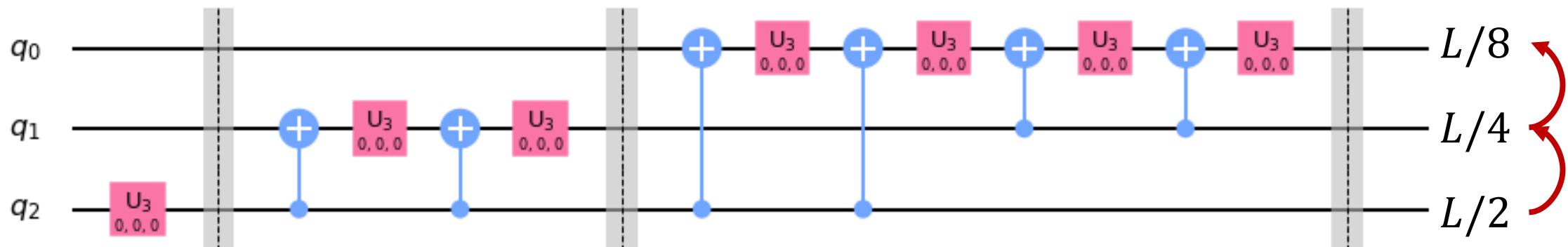
Probability state creation



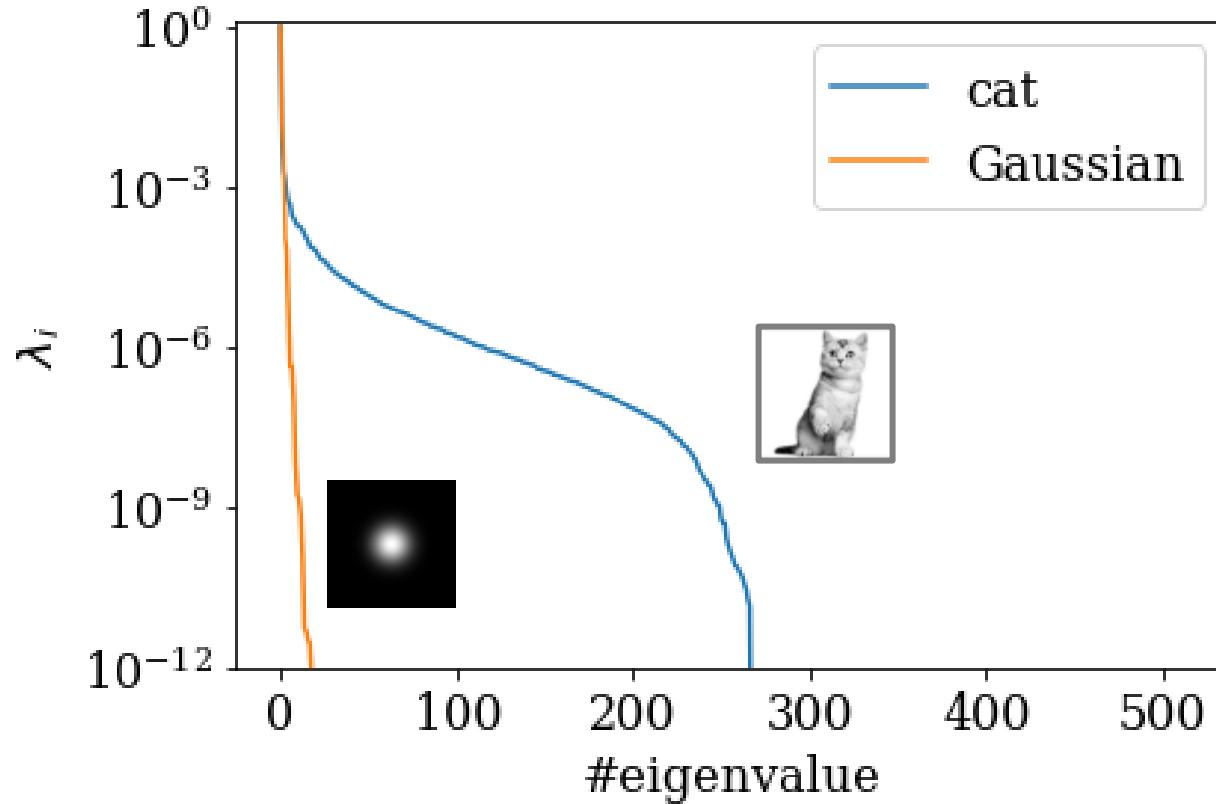
GR-like circuit



Gates propagate “information” or correlations between circuits. The farther / stronger correlations, the more gates we need



Amount of information & entanglement



We analyse how half of the qubits are entangled with the other half, computing the Schmidt decomposition

$$|\psi\rangle = \sum_i \lambda_i |\phi_i^{N/2}\rangle \otimes |\xi_i^{N/2}\rangle$$

The more complex the encoded function, the more states we need.

Quantifying complexity

Schmidt decomposition: an optimal decomposition of bipartite systems

$$|\psi\rangle = \sum_{\alpha} \lambda_{\alpha}^{1/2} |\phi_{\alpha}\rangle |\psi_{\alpha}\rangle \quad \langle \phi_{\alpha} | \phi_{\beta} \rangle = \langle \xi_{\alpha} | \xi_{\beta} \rangle = \delta_{\alpha\beta}$$

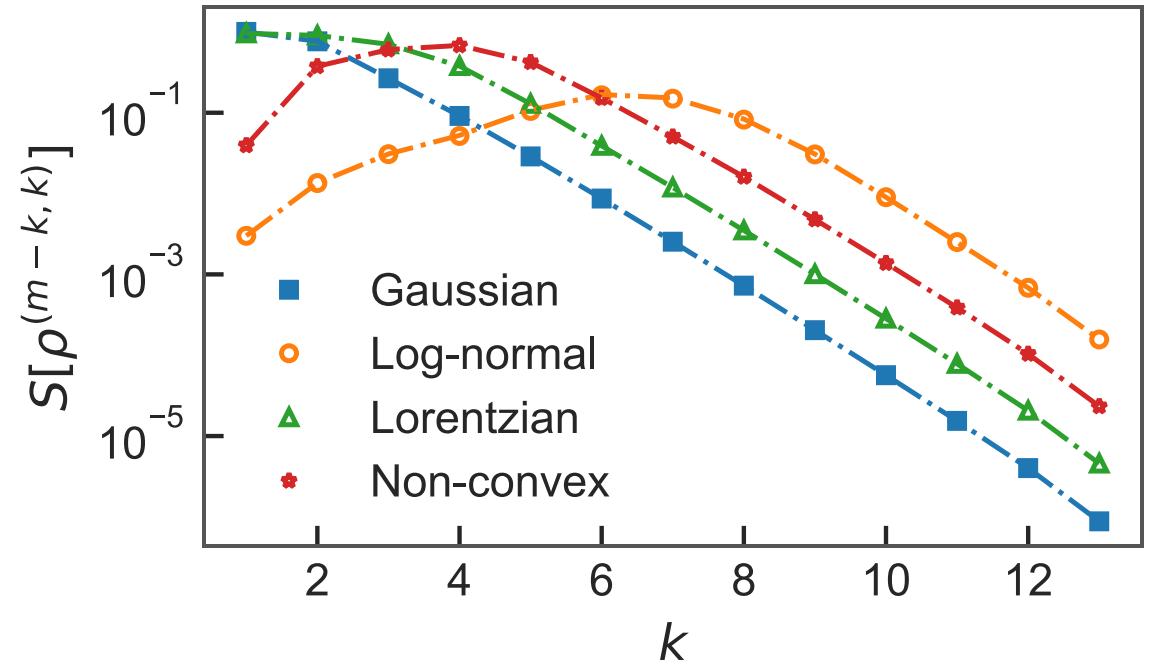
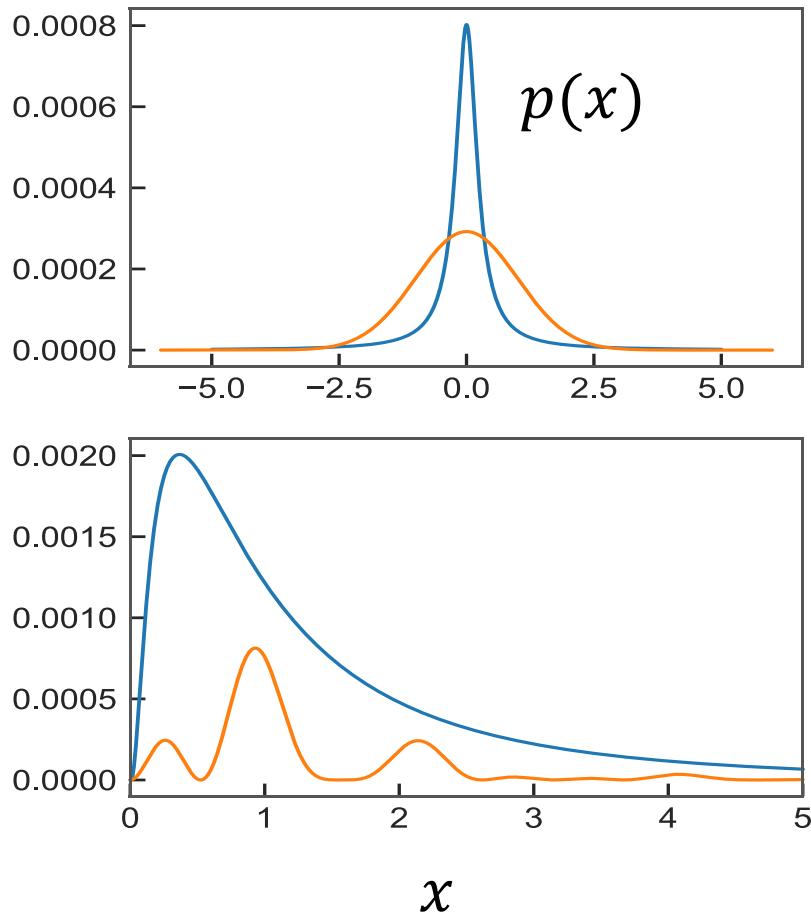
Directly related to entanglement entropy

$$\rho_1 = \text{tr}_2(|\psi\rangle\langle\psi|) = \sum_{s_2} \psi(s_1, s_2) \psi(s'_1, s_2)^* |s_1\rangle\langle s'_1|$$

$$S = \text{tr}(\rho \log_2(\rho)) = - \sum_{\alpha} \lambda_{\alpha} \log_2(\lambda_{\alpha})$$

More entanglement \sim more complex unitary operations to build the state

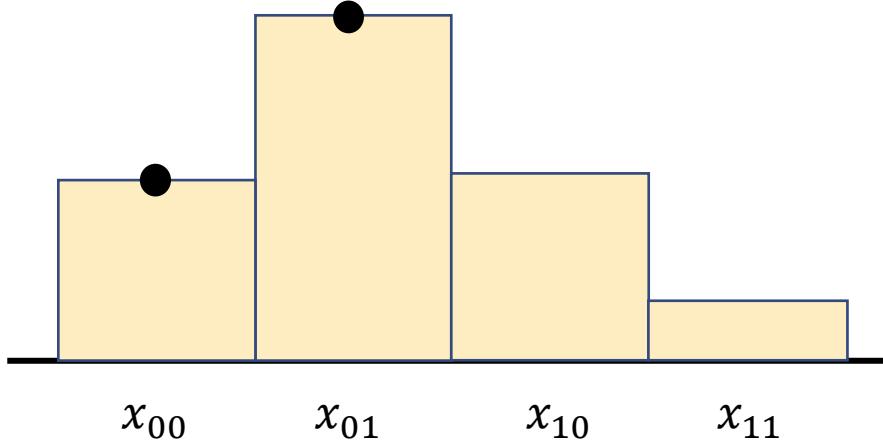
Smooth functions as low-entanglement states



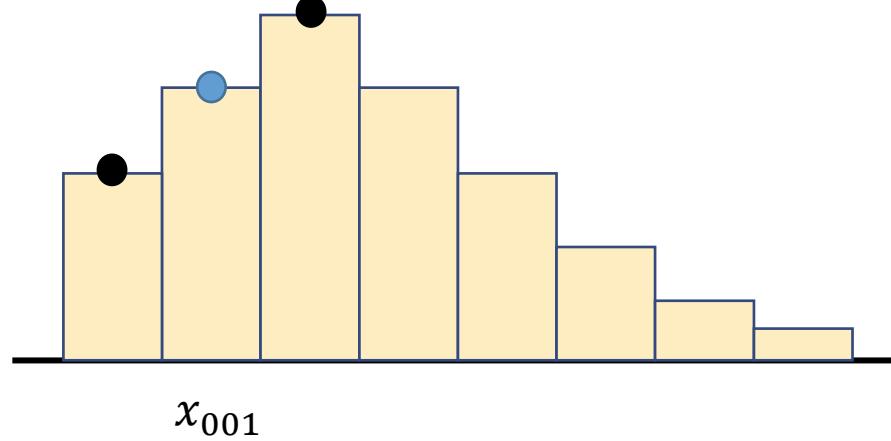
Smooth, differentiable functions require an exponentially small entanglement entropy for each added qubit. **Efficient construction** in a quantum computer.

Intuition

2 qubits



3 qubits

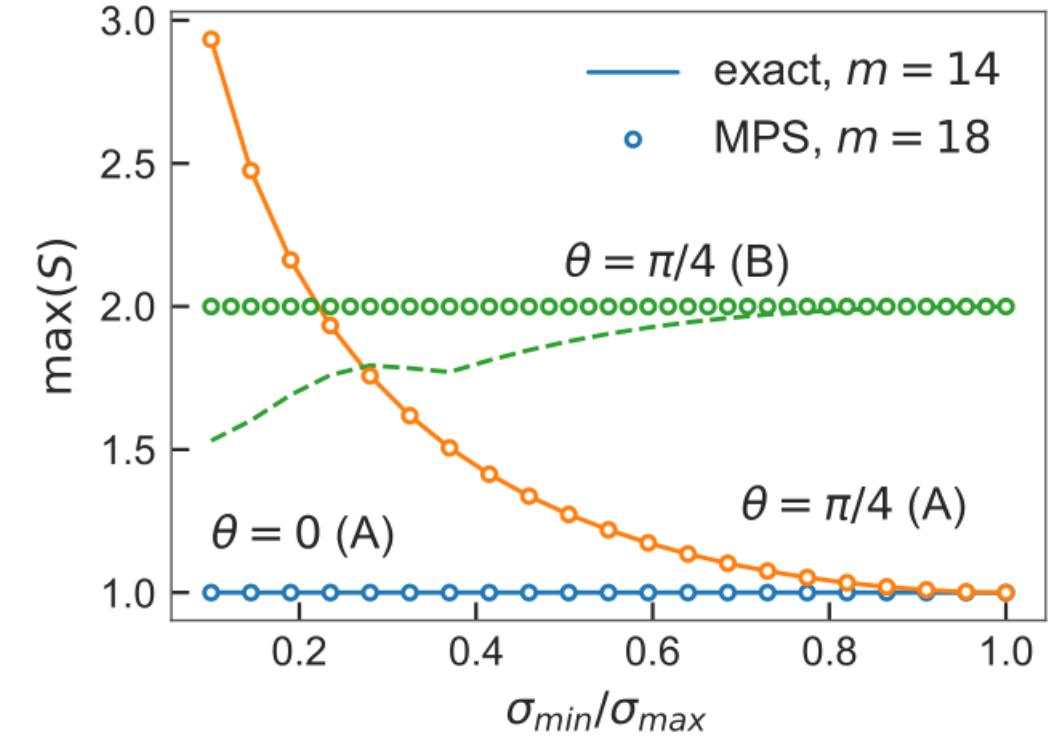
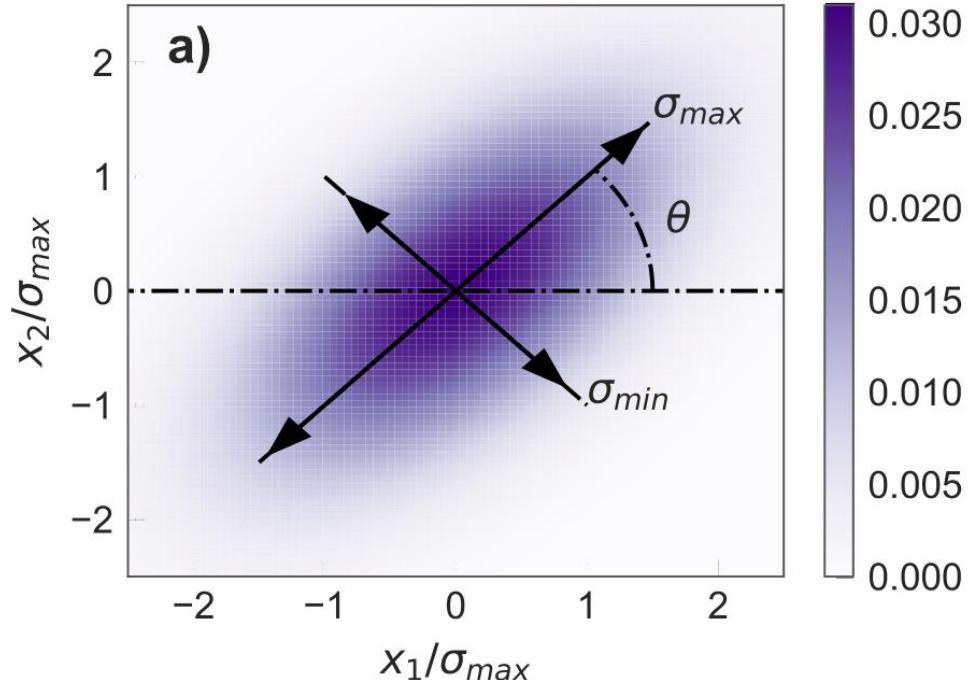


As we refine the discretization,
the angles are exponentially
small perturbations of a
constant.

$$x_{001} \simeq \frac{1}{2}(x_{00} + x_{01})$$

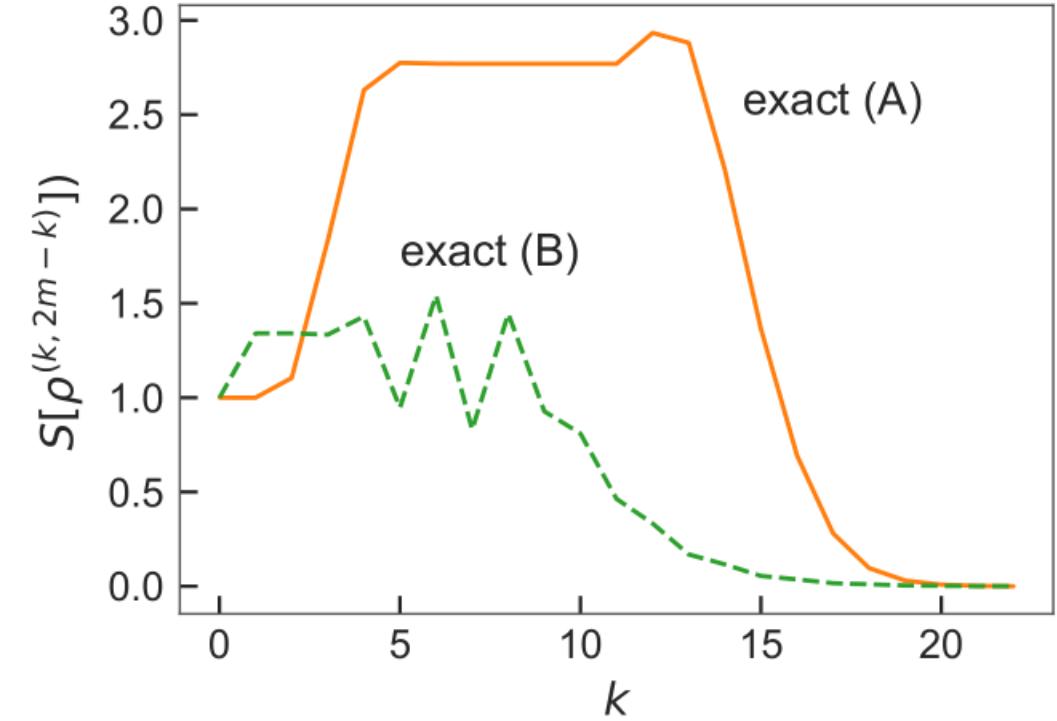
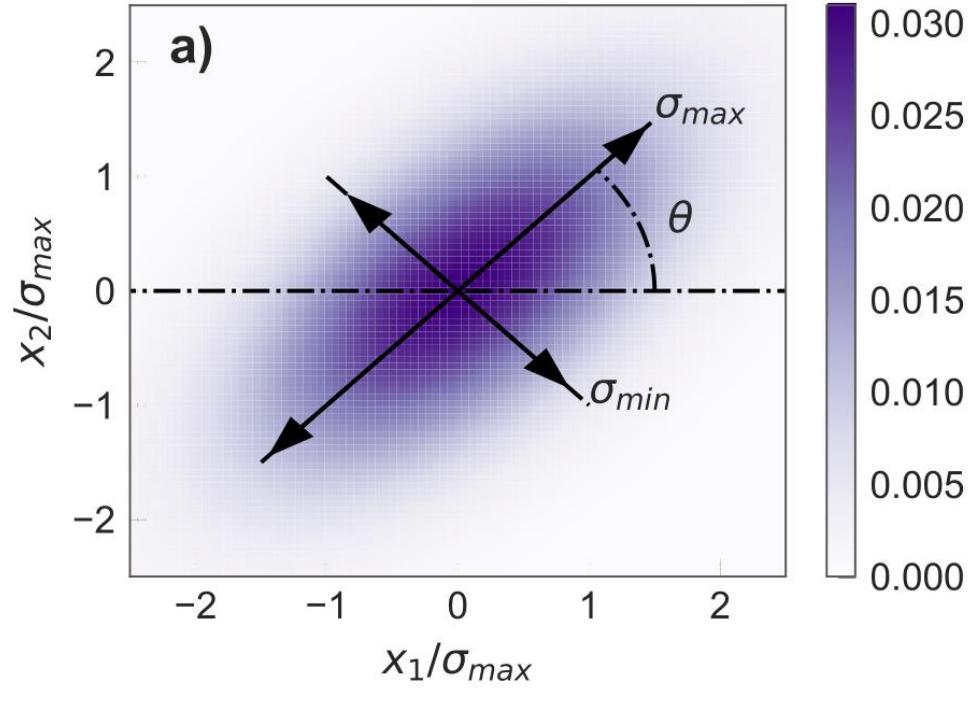
$$\theta_s \simeq ct. + \delta x \simeq ct. + O(2^{-n})$$

Higher dimensions



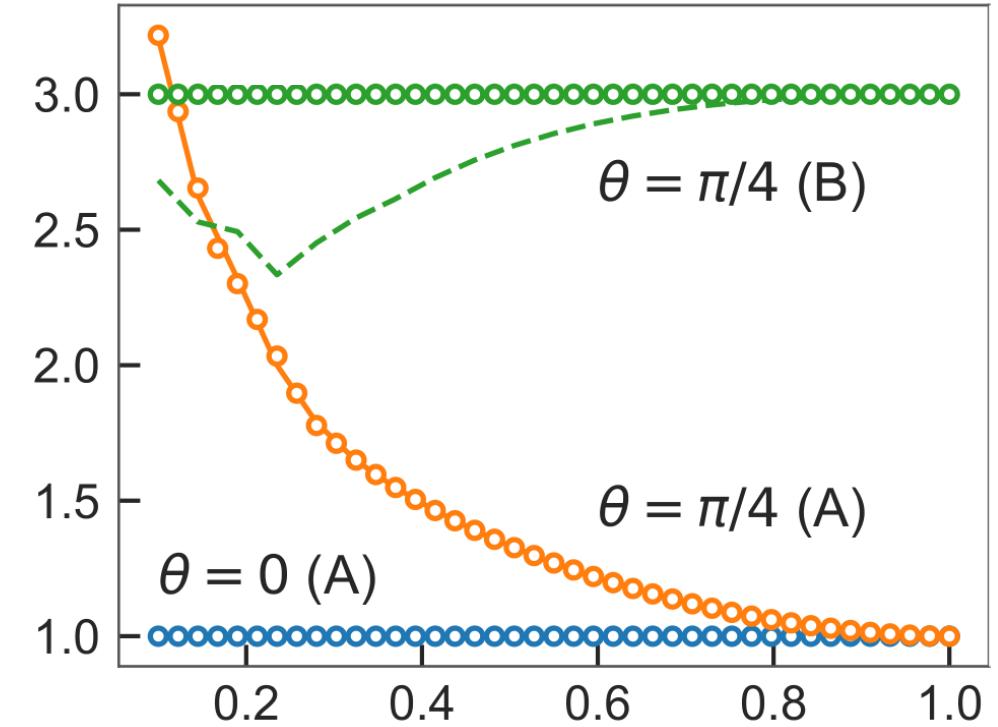
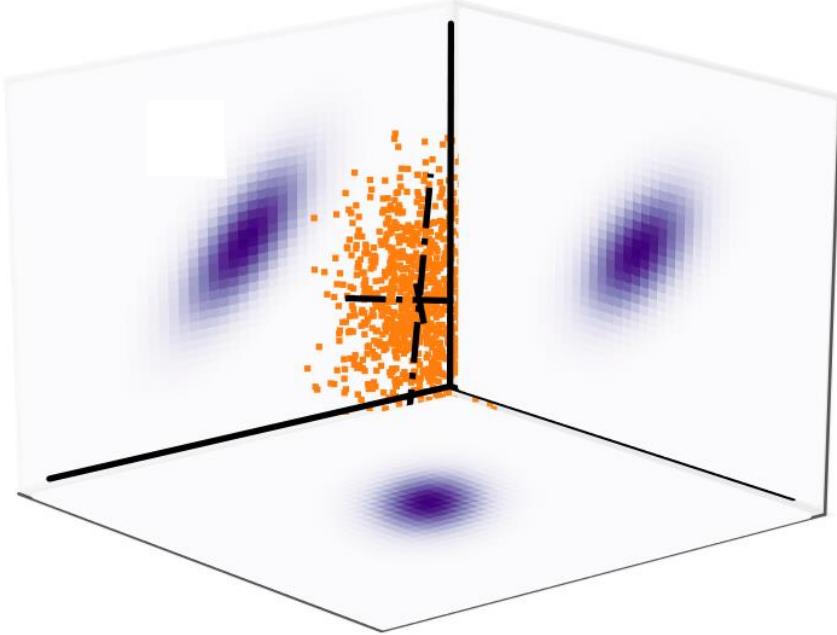
The amount of entanglement is still small, although diverges with correlations

Higher dimensions



The amount of entanglement is still small, although diverges with correlations.
It improves significantly when we shift to the renormalization order.

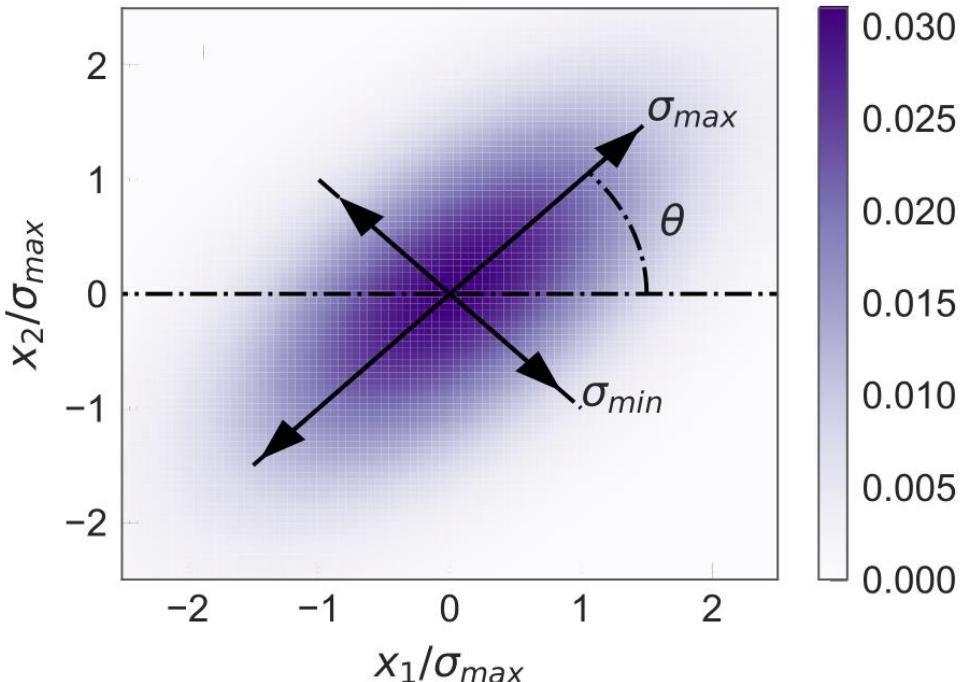
Higher dimensions



Scales up to higher dimensions. Maximum entanglement grows as 2^d , $d=\text{dimension}$

Quantum Numerical Analysis

Encode, manipulate and interrogate multivariate functions in quantum registers.



Q. Algorithm

$$|\psi\rangle = \sum_{\{s_1, s_2\}} f(x_{s_1} x_{s_2}) |s_1, s_2\rangle, s_i \in 2^m - 1$$

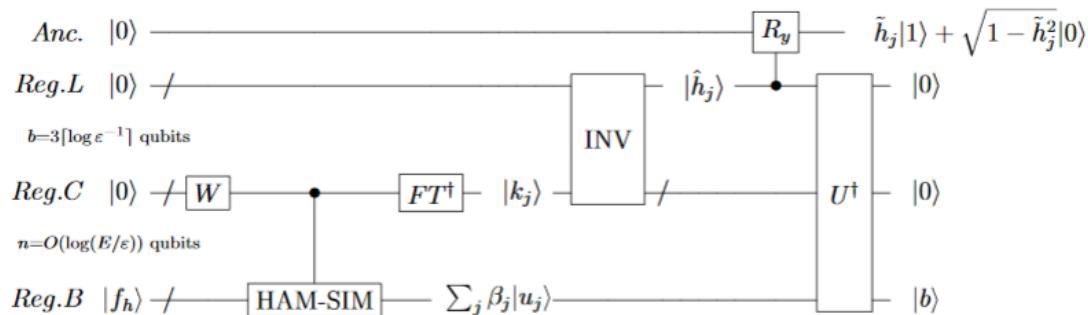
Q. Algorithm

Expected values, risk analysis, PDE's

Algorithms for Poisson equation...

Quantum algorithm and circuit design solving the Poisson equation

Y. Cao et al, NJP 15 (2013)



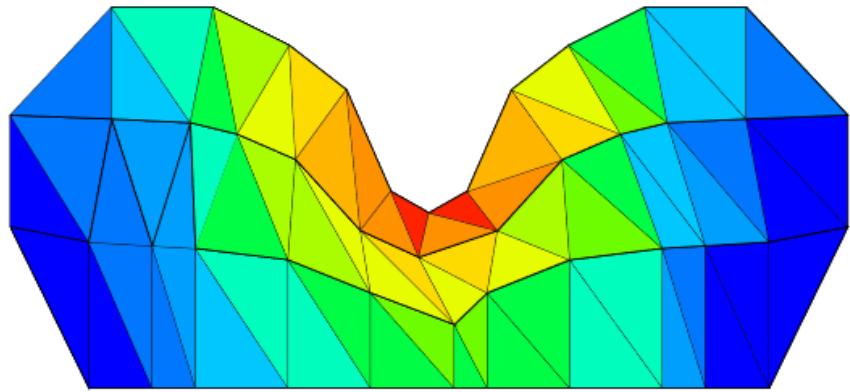
1,3	2,3	3,3	
1,2	2,2	3,2	
1,1	2,1	3,1	
			M = 4

Implement Poisson operator in finite differences using Hamiltonian simulation; invert eigenvalues to obtain solution.

$$-\Delta u(x) = f(x)$$

Quantum algorithms and the finite element method

A. Montanaro, S. Pallister, PRA 93 (2016)



$$u(x_s) = (H^{-1})_{ss'} f(x_{s'})$$

Use finite elements to construct H, f ; use HHL to invert problem

...and in quantum finance



Probability distribution

$$p(s_1, s_2, \dots, s_n)$$

Quantum register

$$|\psi\rangle = \sum_s \sqrt{p(s_1, \dots, s_n)} |s_1, \dots, s_n\rangle$$

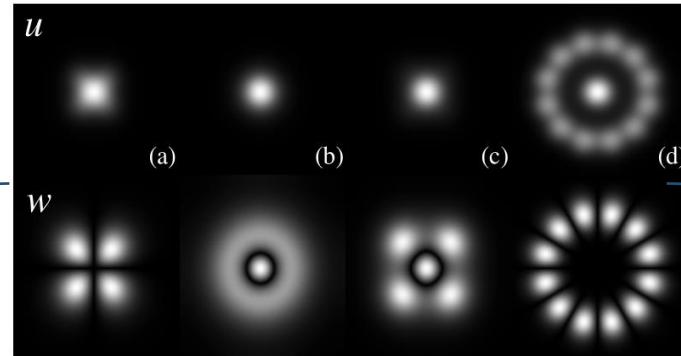
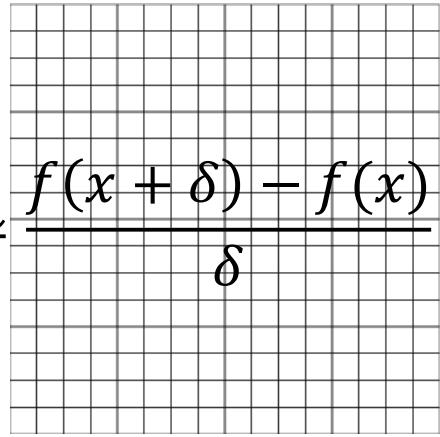
Amplitude estimation

$$\langle s_i \rangle, \langle s_i s_j \rangle, \dots$$

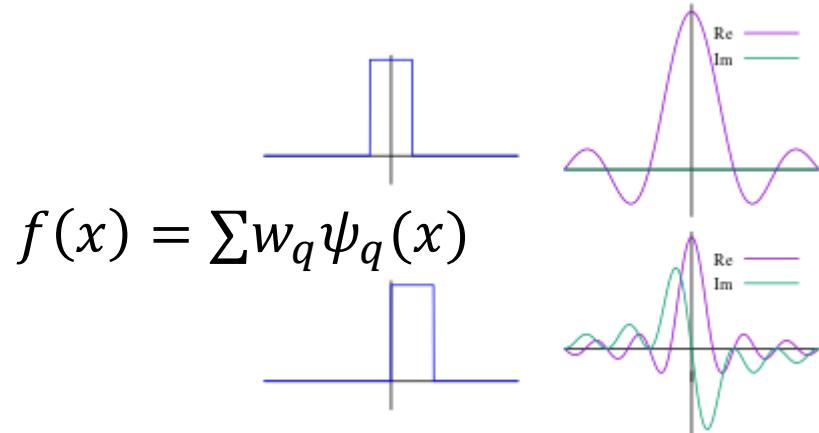
Many classical encodings

Finite differences

$$\frac{df}{dx} \simeq \frac{f(x + \delta) - f(x)}{\delta}$$

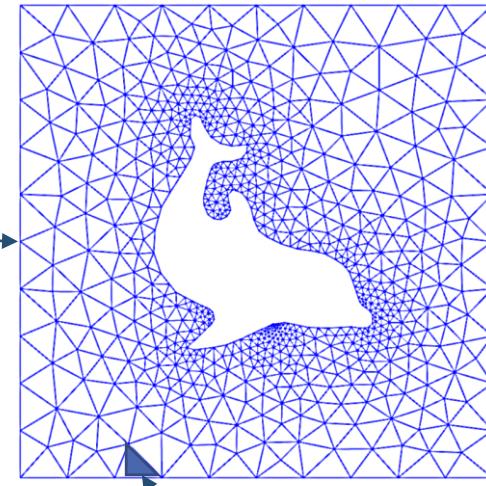


Spectral method

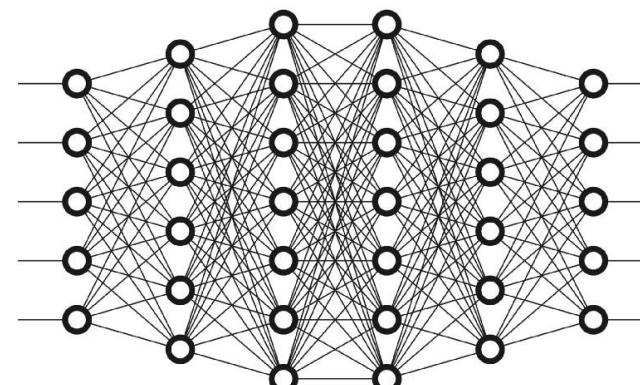


$$f(x) = \sum w_q \psi_q(x)$$

Finite element



Variational methods



$$f(x)_m \simeq \sum_n c_n^m x^n$$

$$f(x_1, x_2, \dots)$$

Algorithms

Problem	Algorithm	Type	Cost
Expected value	Monte Carlo	C	$\mathcal{O}(1/\varepsilon^2)$
	Amplitude estimation	Q	$\mathcal{O}(1/\varepsilon)$
	MPS	QI	$\mathcal{O}(-N\chi^3 \log(\varepsilon))$
Fourier transform	QFT	Q	$\mathcal{O}(N^2 m^2)$
	FFT	C	$\mathcal{O}(Nm 2^{Nm})$
	MPS QFT	QI	$\mathcal{O}(Nm \times \text{Simp}_{Nm})$
Interpolation	Linear ($k = 1$)	C	$\mathcal{O}(2^{Nm})$
	MPS Linear ($k = 1$)	QI	$\sim \text{Simp}_{Nm}$
	FFT	C	$\mathcal{O}(N(m+k)2^{N(m+k)})$
	MPS QFT	QI	$\sim 3 \times \text{QFT}_{N(m+k)}$
PDE Evolution	Finite differences	C	$\mathcal{O}(T_{\text{cgs}} 2^{2Nm})$
	MPS differences	QI	$\mathcal{O}(T_{\text{cgs}} \times \text{Simp}_{Nm})$
	FFT method	C	$\mathcal{O}((Nm+1)2^{Nm})$
	MPS QFT	QI	$\sim 2 \times \text{QFT}_{N(m+k)}$
State construct	GR-like (Sect. 3.3)	Q	$\mathcal{O}(Nm\chi^2)$
	Explicit wavefunction	C	$\mathcal{O}(2^{Nm})$
	MPS	QI	$\mathcal{O}(T_{\text{steps}} \times \text{Simp}_{Nm})$

Fourier analysis

An expansion of functions in a harmonic basis

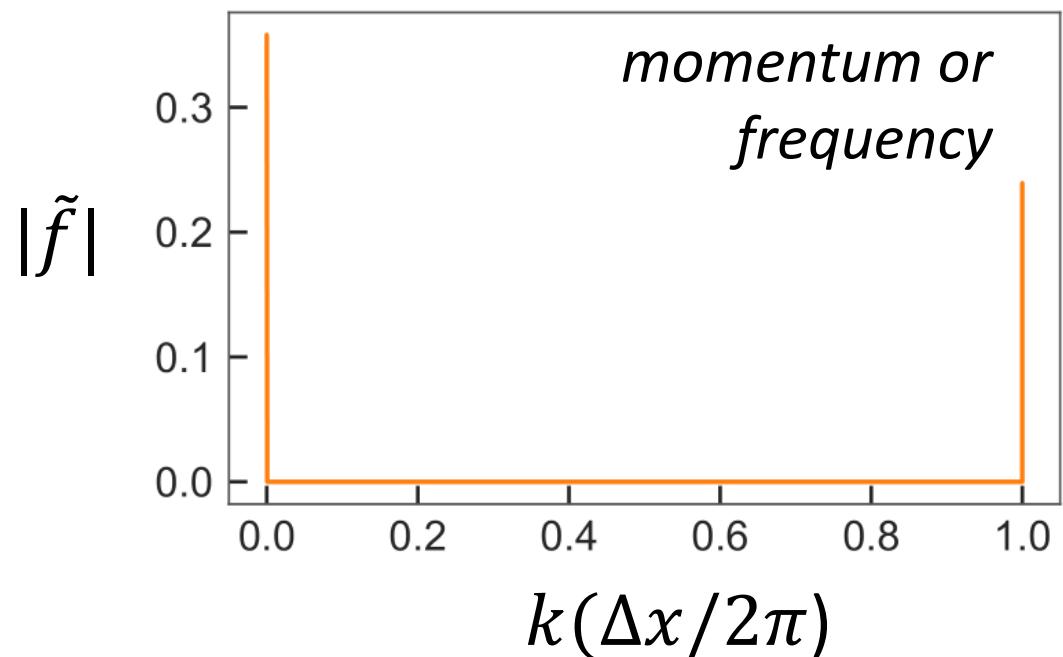
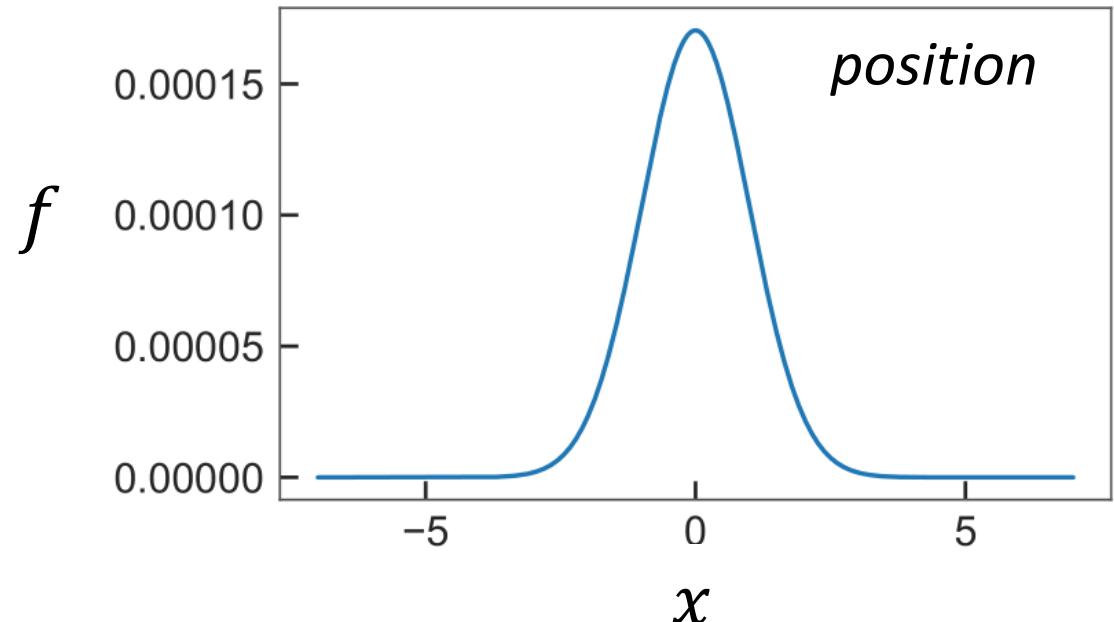
$$f(x_n) = \sum_{k_m} \tilde{f}(k_m) \frac{e^{-ik_m x_n}}{\sqrt{N}}$$

Direct and inverse transform

$$\tilde{f}_m = (Ff)_m$$

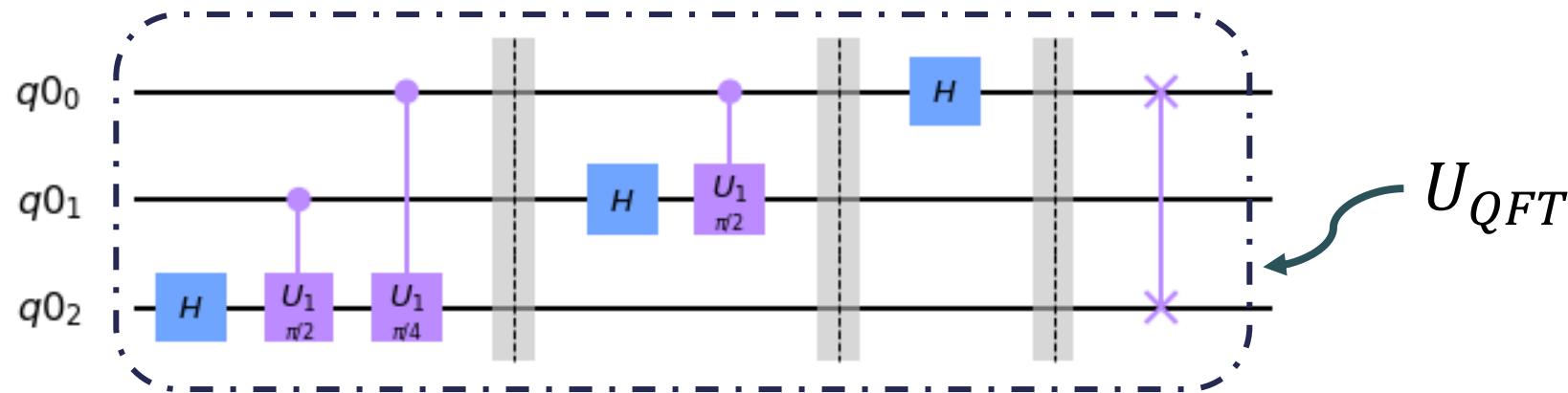
$$f_n = (F^{-1}\tilde{f})_n$$

“F” is a unitary matrix!



Quantum Fourier Transform

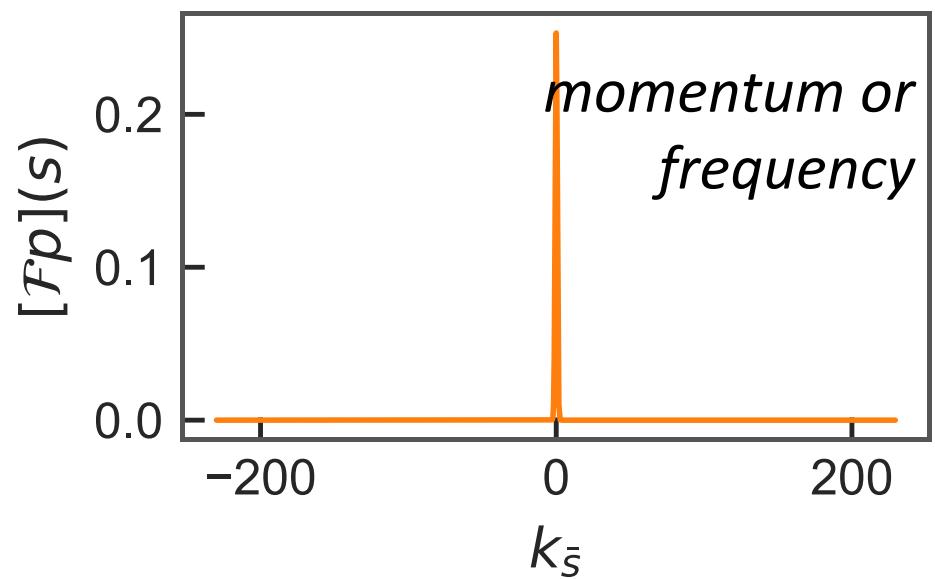
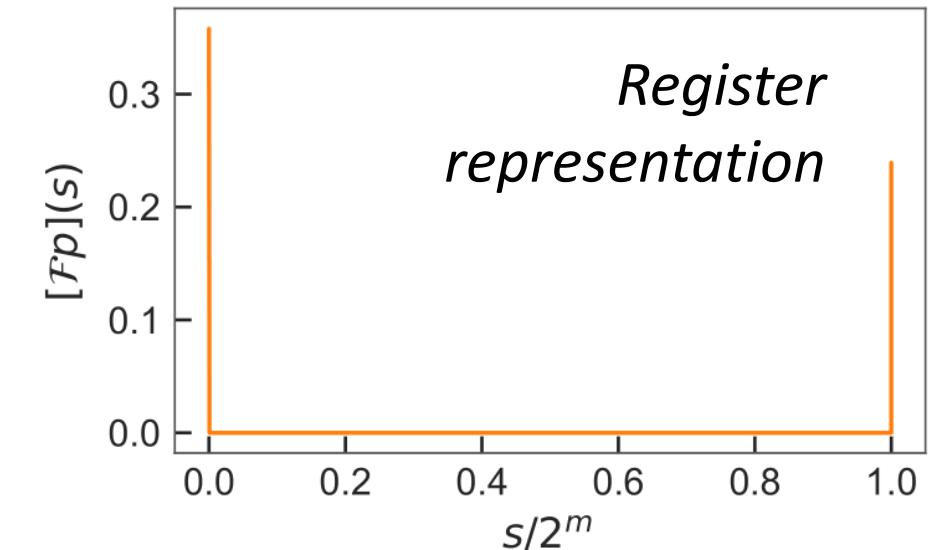
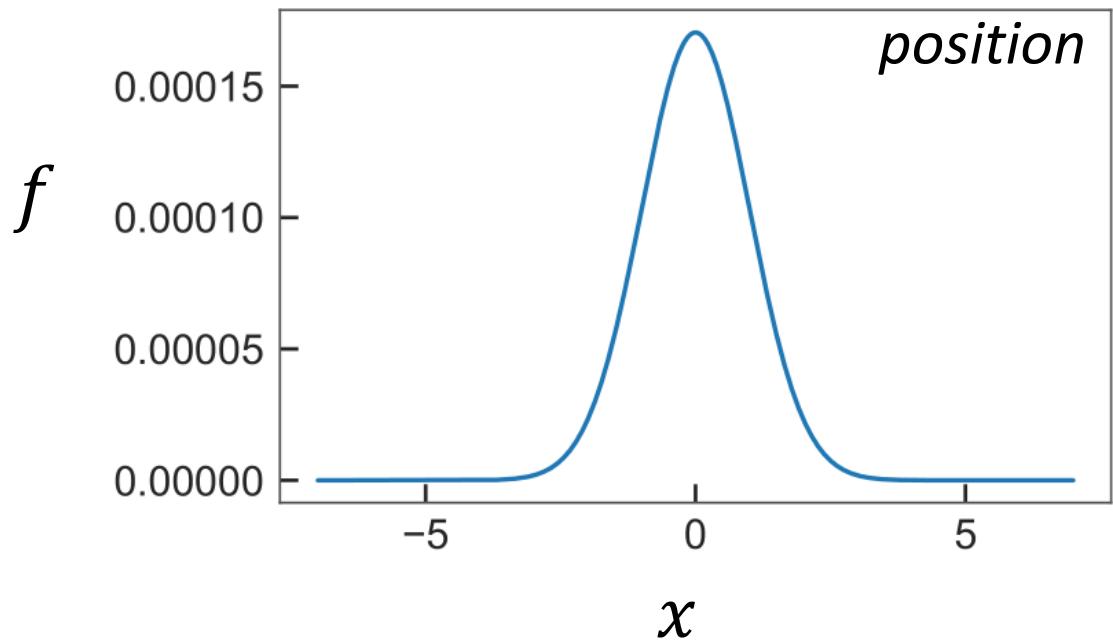
The Fourier transform is a unitary matrix. When dimension is a power of 2, it can be implemented using quantum gates



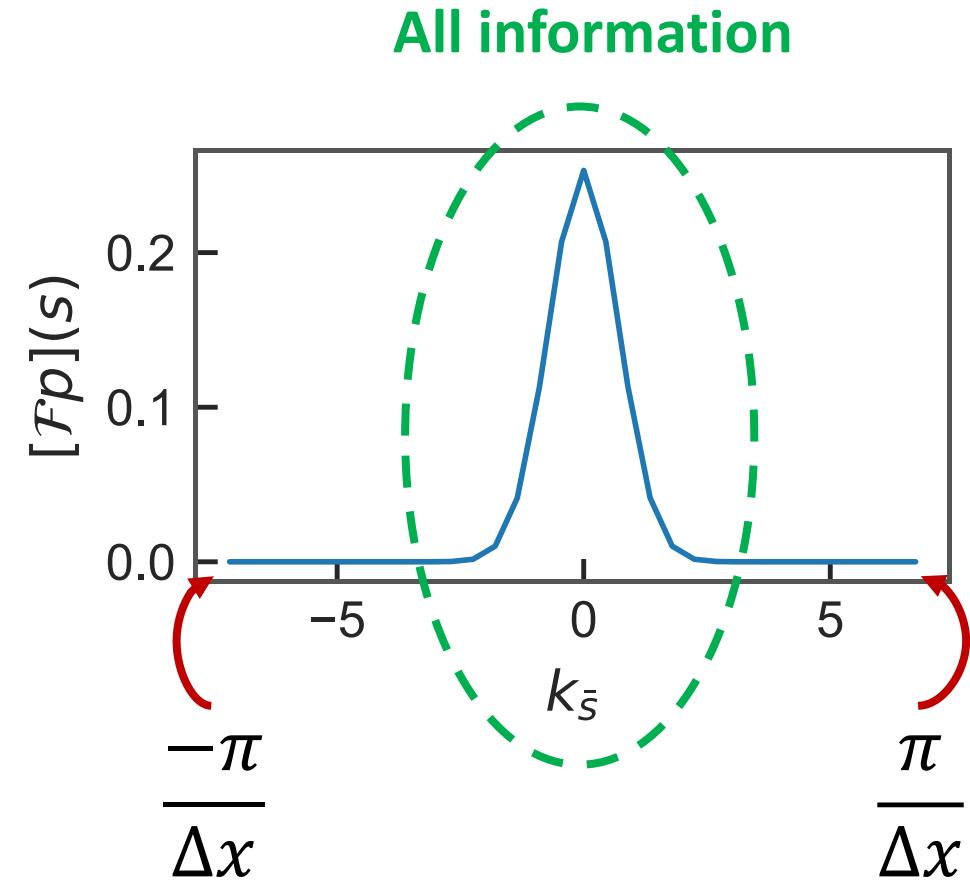
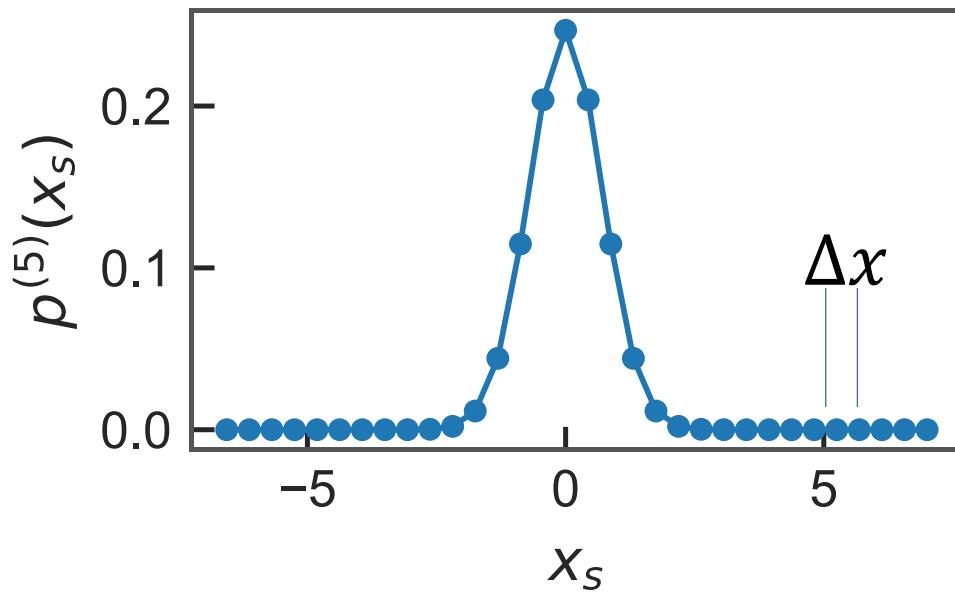
$$|f\rangle = \sum_s f(x_s) |s_1 s_2 \dots s_N\rangle \rightarrow |\tilde{f}\rangle = \sum_s \tilde{f}(k_s) |s_1 s_2 \dots s_N\rangle$$

$$|\tilde{f}\rangle = U_{QFT} |f\rangle$$

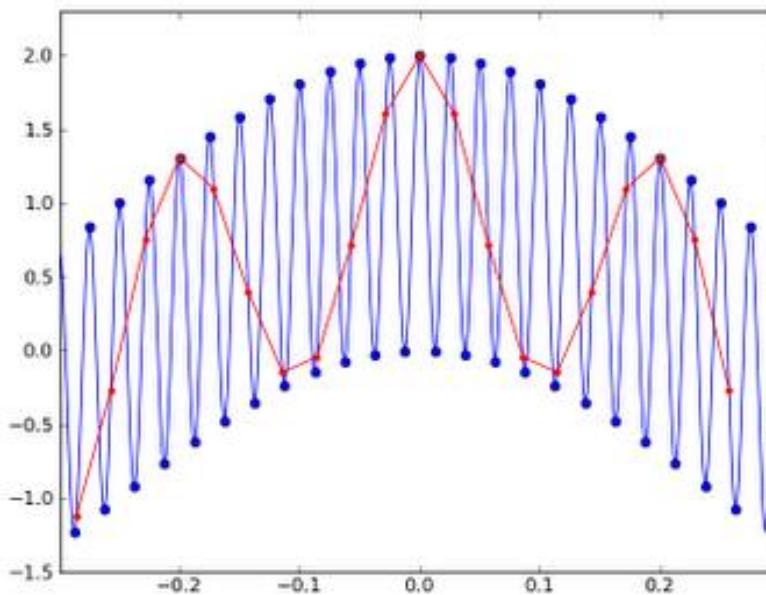
A quirk of DFT encoding



Finite-bandwidth functions

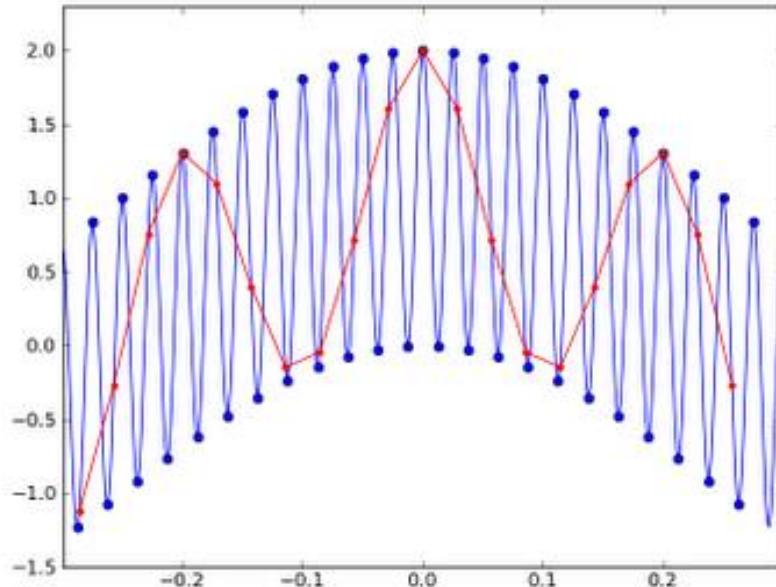


Nyquist-Shannon sampling theorem

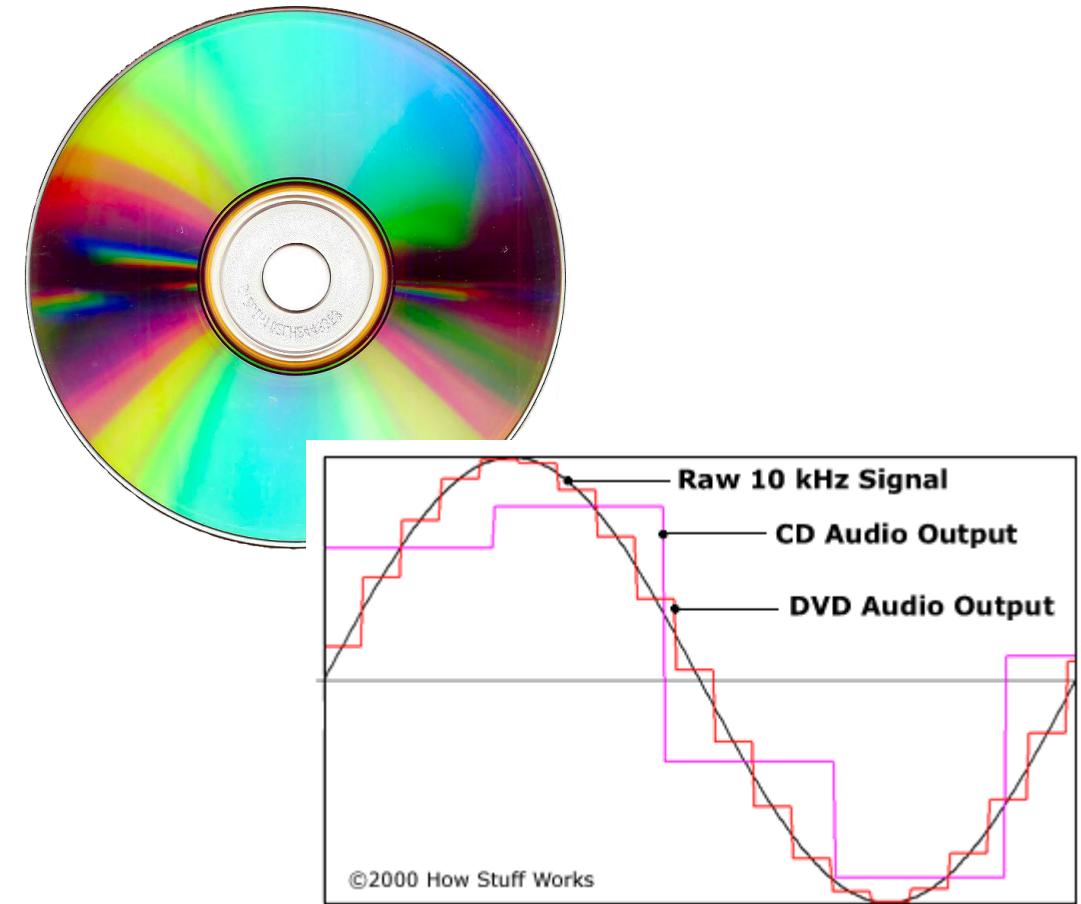


$$\nu_{sampling} \geq 2\nu_{signal}$$

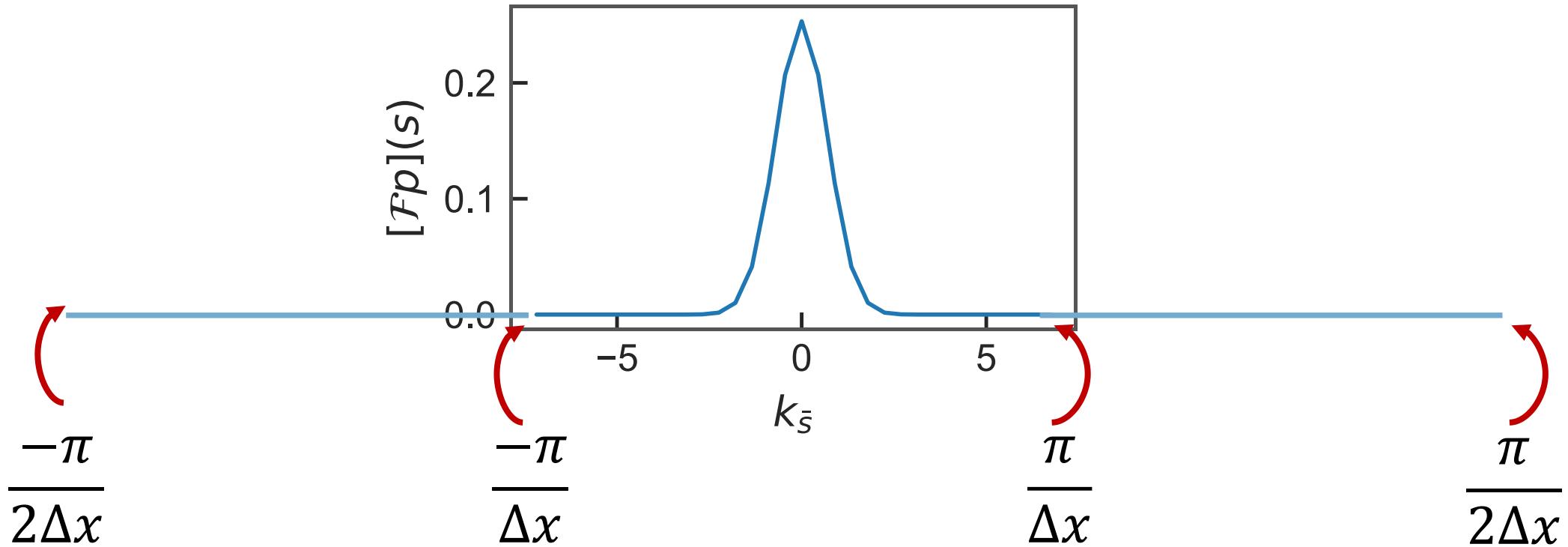
Nyquist-Shannon sampling theorem



$$\nu_{sampling} \geq 2\nu_{signal}$$

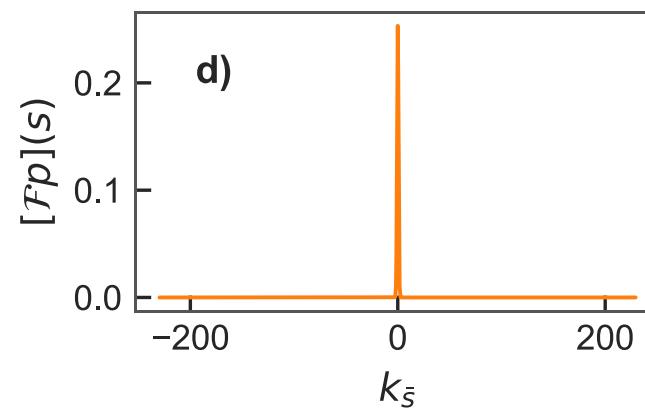
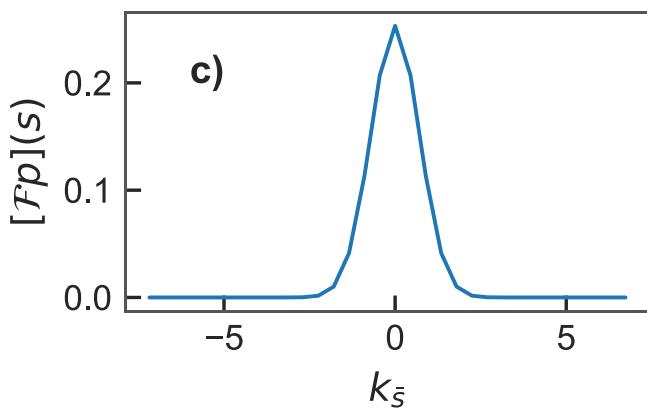
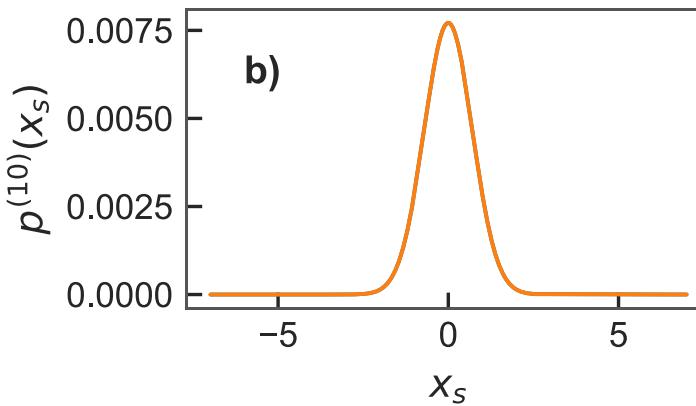
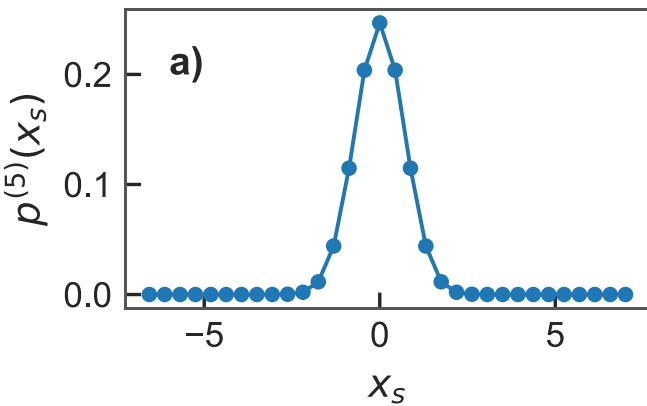


Interpolation in frequency space



By extrapolating (with zeros) we get the Fourier transform of a function defined with finer resolution

Fourier interpolation



$$|p^{(m+k)}\rangle = \hat{\mathcal{F}}^{(m+k)} U_{2c}^{m+k} \left[\left(U_{2c} \hat{\mathcal{F}}^{(m)} |p^{(m)}\rangle \right) \otimes |0_2, 0_3, \dots, 0_{k+1}\rangle \right]$$

Solving differential equations

Partial differential equation (e.g. Schrödinger!)

$$-\frac{d^2}{dx^2}f(x) + V(x)f(x) = Ef(x)$$

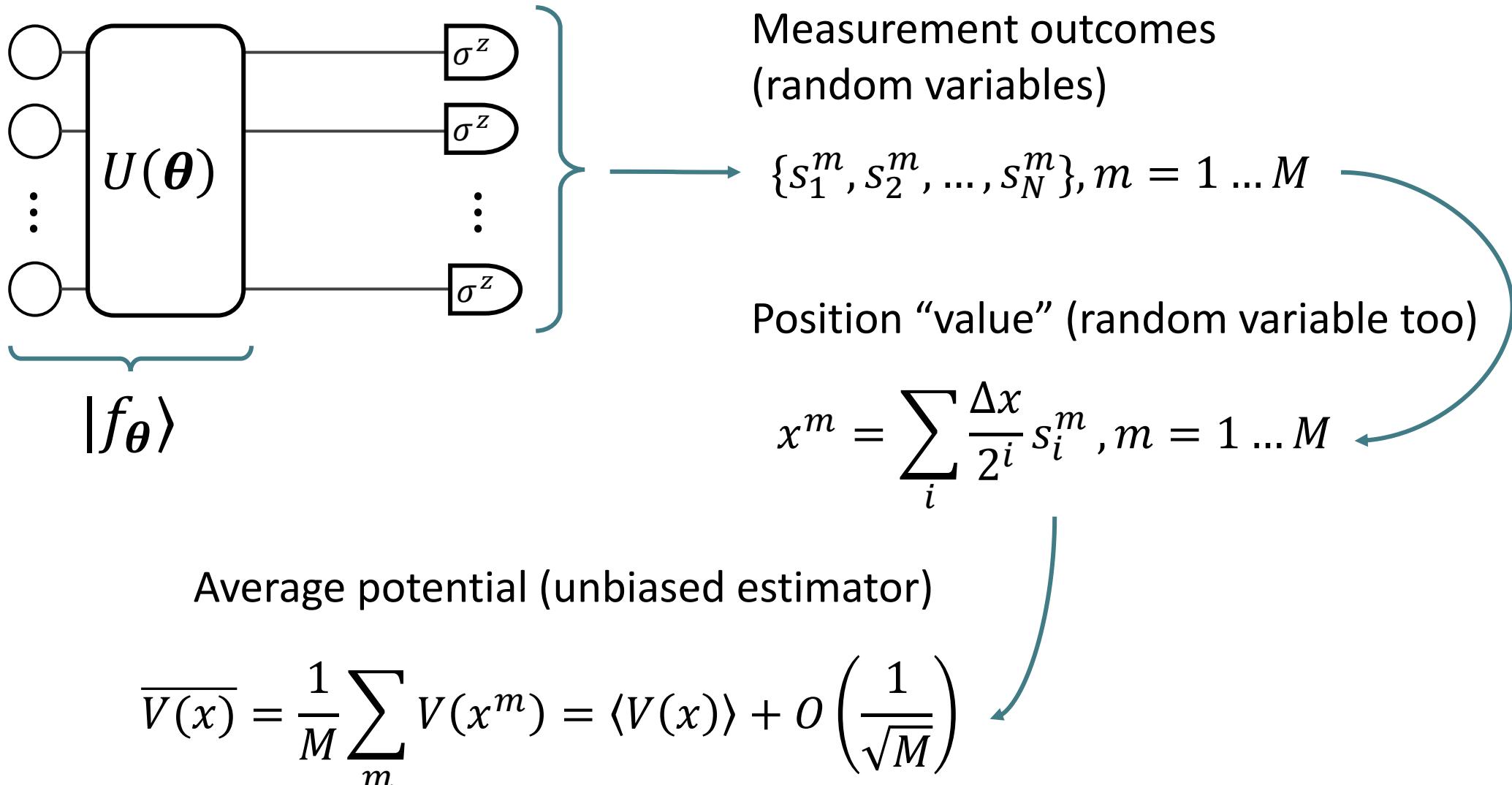
Equivalent variational formulation for min. E

$$\min_{f(x)} \int f(x)^* \left[-\frac{d^2}{dx^2} + V(x) \right] f(x) dx$$

We need to compute

$$\langle V \rangle_f = \int f(x)^* V(x) f(x) dx, \quad \langle \partial_x^2 \rangle_f = \int f(x)^* \frac{d^2}{dx^2} f(x) dx$$

Variational Integration



Differentiation

Fourier interpolation associates a continuous function to discrete values

$$f^{interp}(x) = \sum_{k_m} \tilde{f}(k_m) \frac{e^{-ik_m x}}{\sqrt{N}} \simeq f(x)$$

We can use this to estimate derivatives

$$\frac{d}{dx} f(x) \simeq \frac{d}{dx} f^{interp}(x) = \sum_{k_m} (-ik_m) \tilde{f}(k_m) \frac{e^{-ik_m x}}{\sqrt{N}}$$

“Measure derivatives”

Remember that our “momentum” operator is a combination of bits

$$k_s = \frac{2\pi}{\Delta x} \left(\frac{1}{2}s_0 + \frac{1}{4}s_1 + \dots \right)$$

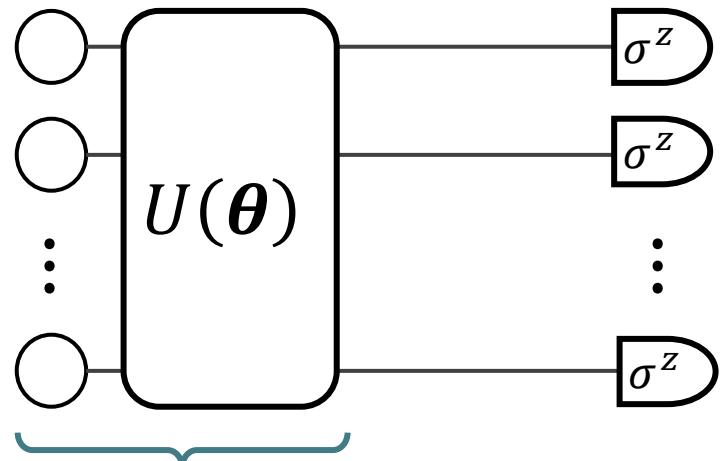
We can use this to compute some interesting integrals

$$\int f(x) \frac{d}{dx} f(x) \simeq \sum_{k_m} (-ik_m) |\tilde{f}(k_m)|^2$$

On the quantum computer we can estimate these integrals with the QFT state

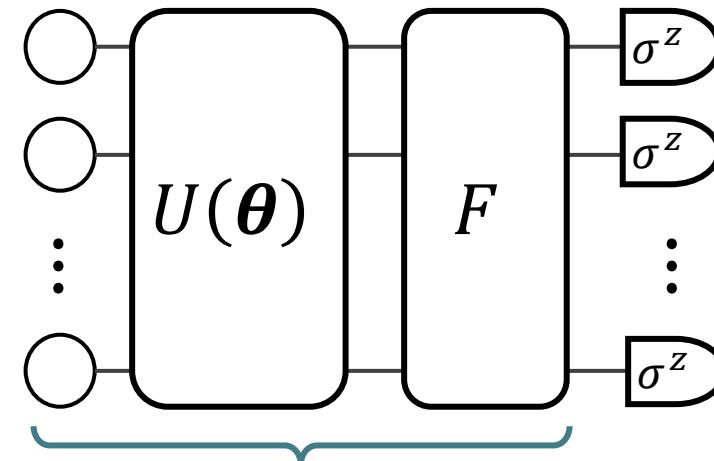
$$\int f(x) \frac{d}{dx} f(x) \simeq -i \frac{2\pi}{\Delta x} \left(\frac{1}{2} \langle \tilde{f} | \sigma_0^z | \tilde{f} \rangle + \frac{1}{4} \langle \tilde{f} | \sigma_1^z | \tilde{f} \rangle + \dots \right)$$

Variational formulation



$|f_\theta\rangle$

$$\langle \tilde{f}_\theta | \sigma_i^z | \tilde{f}_\theta \rangle, \langle \sigma_i^z \sigma_j^z \rangle, \dots$$



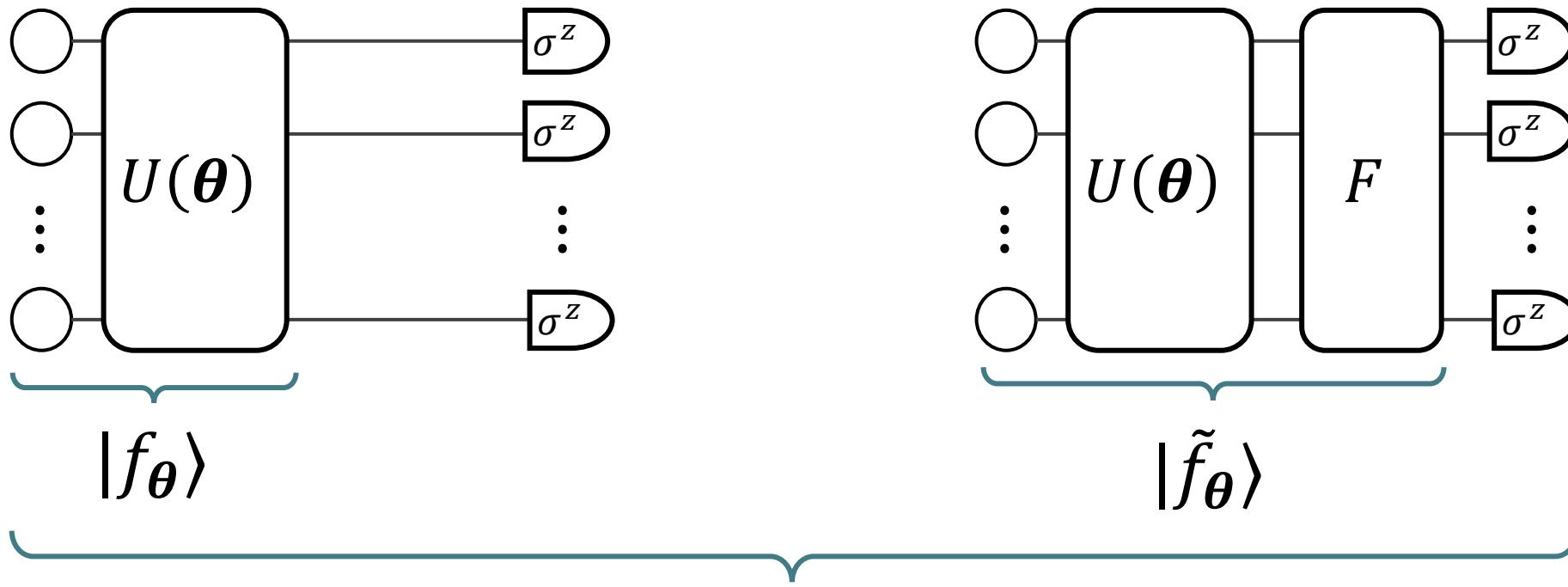
$|\tilde{f}_\theta\rangle$

$$\langle \tilde{f}_\theta | \sigma_i^z | \tilde{f}_\theta \rangle, \langle \sigma_i^z \sigma_j^z \rangle, \dots$$

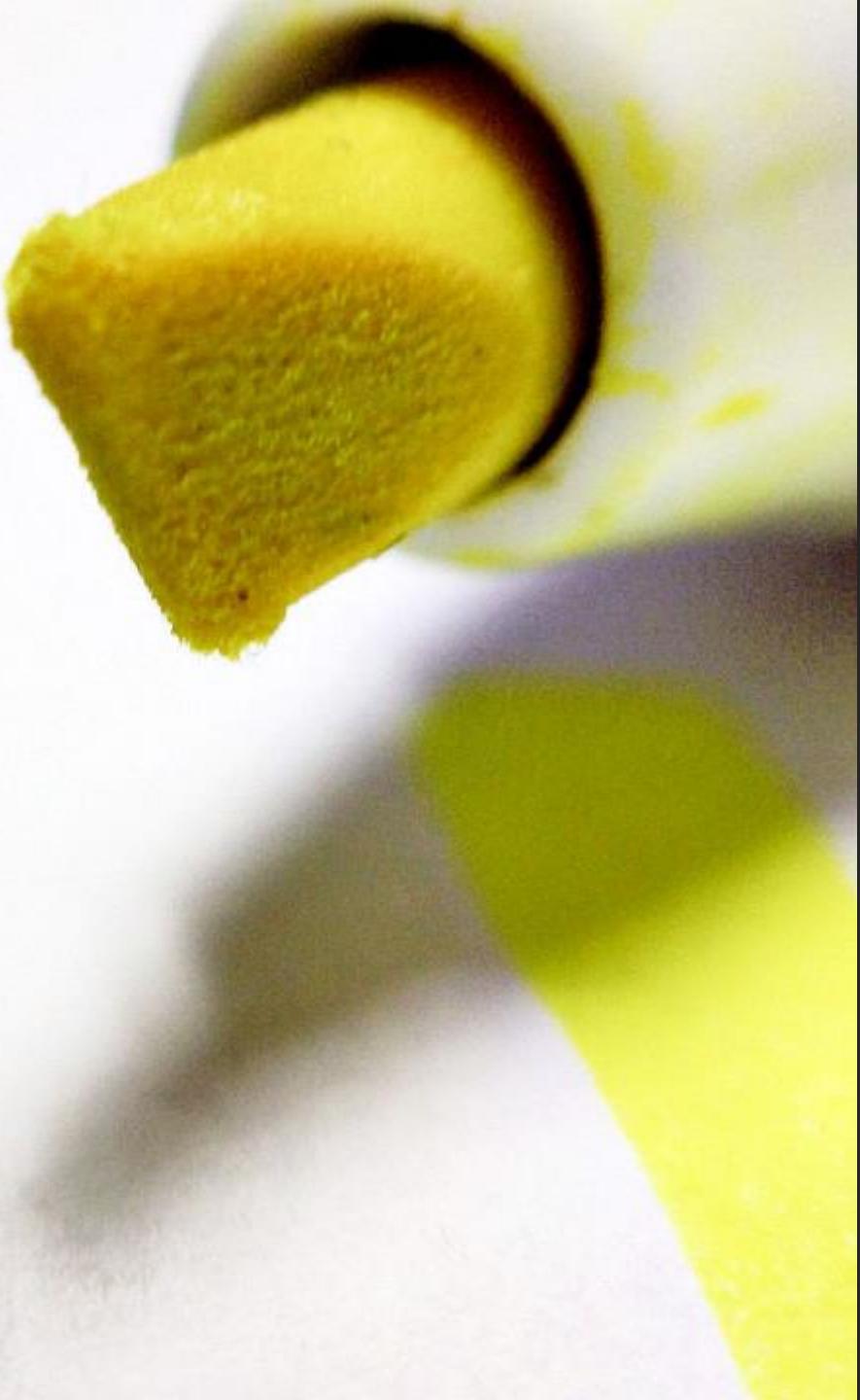
$$\langle V(x) \rangle = \int f_\theta(x) V(x) f_\theta(x)$$

$$\langle -i\partial_x \rangle = \int f_\theta(x) \left(-i \frac{d}{dx} \right) f_\theta(x), \langle \partial_x^2 \rangle, \dots$$

Variational formulation

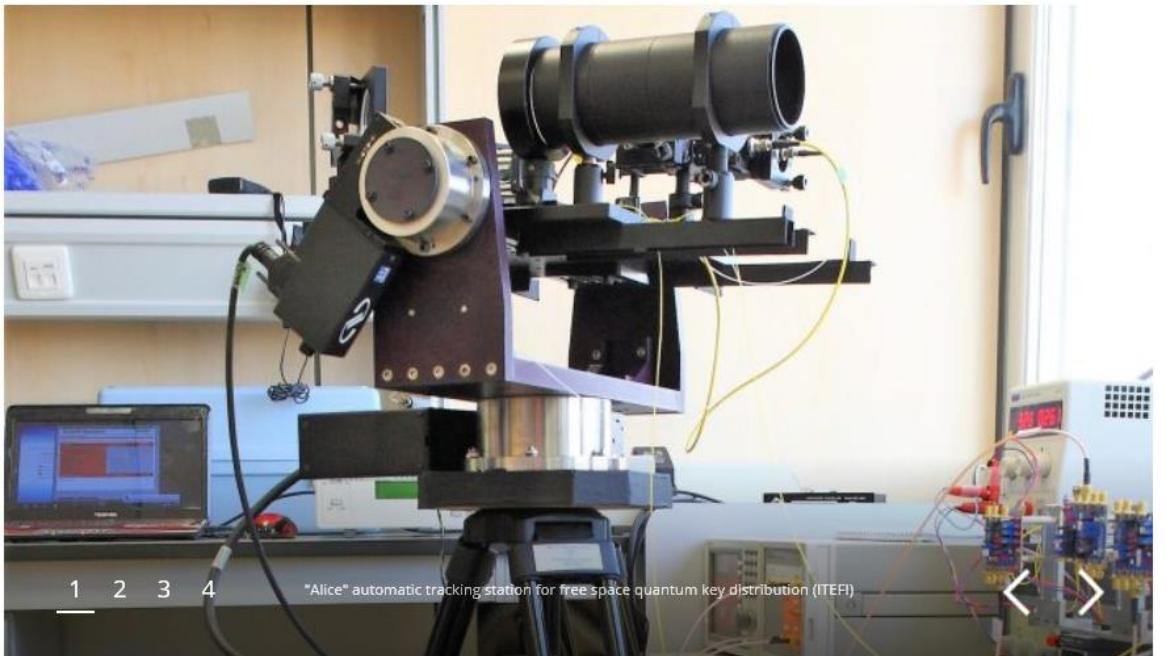


$$\text{argmin}_{\theta} \left\langle f_{\theta}(x) \left| -\frac{d^2}{dx^2} + V(x) \right| f_{\theta}(x) \right\rangle$$



Main ideas

- Quantum registers can encode efficiently multivariate functions.
- Quantum computers can construct, manipulate and interrogate functions.
- There are many algorithms with a potential gain, even if not exponential.
- Applications to other domains: numerical analysis, finances, Physics, engineering...



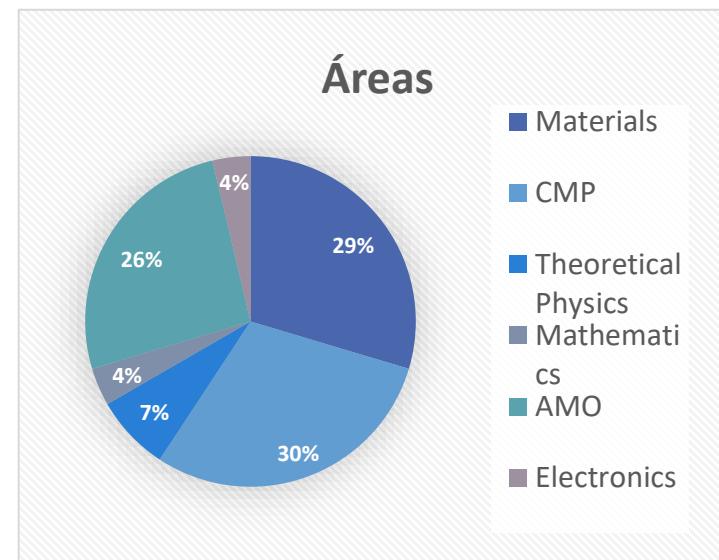
CSIC enters the IBM-Q network

CSIC and IBM have signed a contract to allow researchers at CSIC and Universidad Autónoma de Madrid to work with IBM's superconducting quantum computers, collaborate in training a new generation of quantum software developers and translating quantum computing technologies to Spain's industrial ecosystem. This agreement was celebrated in an event that took place at CSIC's...

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Alejandro González Tudela



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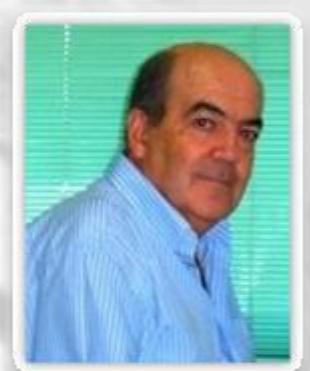
Manuel Pino



Érik Torrontegui



Tomás Ramos



Juan León



Alejandro Valido



Diego G. Olivares

Thanks!

