Quantum Algorithms and Monte Carlo Estimation

Patrick Rall

The University of Texas at Austin
Quantum Information Center

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Feynman's vision

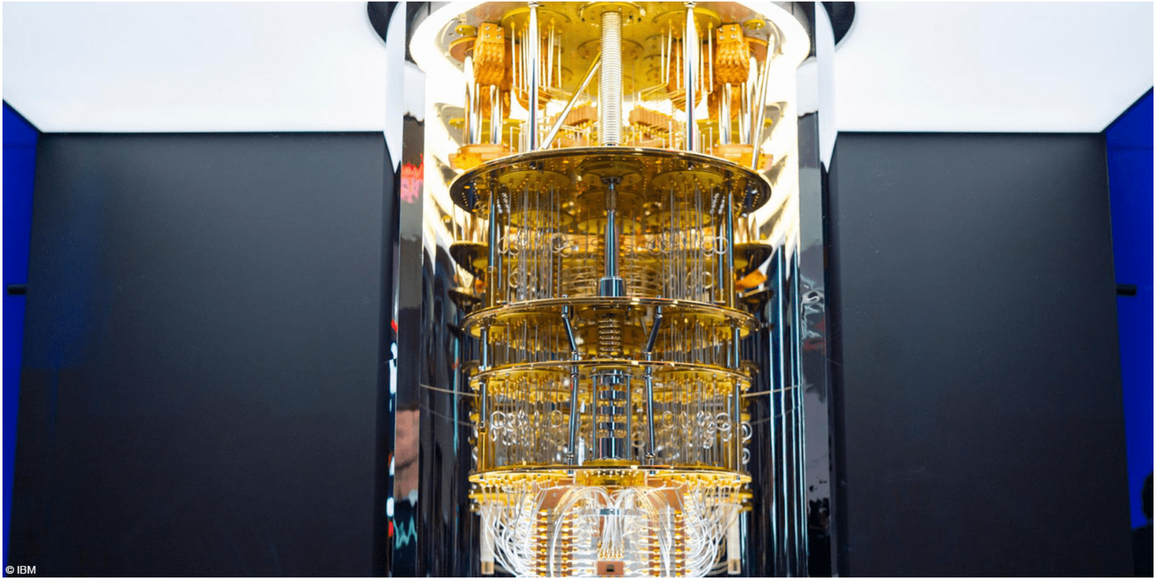
"What kind of computer are we going
to use to simulate physics?"

'Simulating Physics with Computers' 1981

"What kind of computer are we going
to use to simulate physics?"

"If you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."

'Simulating Physics with Computers' 1981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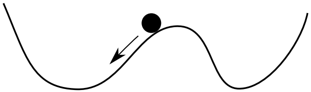

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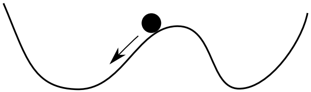
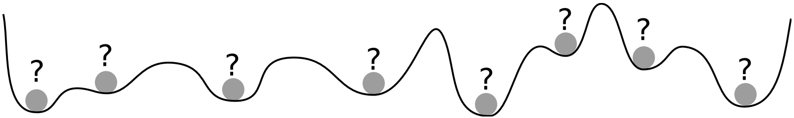
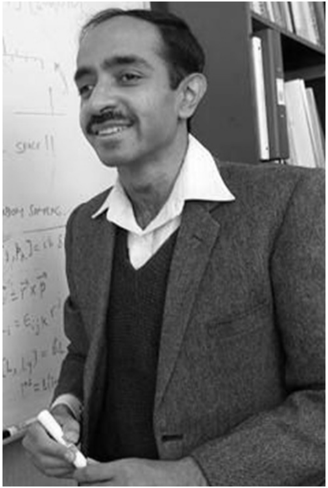


- 'Statics Questions':

  Input: Description of the energy landscape.
  In what state are we likely to find the system?



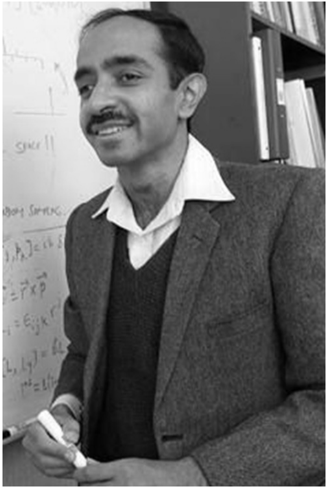


Lov Grover

“Quantum mechanical systems can be in a superposition of states and simultaneously examine multiple possibilities.”

‘A fast quantum mechanical algorithm for database search’ 1996

Quantum Computers and Monte Carlo



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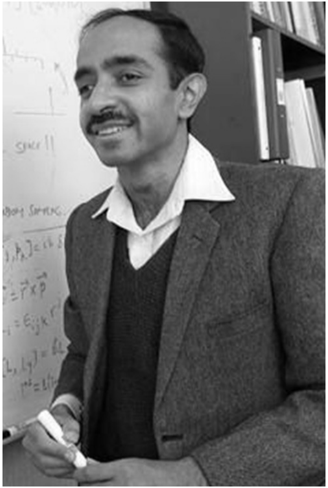

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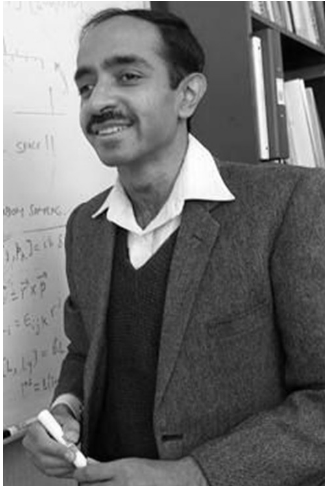

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Estimating p to accuracy ε:

$$\text{classical} \sim \frac{1}{\varepsilon^2} \qquad \text{quantum} \sim \frac{1}{\varepsilon}$$

Brassard, Høyer, Mosca, Tapp (BHMT) 1998

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1. An introduction to quantum computing and Grover's algorithm

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In the dissertation but not in the defense:
Efficiently simulating certain quantum circuits using classical Monte Carlo
Rall, Liang, Cook, Kretschmer, arXiv:1901.09070, Phys. Rev. A 99, 062337

Quantum Circuits

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The power of quantum circuits

$$|+\rangle := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \cdot |0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

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Not quite so simple.

"The only difference between a probabilistic classical world
and the equations of the quantum world is that
somehow or other it appears as if **the probabilities would have to go negative.**"

Feynman 1981

Grover's search and negative probability

$|\Psi\rangle := |+\rangle^{\otimes n} \sim$ superposition over all possibilities $\quad \rightarrow \quad R_\Psi :=$ reflection about Ψ

$\Pi :=$ projection matrix onto good possibilities $\quad \rightarrow \quad R_\Pi :=$ reflection about Π

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$$p := |\Pi |\Psi\rangle |^2 = \sin^2(\theta)$$

$$|\Psi\rangle = \sin(\theta) |\text{good}\rangle + \cos(\theta) |\text{bad}\rangle$$

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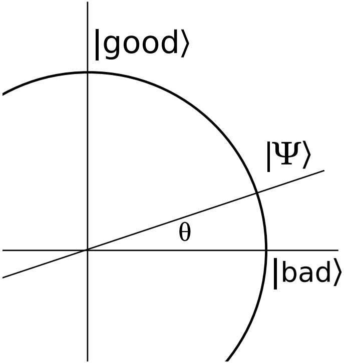

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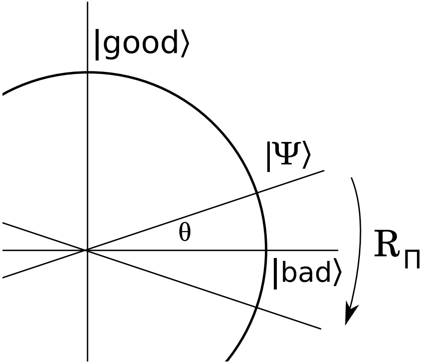

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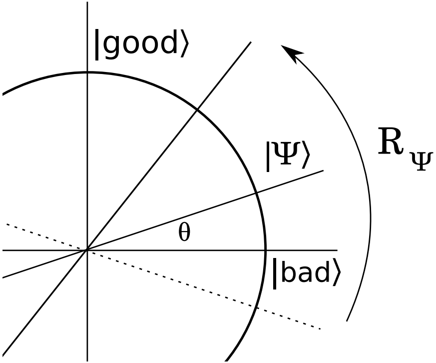

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$$R_\Psi \cdot R_\Pi \cdot |\Psi\rangle = \sin(3\theta)\,|\text{good}\rangle + \cos(3\theta)\,|\text{bad}\rangle$$

$$(R_\Psi \cdot R_\Pi)^k \cdot |\Psi\rangle = \sin((2k+1)\theta)\,|\text{good}\rangle + \cos((2k+1)\theta)\,|\text{bad}\rangle$$

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For every odd r, we can toss a coin:

$$\Pr[\text{coin comes up heads}] = \sin^2(r\theta)$$

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- **Search:** Make the event happen / find a good possibility.

$$r \sim 1/\theta \sim \sqrt{1/p}$$

$$\sin^2(r\theta) \sim \text{const}$$

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    - Finance: stochastic option pricing, financial derivatives
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- Traditional method: BHMT 1998

  Very complicated: uses quantum Fourier transform, conditional rotations, median amplification.

Quantum Approximate Counting, Simplified Aaronson, SOSA '20 24-32

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- Pick $r \sim 1/(\theta_{\text{max}} - \theta_{\text{min}})$ so that:

$$\begin{aligned} r\theta_{\text{min}} &\approx \pi k & r\theta_{\text{max}} &\approx \pi k + \frac{\pi}{2} \\ \sin^2(r\theta_{\text{min}}) &\approx 0 & \sin^2(r\theta_{\text{max}}) &\approx 1 \end{aligned}$$

Quantum Approximate Counting, Simplified [Aaronson, SOSA '20 24-32]

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$$\sin^2(r\theta_{\text{min}}) \approx 0 \qquad \sin^2(r\theta_{\text{max}}) \approx 1$$

- Toss r-coin very many times to test if:

$$\sin^2(r\theta) \leq \frac{1}{3} \quad \text{or} \quad \sin^2(r\theta) \geq \frac{2}{3}$$

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$$\rho(E) = \frac{1}{D} \sum_i \delta(E_i - E)$$

$\rightarrow$ Lots of non-unitary matrices: cannot write into a quantum circuit.

Block Encodings

- Main idea: encode M into top left corner of a unitary matrix.

$$U_M = \begin{bmatrix} M & \cdot \\ \cdot & \cdot \end{bmatrix} \qquad (\langle 0| \otimes I) U_M (|0\rangle \otimes I) = M$$

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\end{aligned}$$

- Linear combinations of Paulis $\rightarrow$ block encodings of any Hamiltonian or observable

Estimating observables: $\mathrm{Tr}(\rho O)$ Rall, arXiv:2004.06832, Phys. Rev. A 102, 022408

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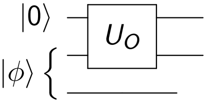
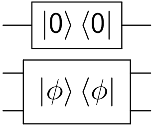
$|\Psi\rangle :=$

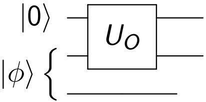


$\Pi :=$



- Given a block encoding U_O of O, and $|\phi\rangle$, a purification of ρ

$|\Psi\rangle :=$



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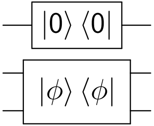

- "Approximate counting simplified" gives an estimate of:

$$\begin{aligned} p := |\Pi\,|\Psi\rangle\,|^2 &= |\,\langle 0|\,\langle\phi|\,(U_O \otimes I)\,|0\rangle\,|\phi\rangle\,|^2 \\ &= |\,\langle\phi|\,(O \otimes I)\,|\phi\rangle\,|^2 \\ &= |\mathrm{Tr}\,[|\phi\rangle\,\langle\phi|\,(O \otimes I)]\,|^2 = |\mathrm{Tr}\,(\rho O)\,|^2 \end{aligned}$$

n-time correlation functions

- An observable in Heisenberg picture:

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- Γ is not Hermitian, so expectation is complex.

$$\text{Real part:} \qquad \mathrm{Tr}\left(\rho \frac{\Gamma + \Gamma^\dagger}{2}\right)$$

$$\text{Imaginary part:} \qquad \mathrm{Tr}\left(\rho \frac{\Gamma - \Gamma^\dagger}{2i}\right)$$

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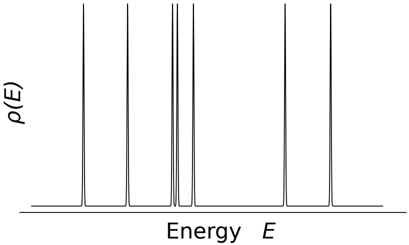

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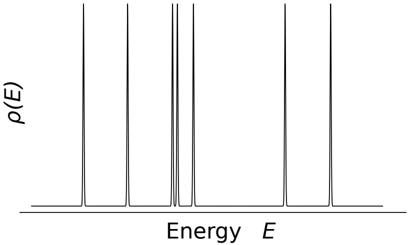

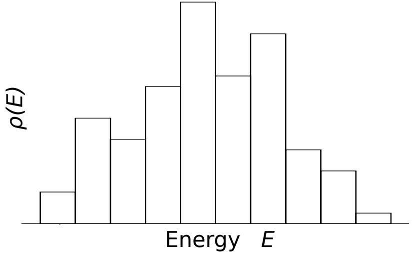

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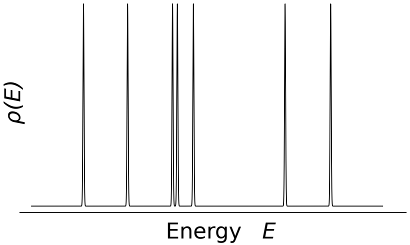
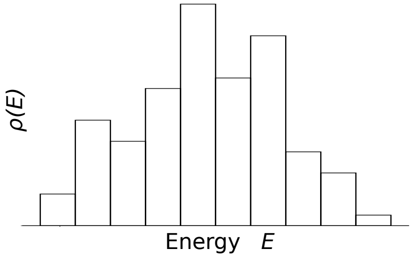
- Map to observable estimation:

$$\int_{E_1}^{E_2} \rho(E)dE = \mathrm{Tr}\left(\frac{I}{D}\cdot w(H)\right)$$

$w(E) :=$ polynomial indicating $E_1 \leq E \leq E_2$





Outline

1. An introduction to quantum computing and Grover's algorithm
2. Simplified quantum Monte Carlo estimation
3. An introduction to block encodings
4. Quantum algorithms for estimating physical quantities
5. A quantum algorithm for measuring in the energy eigenbasis

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- 'Textbook' method: Phase Estimation Nielsen, Chuang
  Uses Hamiltonian simulation, quantum Fourier transform, median amplification, and a quantum sorting network.

Block Measurement Lemma

Say we have a block encoding of a projector Π.
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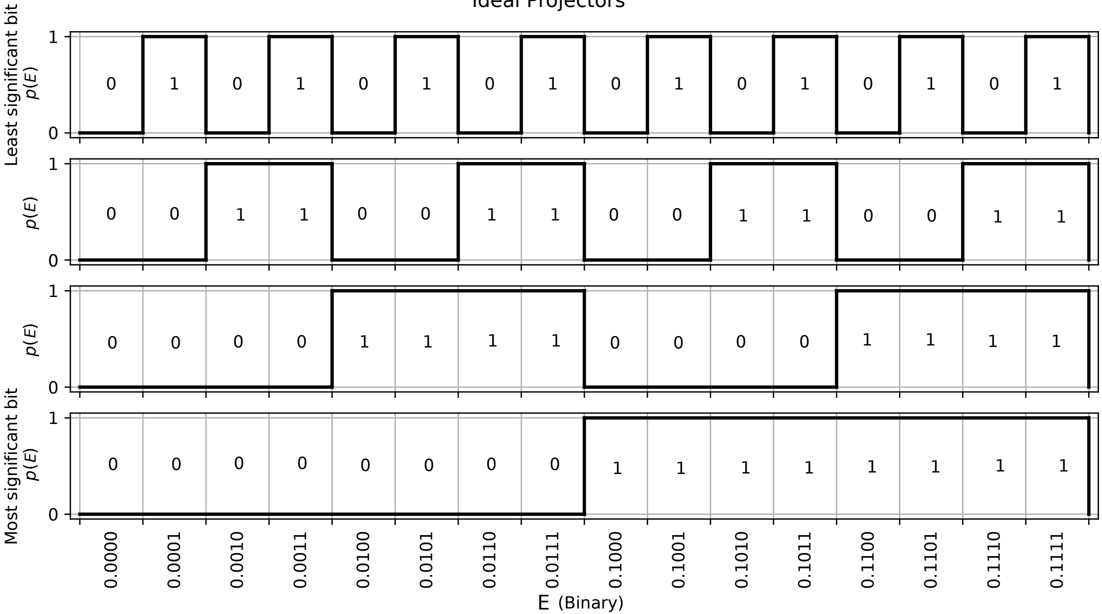
Ideal Projectors



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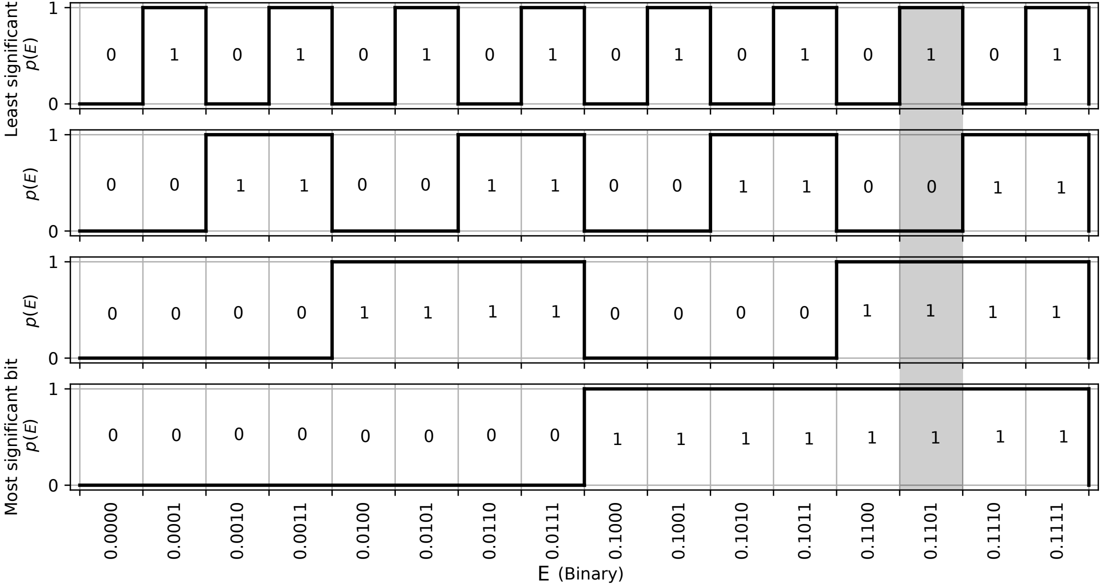
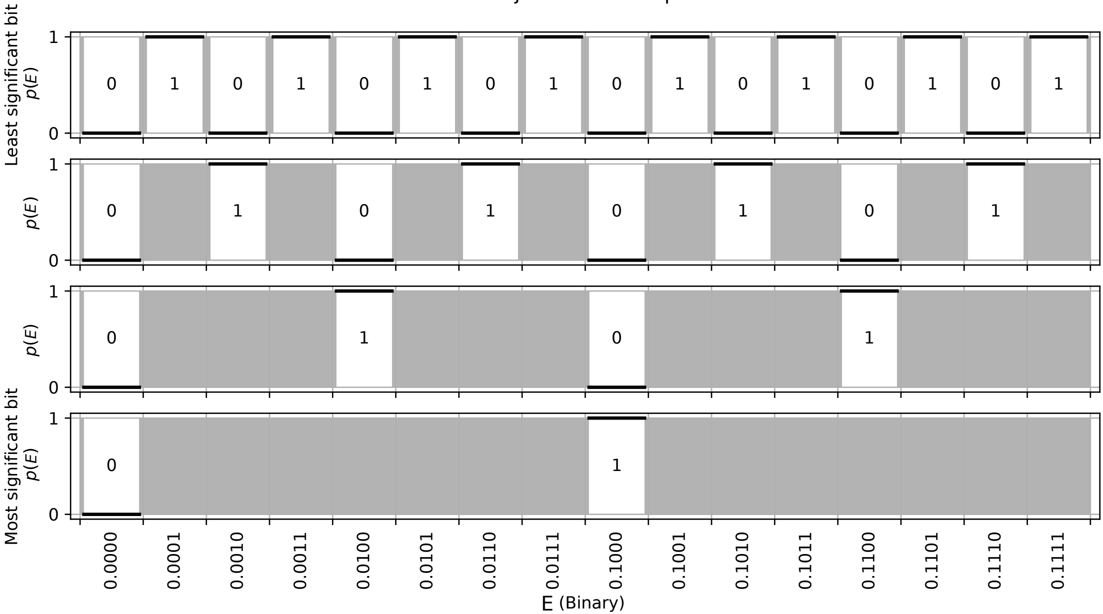


Projectors with Gaps



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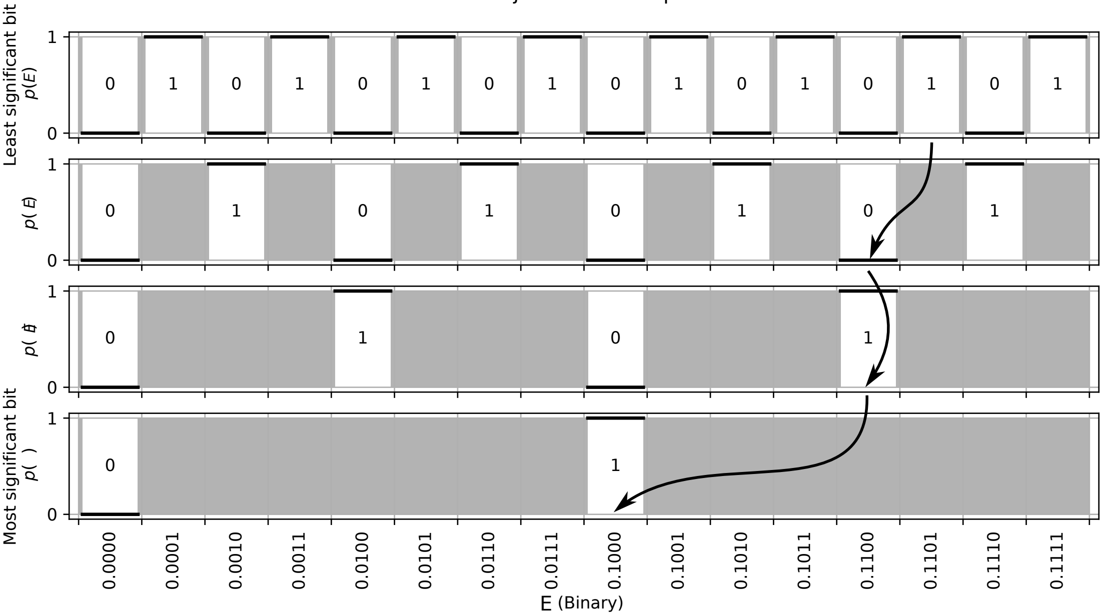

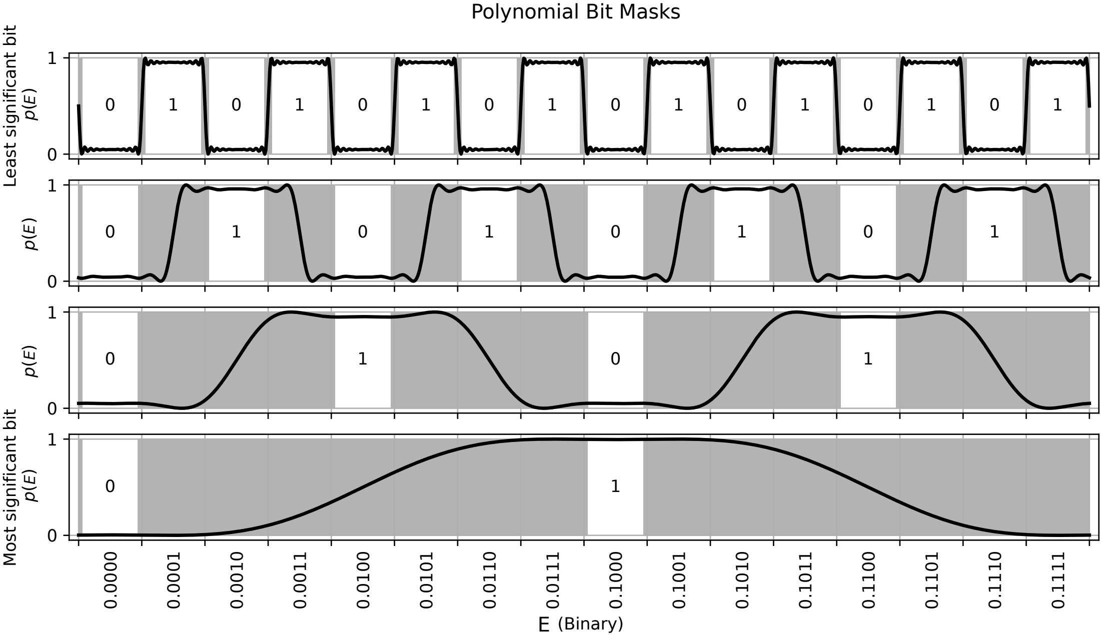

Polynomial Bit Masks
Least significant bit
p(E)
Most significant bit
0
1
0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1
0 1 0 1 0 1 0 1
0 1 0 1
0 1
0.0000
0.0001
0.0010
0.0011
0.0100
0.0101
0.0110
0.0111
0.1000
0.1001
0.1010
0.1011
0.1100
0.1101
0.1110
0.1111
E (Binary)

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  Harrow, Wei arXiv:1908.10856 Arunachalam et al arXiv:2009.11270

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- Energy measurement is simpler and more efficient using eigenvalue transformation
  Rall, arXiv:2103.09717, Quantum 5 556
  Next steps: modernize the quantum algorithms literature with eigenvalue transformation

Thank you for your attention!

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Contact me at `patrickjrall@gmail.com`