7- Quantum Simulation

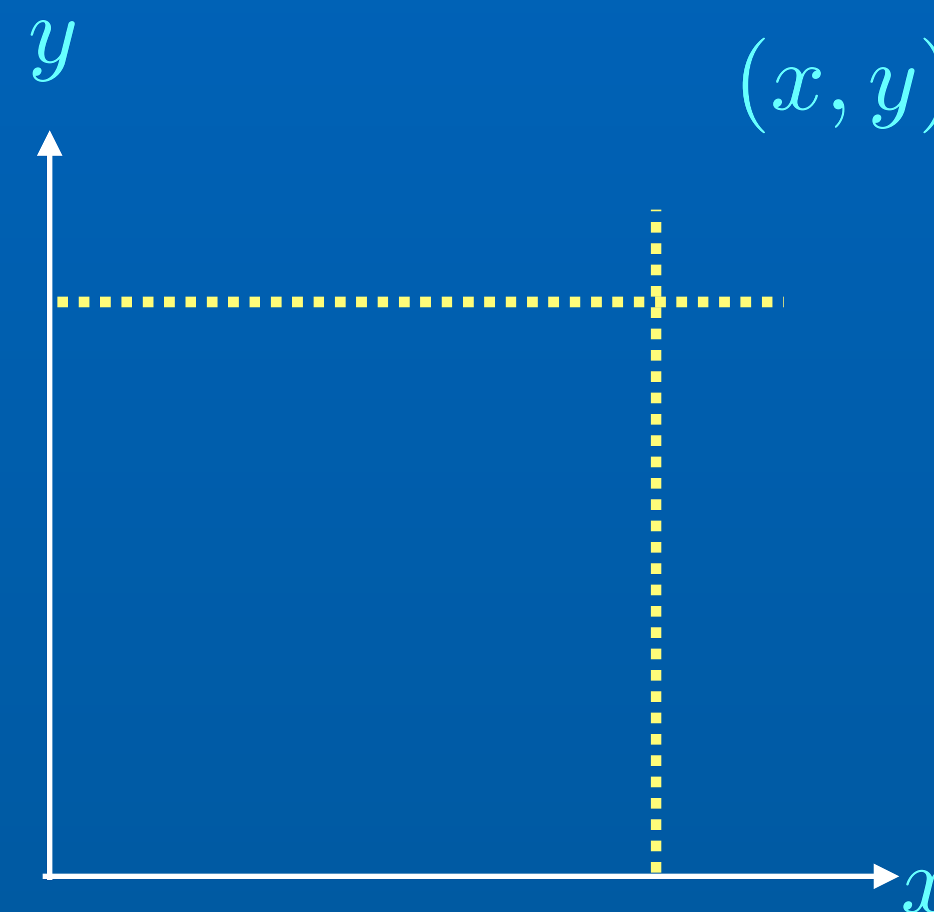
گام های بزرگ در علوم

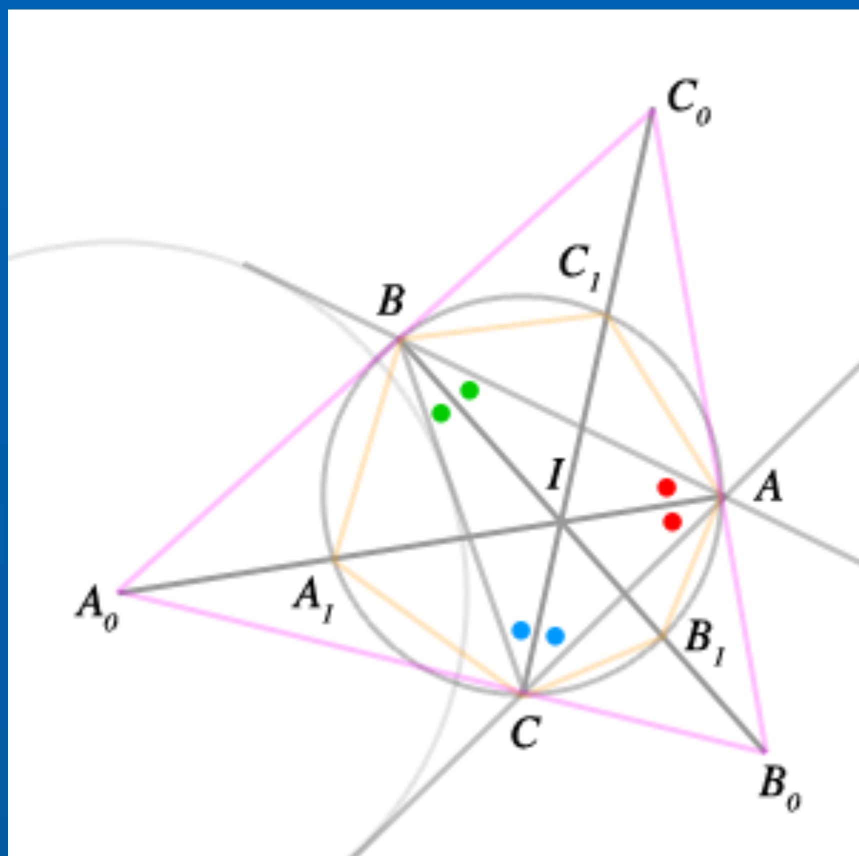
یا

در شیوه های مطالعه علوم

هندسه تحلیلی

هندسه قدیمی

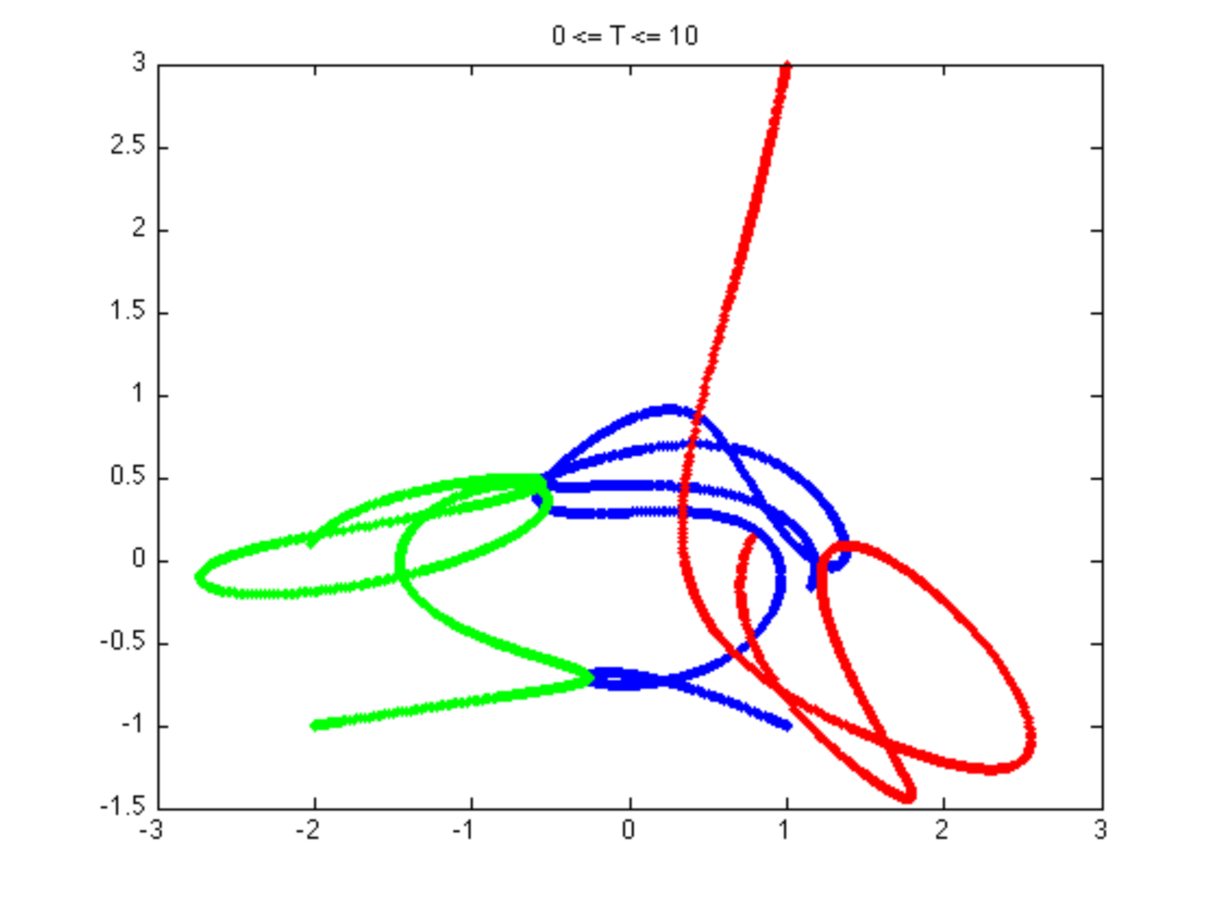




محاسبات جبری

خلاقیت

حل های عددی و
شبیه سازی عددی



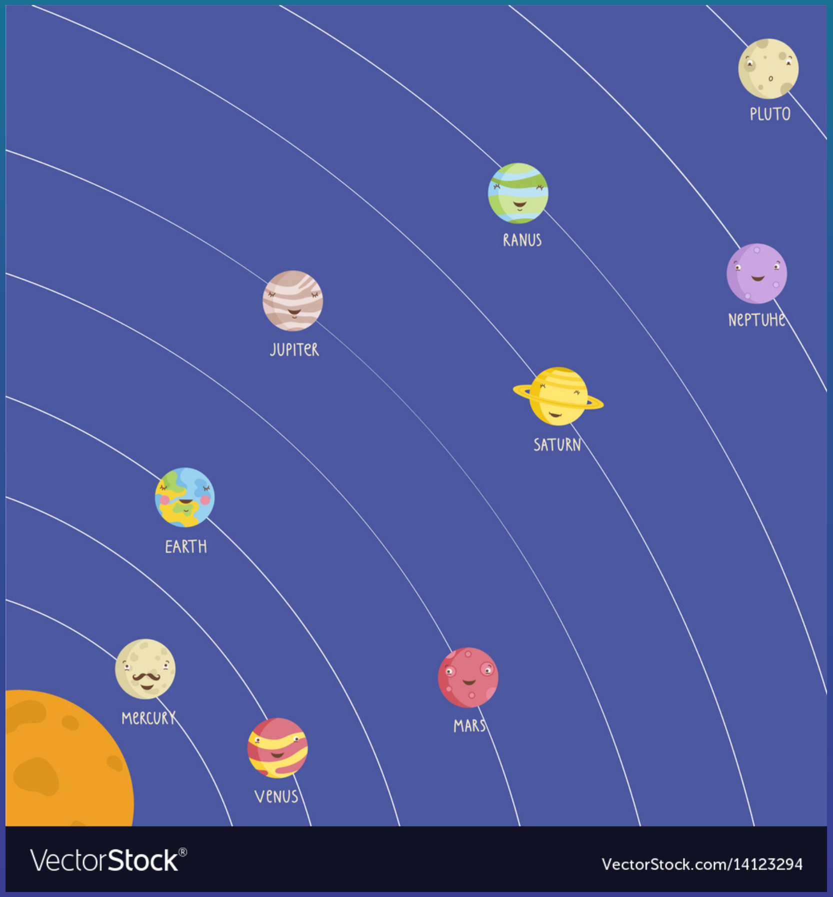
حل های تحلیلی

$$\ddot{\mathbf{r}}_1 = -Gm_2\frac{\mathbf{r}_1-\mathbf{r}_2}{|\mathbf{r}_1-\mathbf{r}_2|^3} - Gm_3\frac{\mathbf{r}_1-\mathbf{r}_3}{|\mathbf{r}_1-\mathbf{r}_3|^3},$$

$$\ddot{\mathbf{r}}_2 = -Gm_3\frac{\mathbf{r}_2-\mathbf{r}_3}{|\mathbf{r}_2-\mathbf{r}_3|^3} - Gm_1\frac{\mathbf{r}_2-\mathbf{r}_1}{|\mathbf{r}_2-\mathbf{r}_1|^3},$$

$$\ddot{\mathbf{r}}_3 = -Gm_1\frac{\mathbf{r}_3-\mathbf{r}_1}{|\mathbf{r}_3-\mathbf{r}_1|^3} - Gm_2\frac{\mathbf{r}_3-\mathbf{r}_2}{|\mathbf{r}_3-\mathbf{r}_2|^3}.$$

شبیه سازی منظومه شمس



تعداد متغیرها $6 \times N$

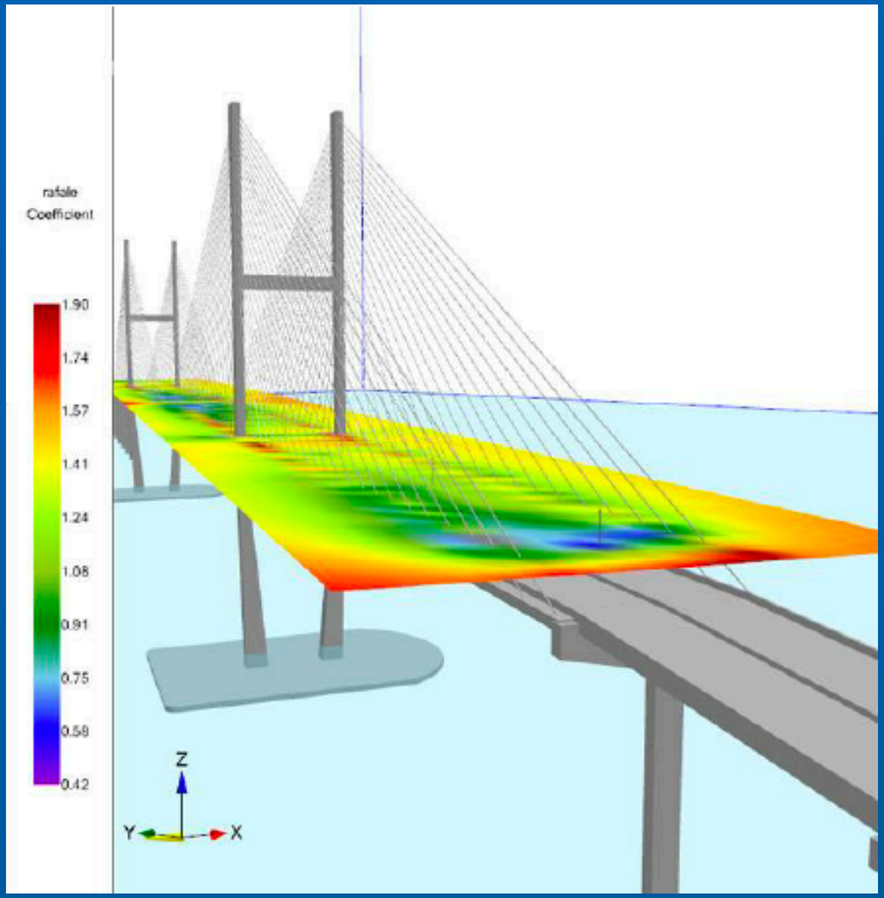
$$\frac{d}{dt} x_i = f_i(x_1, \cdots x_{6N})$$

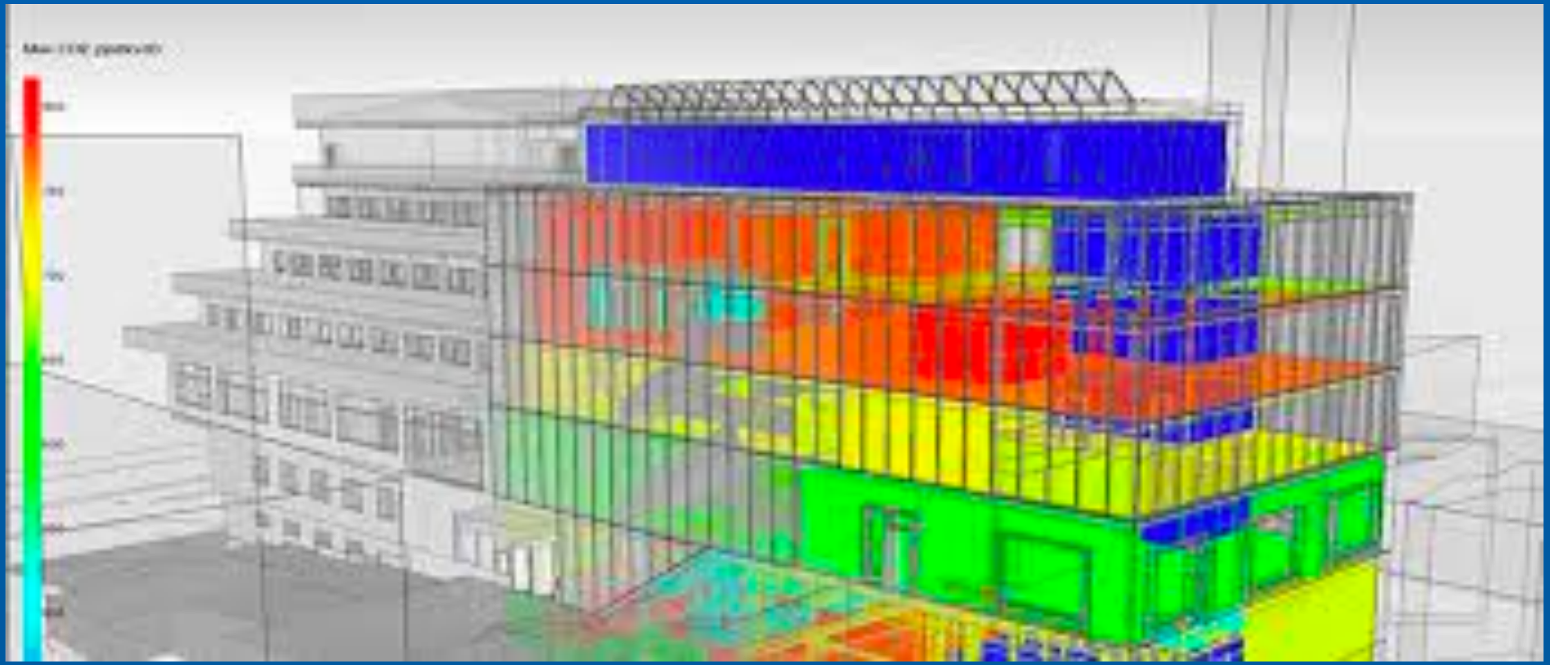
شبیه سازی یک خوشه ستاره ای

تعداد متغیرها $6 \times N$

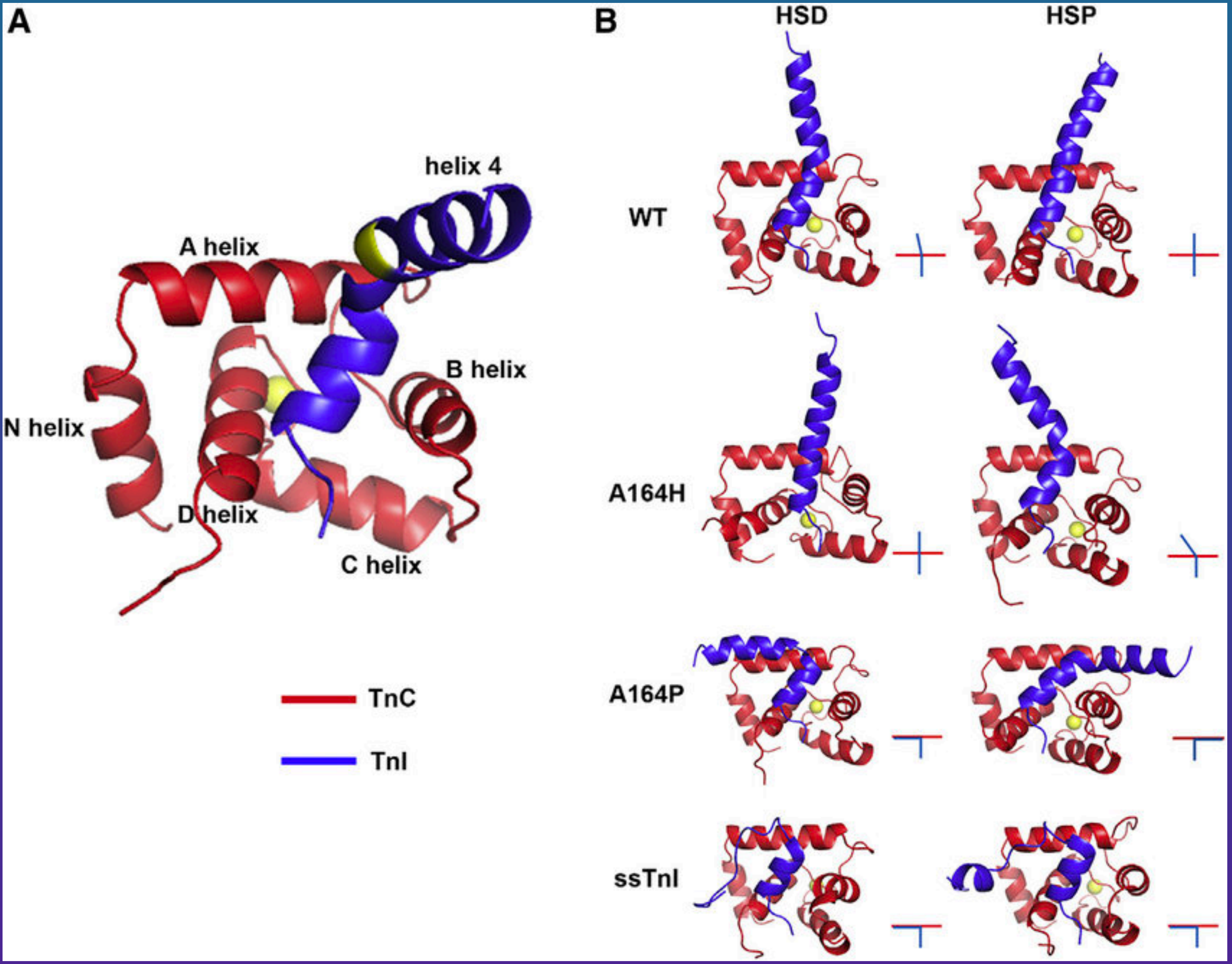
$$\frac{d}{dt}x_i = f_i(x_1, \cdots x_{6N})$$

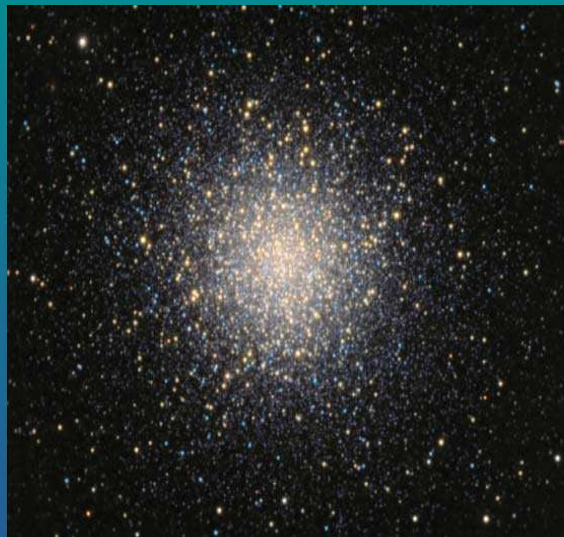
شبیه سازی در مهندسی

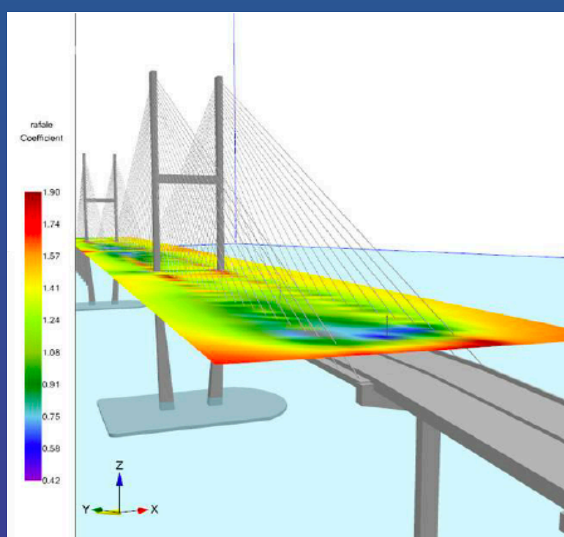


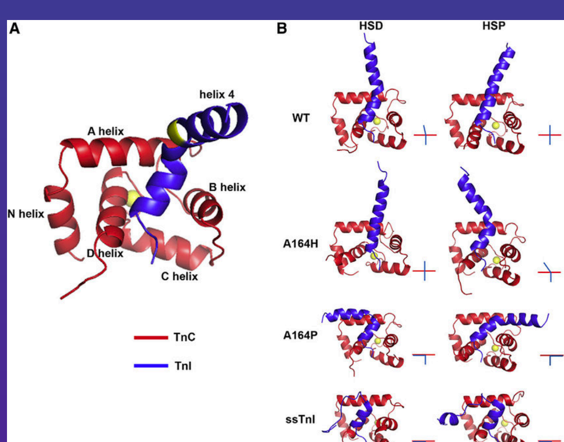


شبیه سازی محدود در شیمی و بیوشیمی



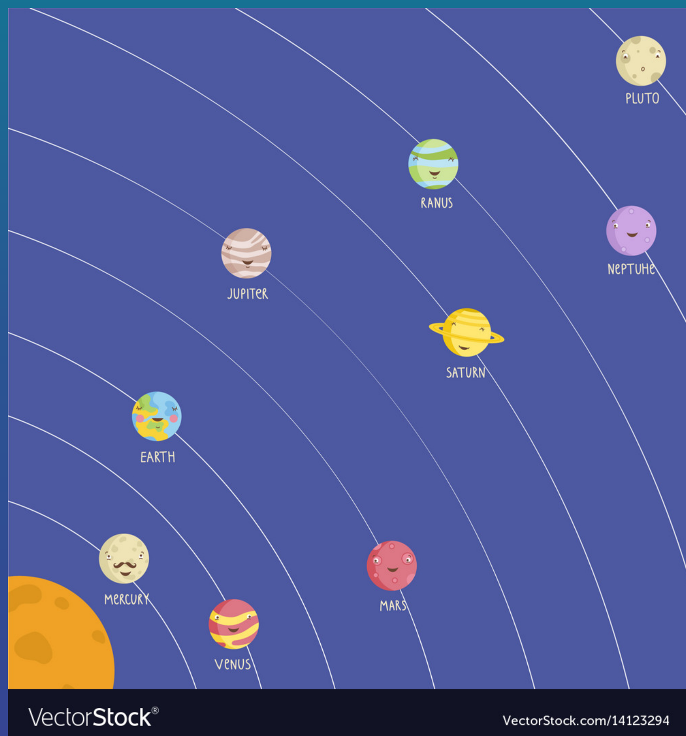


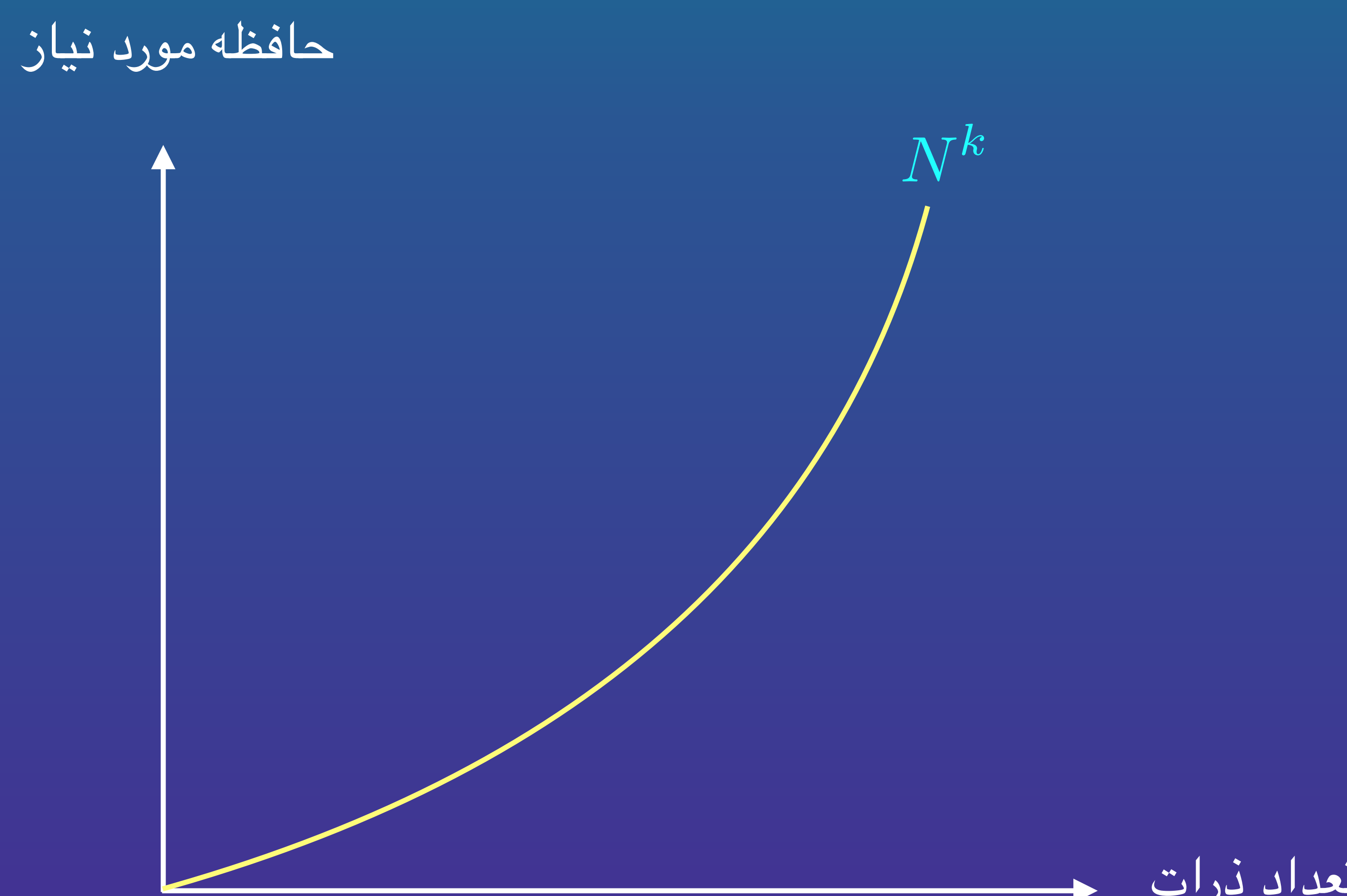


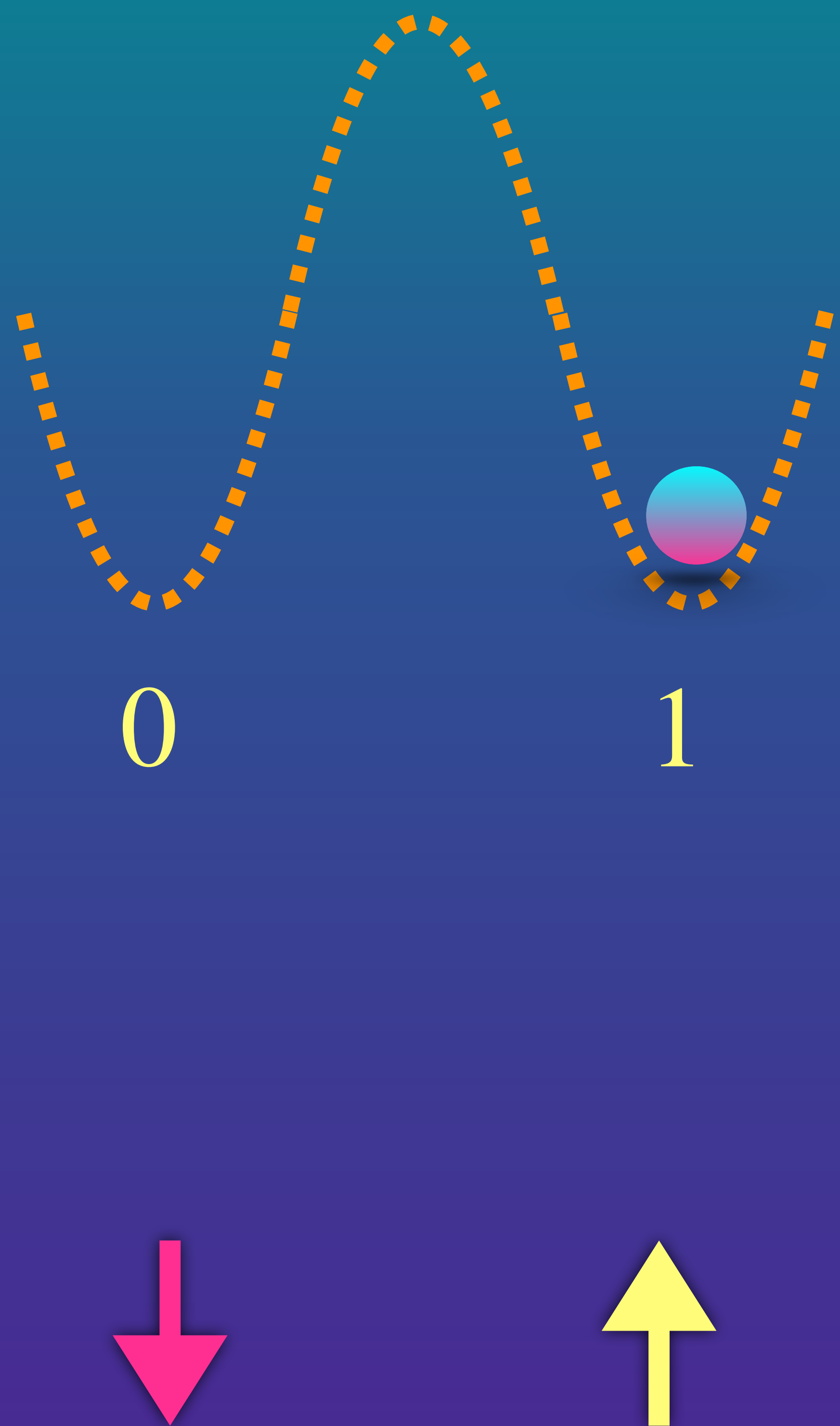


Classical Simulator

مسائل آسان


PLUTO
RANUS
JUPITER
NEPTUNE
SATURN
EARTH
MERCURY
MARS
VENUS
VectorStock®
VectorStock.com/14123294


حافظه مورد نیاز
N^k
تعداد ذرات



$$|\psi\rangle = a\,|0\rangle + b\,|1\rangle$$

$$a \longrightarrow \quad 0101010001011011$$

$$b \longrightarrow \quad 1011010010110101$$

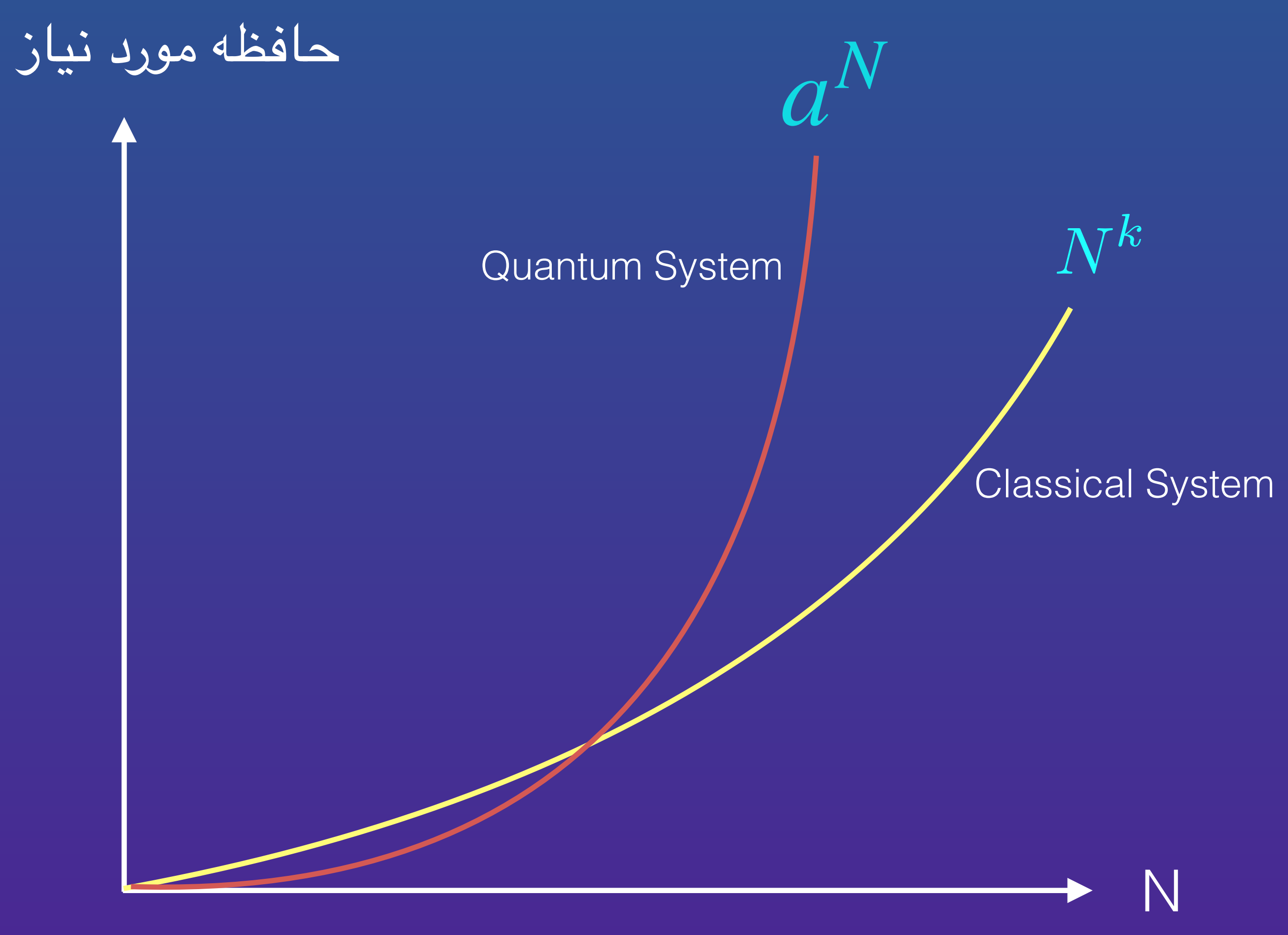
$$dim(H) = 2^N$$

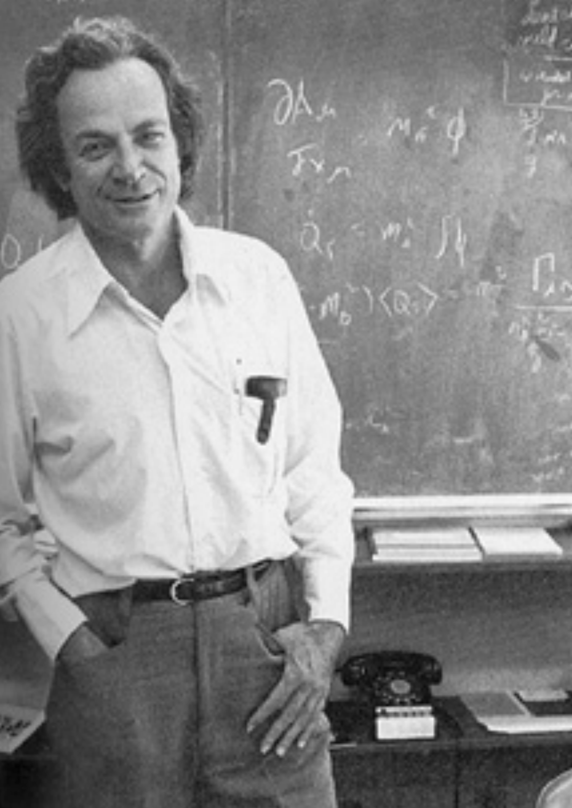
$$|\Psi\rangle = a_1|1\rangle + a_2|2\rangle + \cdots a_{2^N}|2^N\rangle$$

$2^{10} = 1024$ Bytes

$2^{100} \approx 10^{24}$ Giga Bytes

حتی یک سیستم ساده
کوانتومی را نیز نمی توانیم در یک کامپیوتر کلاسیک شبیه سازی کنیم.





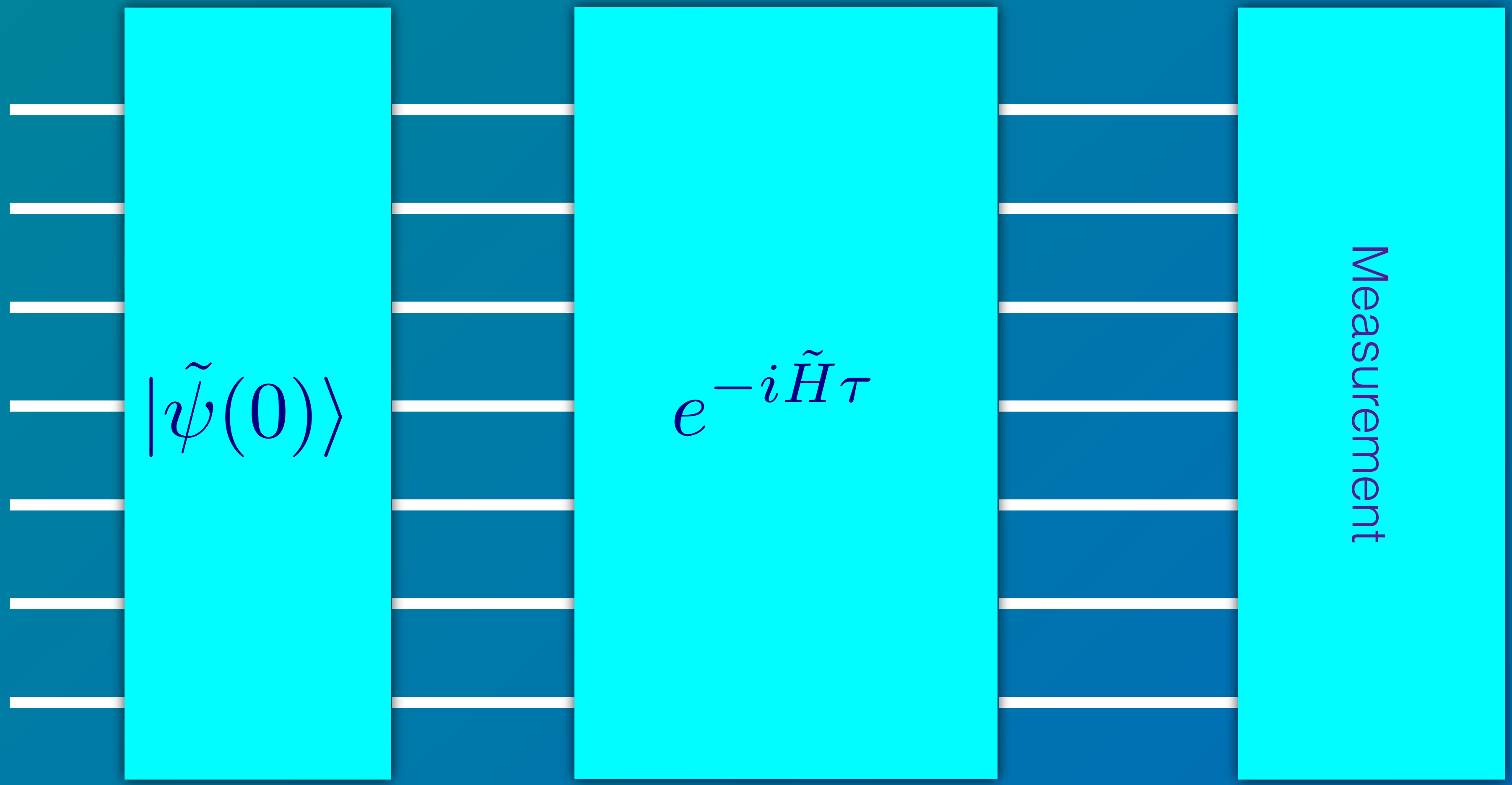
شبیه سازی کوانتومی

استفاده از یک سیستم کوانتومی ساده برای
شبیه سازی یک سیستم کوانتومی دیگر

$$i\frac{d}{dt}|\psi\rangle = H|\psi(t)\rangle$$

A-Digital Quantum Simulation

A1-Dynamics of a particle in one dimension



$$|\tilde{\psi}\rangle = e^{-i\tilde{H}\tau}|\tilde{\psi}(0)\rangle$$

یک مثال خیلی ساده

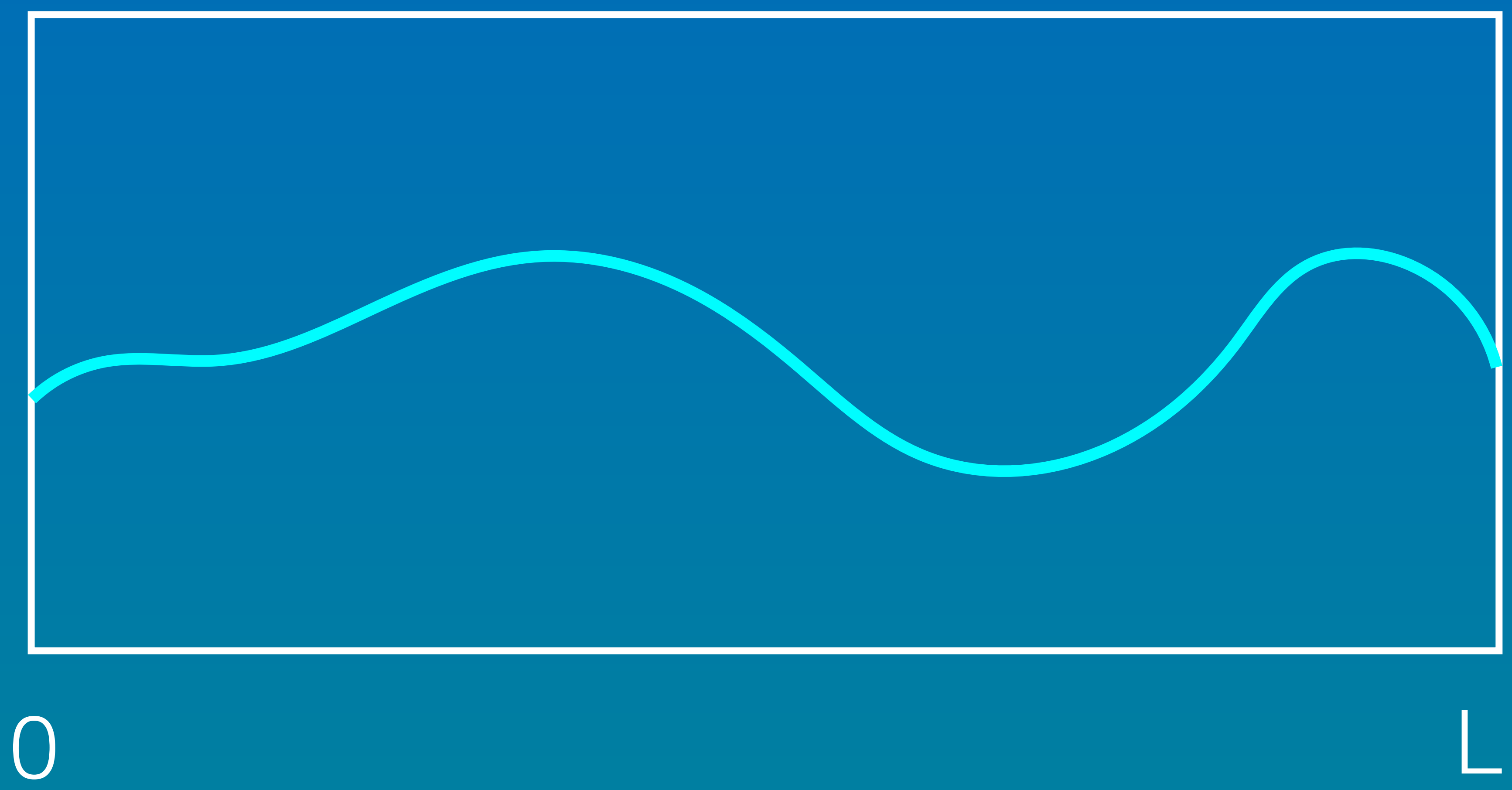
Simulation of the dynamics of a single particle

$$i\frac{d}{dt}|\psi\rangle = H|\psi(t)\rangle$$

Efficient Simulation of Quantum Systems by Quantum Computers

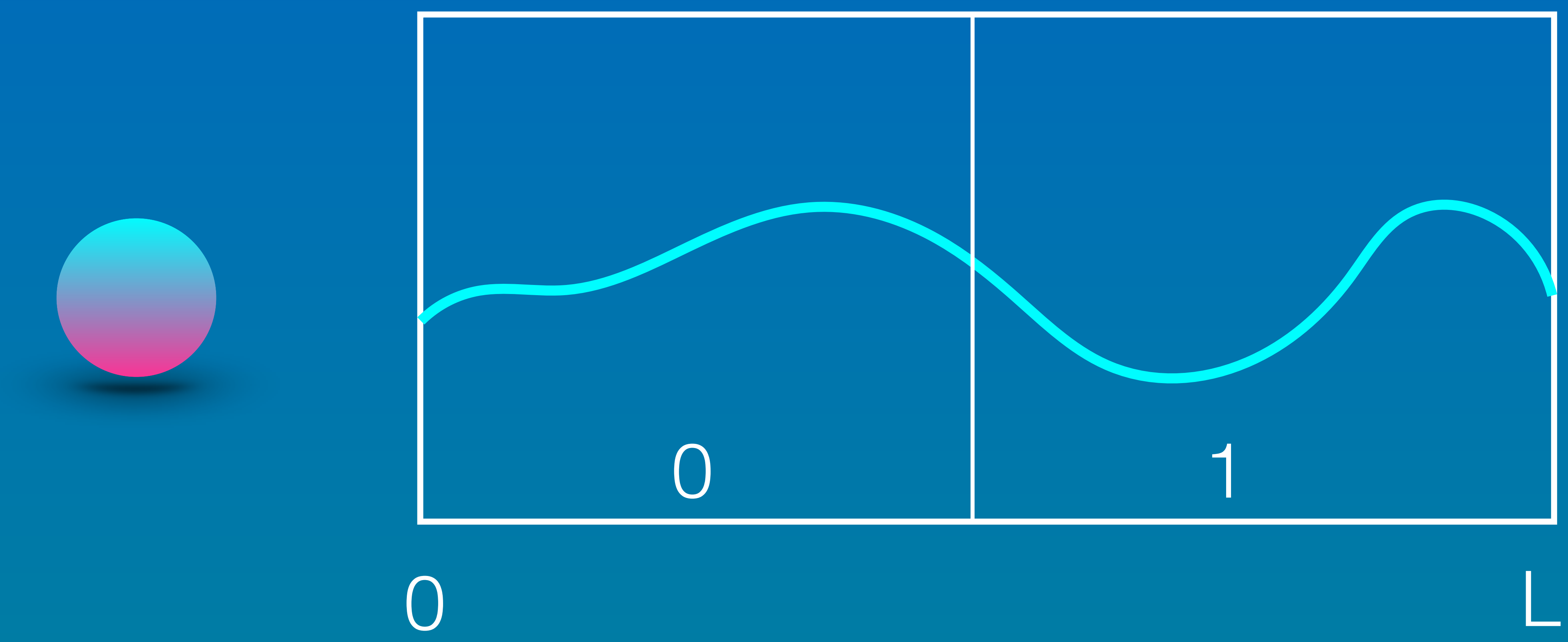
Christoff Zalka

Preparation of the initial state



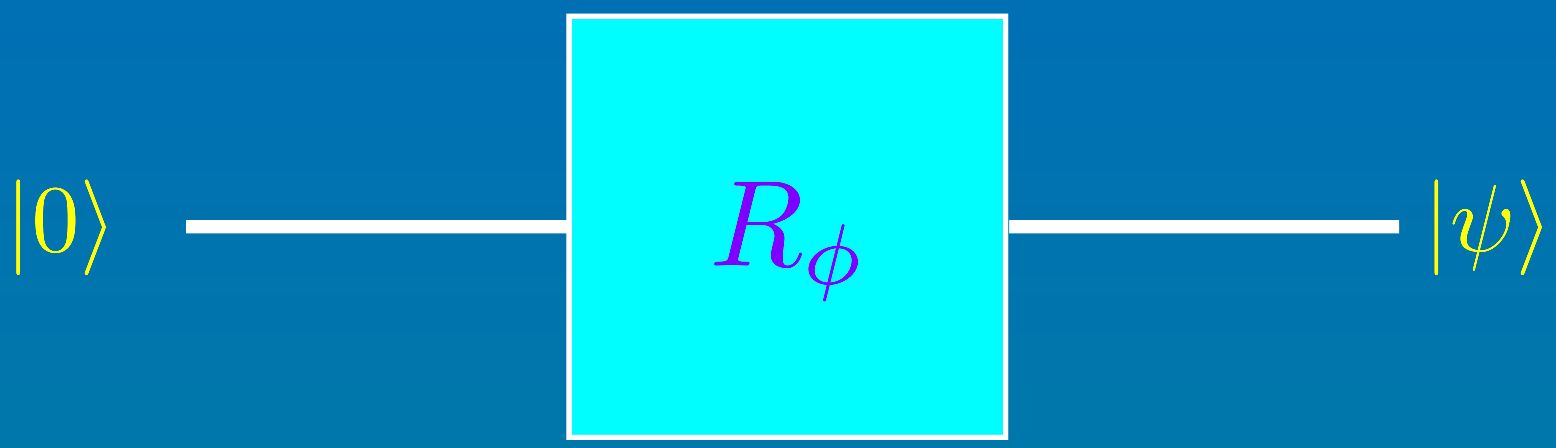
$$|\psi\rangle = \int_0^L \psi(x)|x\rangle$$

If we have only one qubit, we approximate the wave function as follows



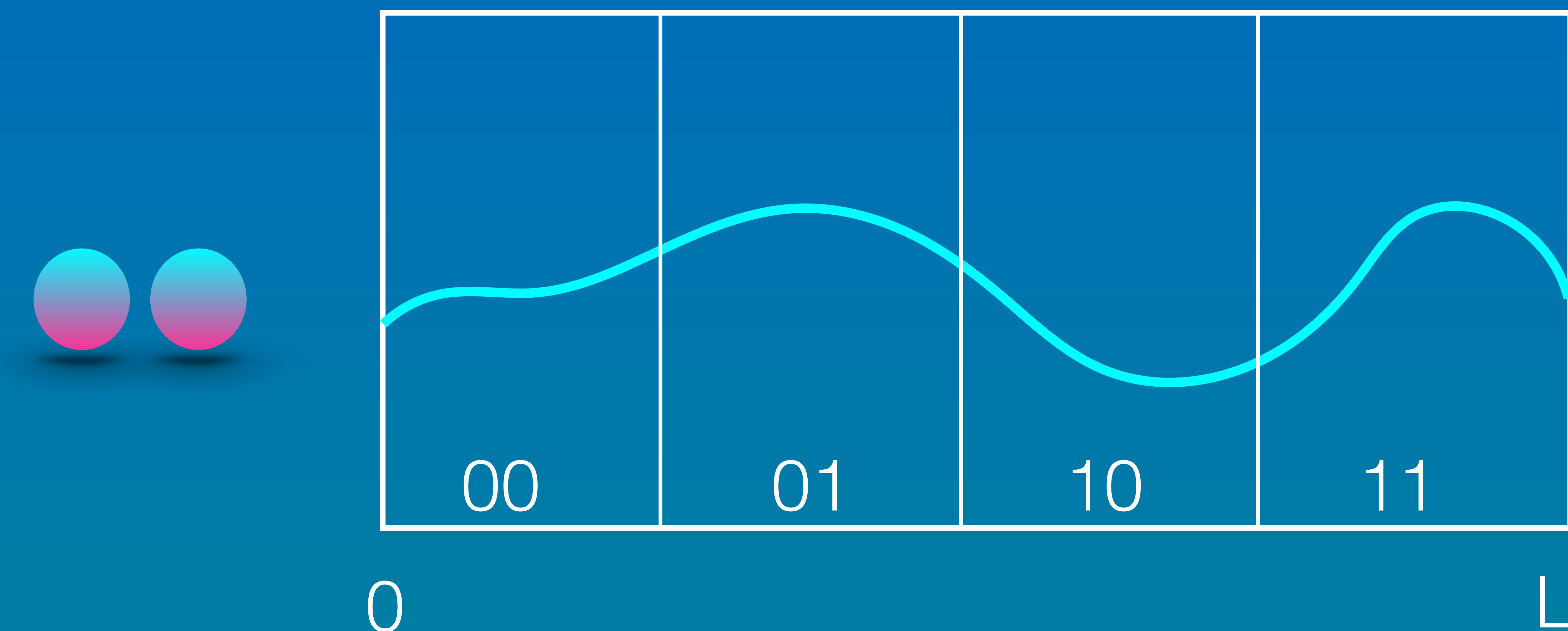
$$|\psi\rangle = \cos\phi|0\rangle + \sin\phi|1\rangle$$

$$\cos^2\phi = \int_0^{\frac{L}{2}} |\psi(x)|^2 dx \qquad \sin^2\phi = \int_{\frac{L}{2}}^{L} |\psi(x)|^2 dx$$



$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad R_\phi = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \qquad \begin{pmatrix} \cos\phi \\ \sin\phi \end{pmatrix}$$

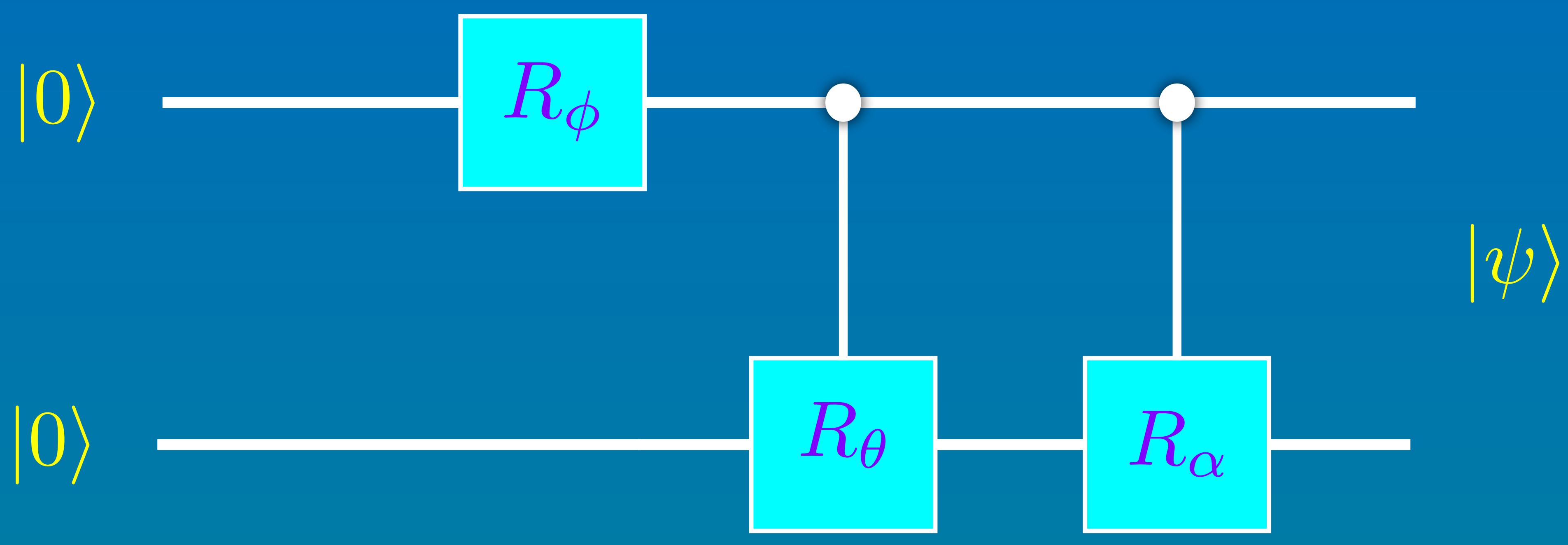
If we have only two qubits, we can do a better approximation



$$|\psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$$

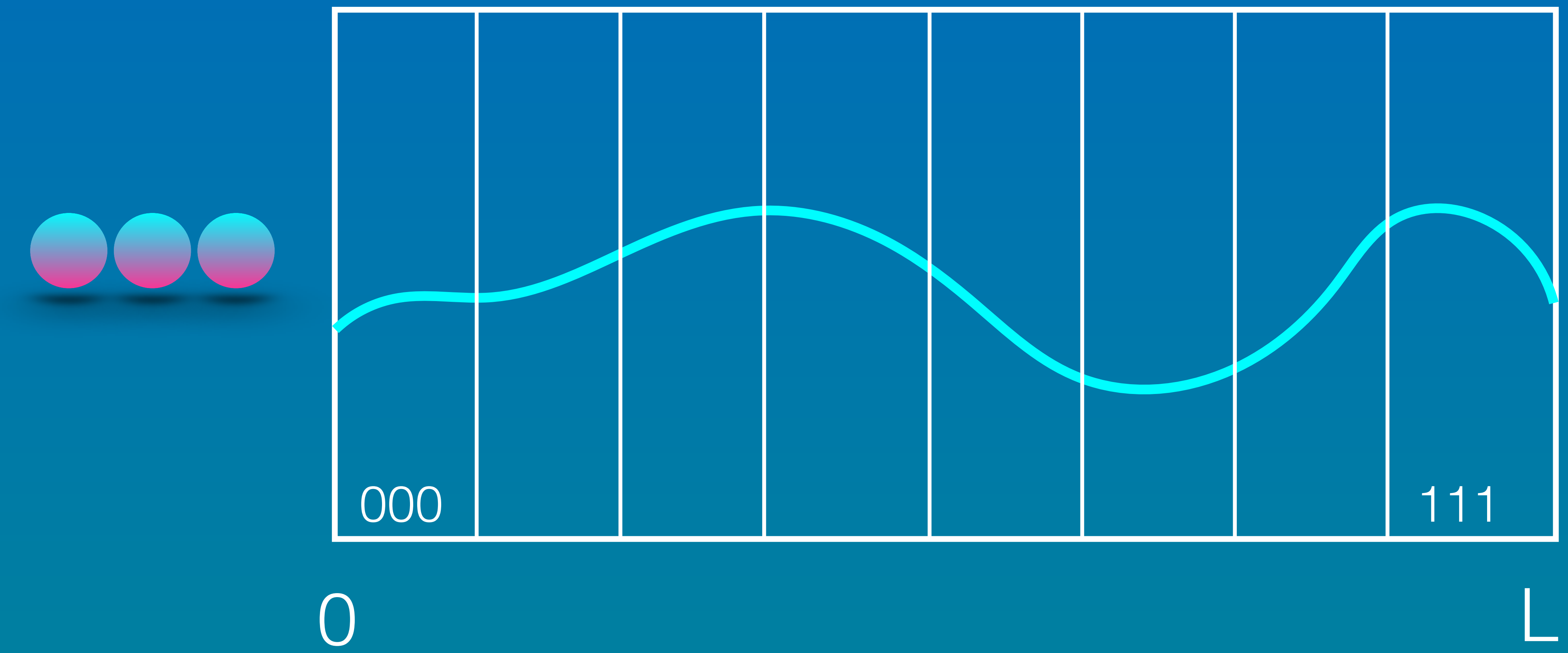
$$a_n = \psi(n\Delta) \qquad |\psi\rangle = \sum_{n=0}^{N-1} a_n |n\rangle, \qquad N = 2^{\text{number of bins}}$$

Assuming that a, b, c, and d are real, we can choose the three rotation angles to produce the state.

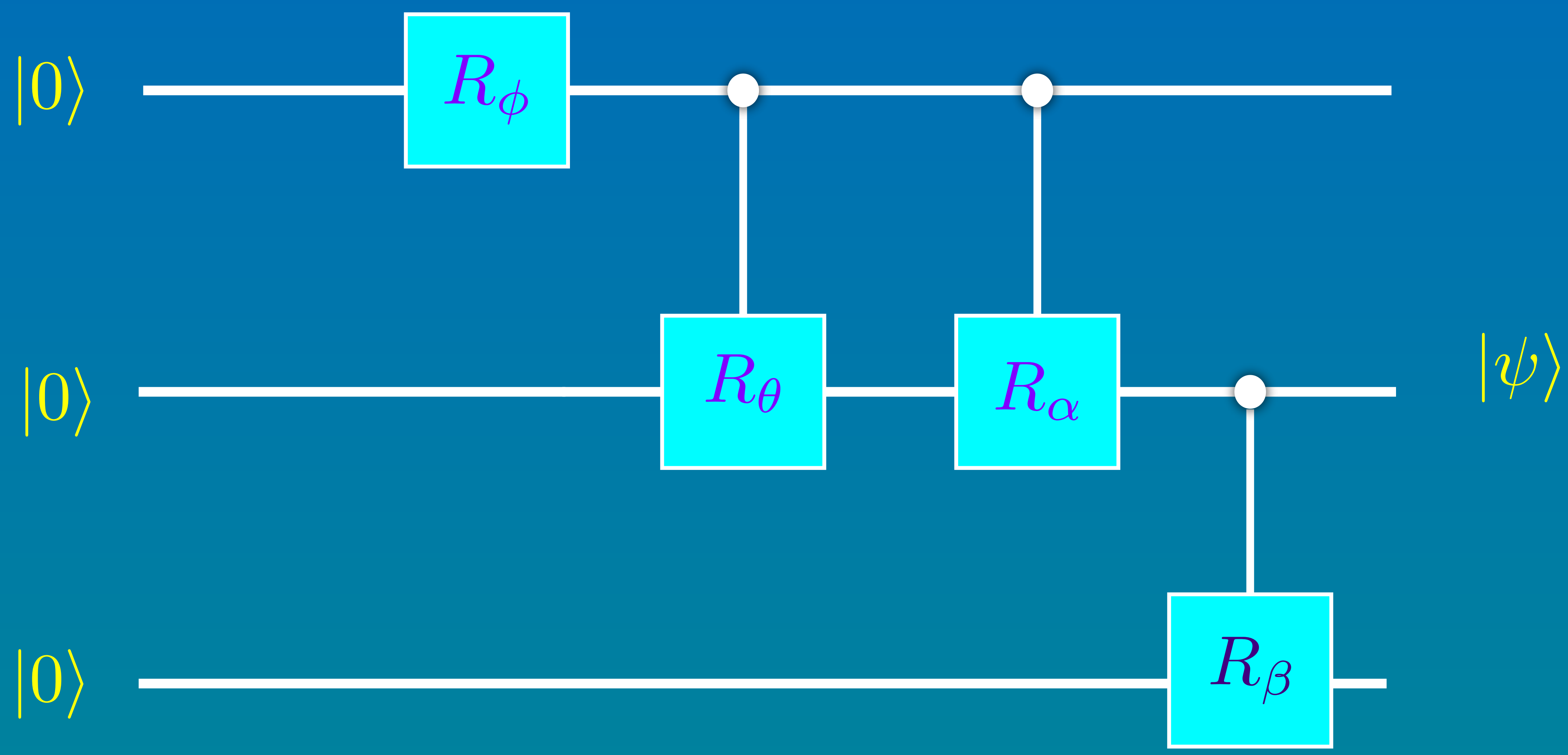


$$|\psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$$

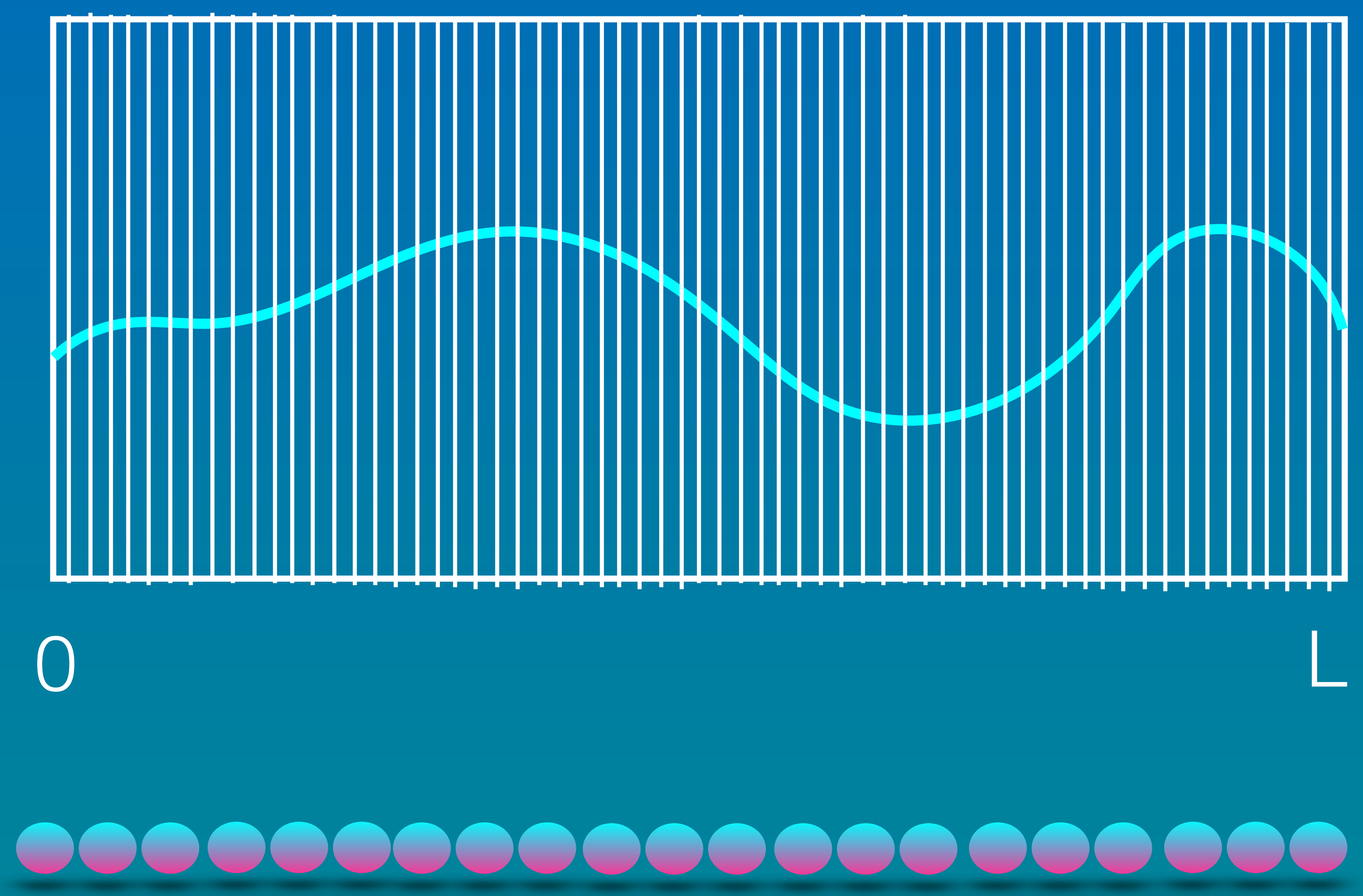
With 3 qubits, we can have 8 bins.



With 3 qubits

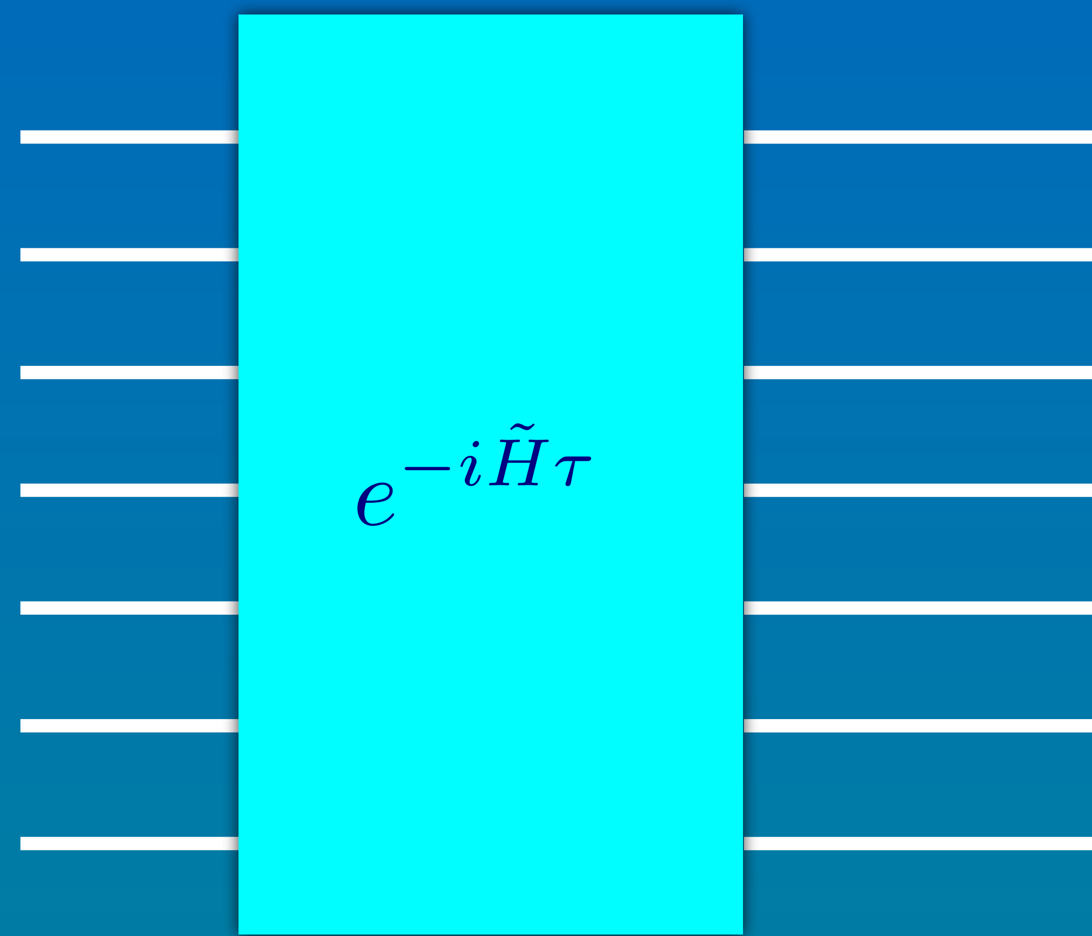

$|0\rangle$
$|0\rangle$
$|0\rangle$
R_ϕ
R_θ
R_α
R_β
$|\psi\rangle$

With 20 qubits, we can have 1 million bins.



$$2^{20} = 1048576 \approx 1,000,000$$

Dynamics



$$G(x_1, x_2, t) = k e^{i\frac{m}{2}\frac{(x_1 - x_2)^2}{\tau} - iV(x_1)\tau}$$

$$G(n_1, n_2, t) = \frac{1}{\sqrt{N}} e^{i\frac{m}{2}\frac{(n_1 - n_2)^2\Delta^2}{\tau} - iV(n_1\Delta)\tau}$$

$$G(n_1, n_2, t) = \frac{1}{\sqrt{N}} e^{-i\frac{m}{2}\frac{n^2\Delta^2}{\tau}+iV(n\Delta)\tau} \times \sum_{n'=0}^{N-1} e^{im\frac{nn'\Delta^2}{\tau}} \times e^{-im\frac{n'^2\Delta^2}{\tau}}$$

Diagonal

Fourier transform

Diagonal

But for one single particle or for a few particles,
we do not need quantum simulators.

The real power of quantum simulators, becomes apparent,
when we have many particles.

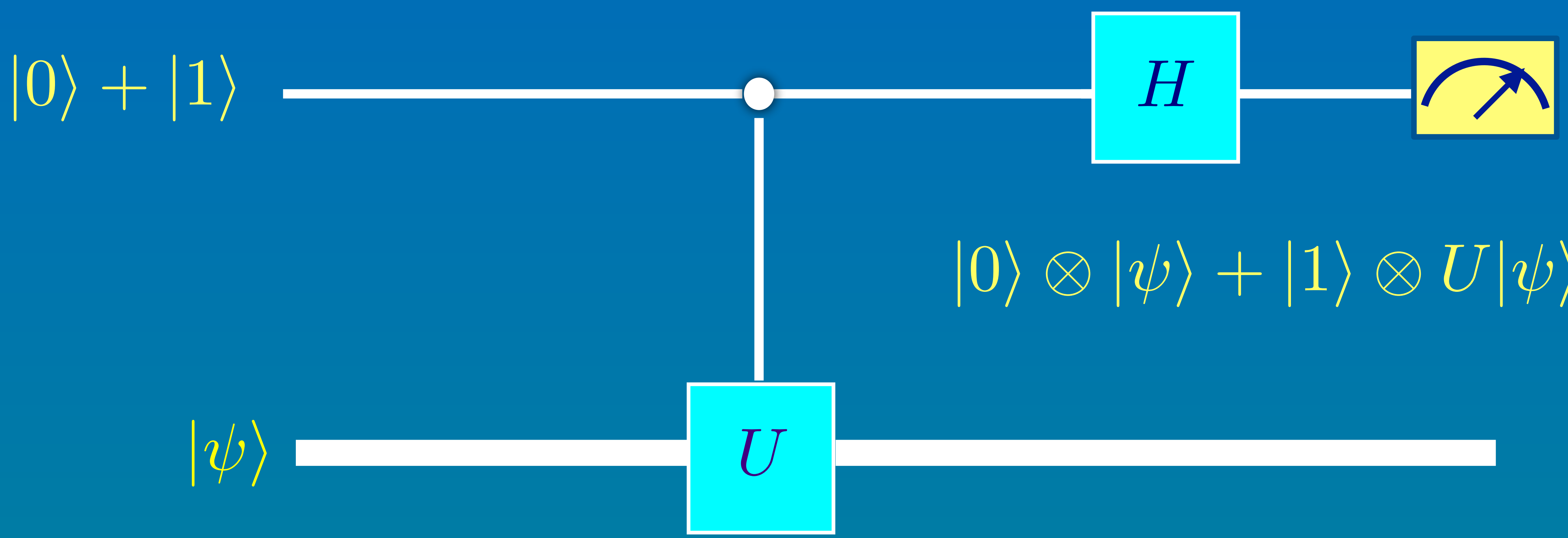
Efficient Simulation of Quantum Systems by Quantum Computers

Christoff Zalka

Universal Quantum Simulators

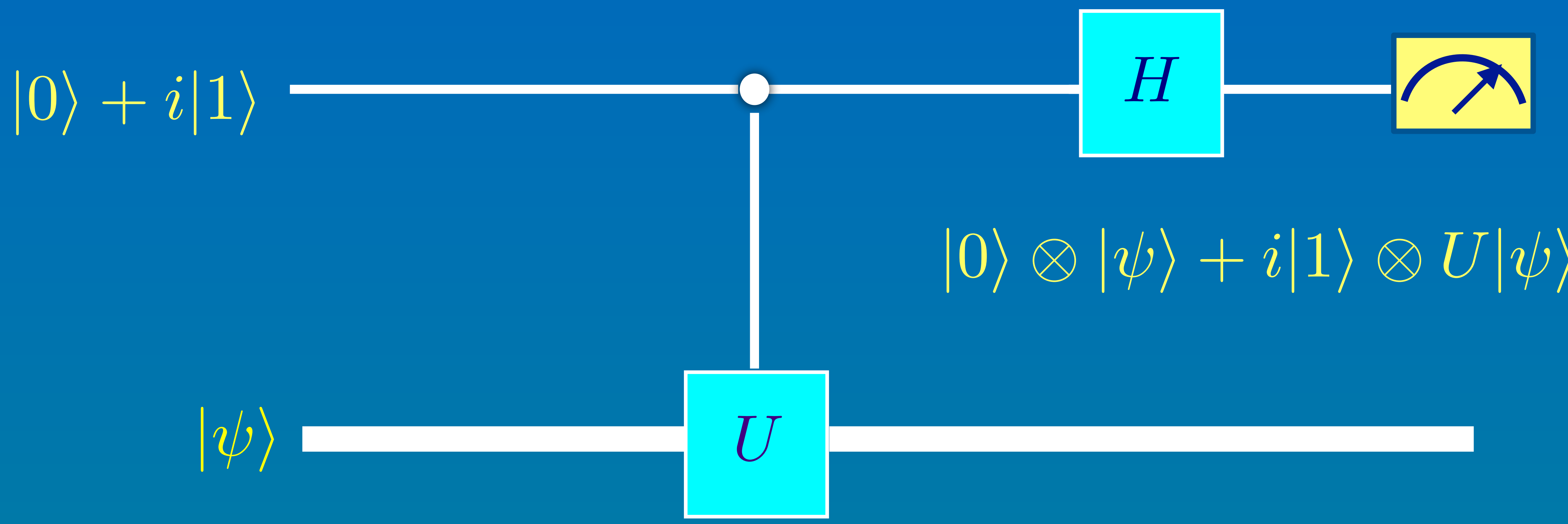
Seth Lloyd

Expectation Values



$$P(0) = \frac{1}{4}||(I + U)|\psi\rangle|| \qquad P(0) = \frac{1}{2}(1 + Re\langle\psi|U|\psi\rangle)$$

$$P(1) = \frac{1}{4}||(I - U)|\psi\rangle|| \qquad P(1) = \frac{1}{2}(1 - Re\langle\psi|U|\psi\rangle)$$

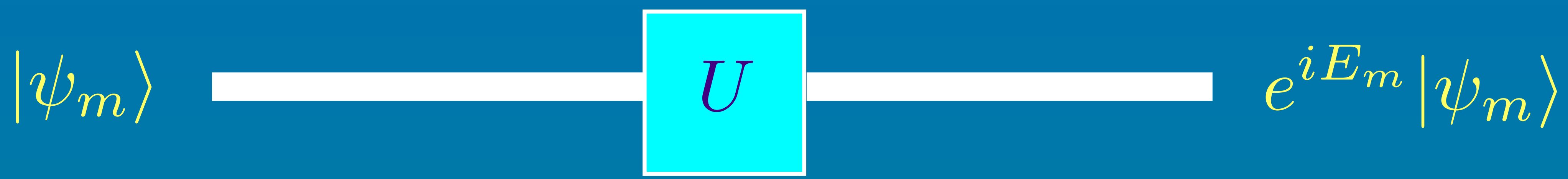


$$P(0) = \frac{1}{4}||(I + iU)|\psi\rangle||^2 \qquad P(0) = \frac{1}{2}(1 - Im\langle\psi|U|\psi\rangle)$$

$$P(1) = \frac{1}{4}||(I - iU)|\psi\rangle||^2 \qquad P(1) = \frac{1}{2}(1 + Im\langle\psi|U|\psi\rangle)$$

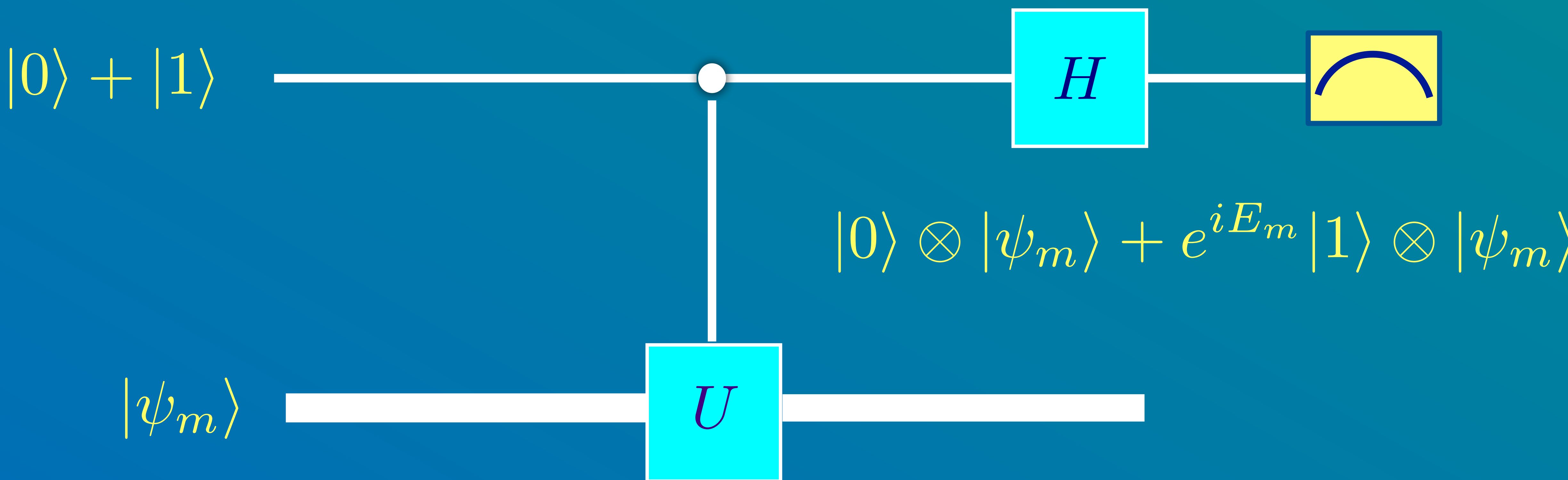
Finding the spectrum of a Hamiltonian

$$U = e^{iH}$$



$$H|\psi_m\rangle = E_m|\psi_m\rangle$$

$$U|\psi_m\rangle = e^{iE_m}|\psi_m\rangle$$

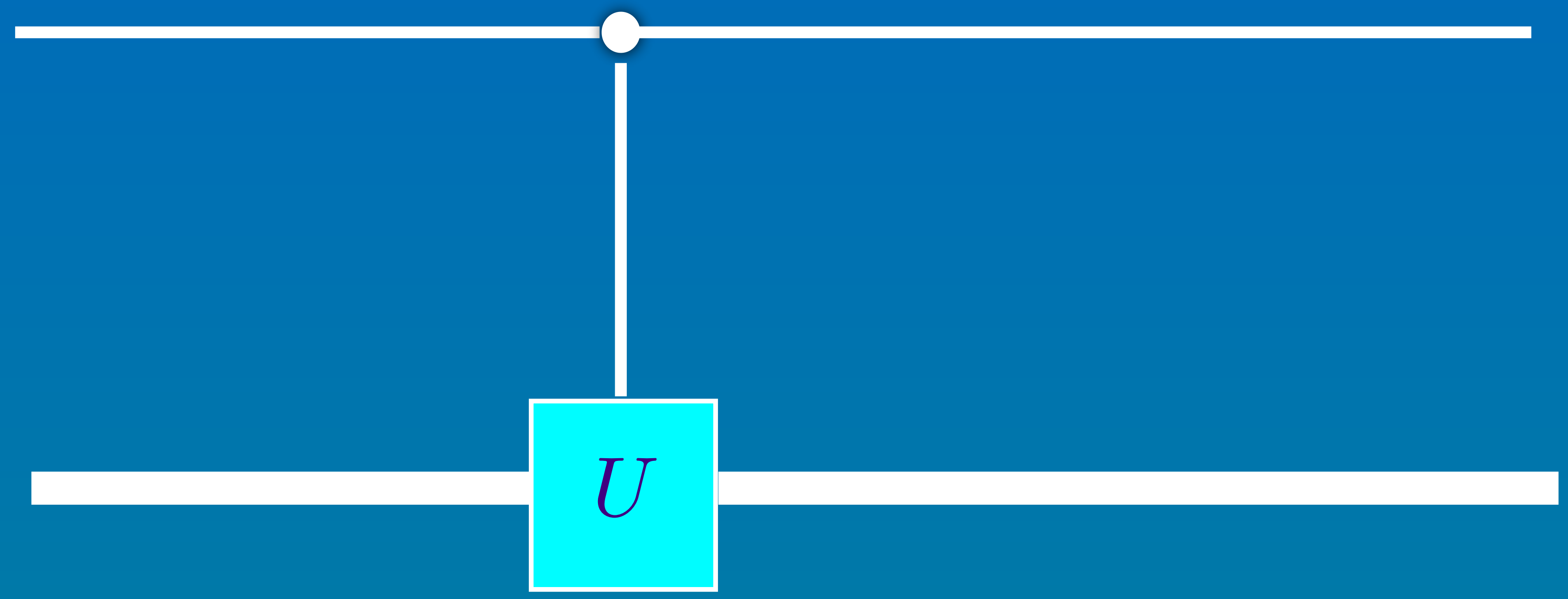


$$P(0) = \frac{1}{2}(1 + \cos E_m)$$

$$P(1) = \frac{1}{2}(1 - \cos E_m)$$

$$\frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}|k\rangle$$

$$\sum_m \alpha_m|\psi_m\rangle$$



$$\sum_{m,k}\alpha_m|k\rangle\otimes U^k|\psi_m\rangle$$

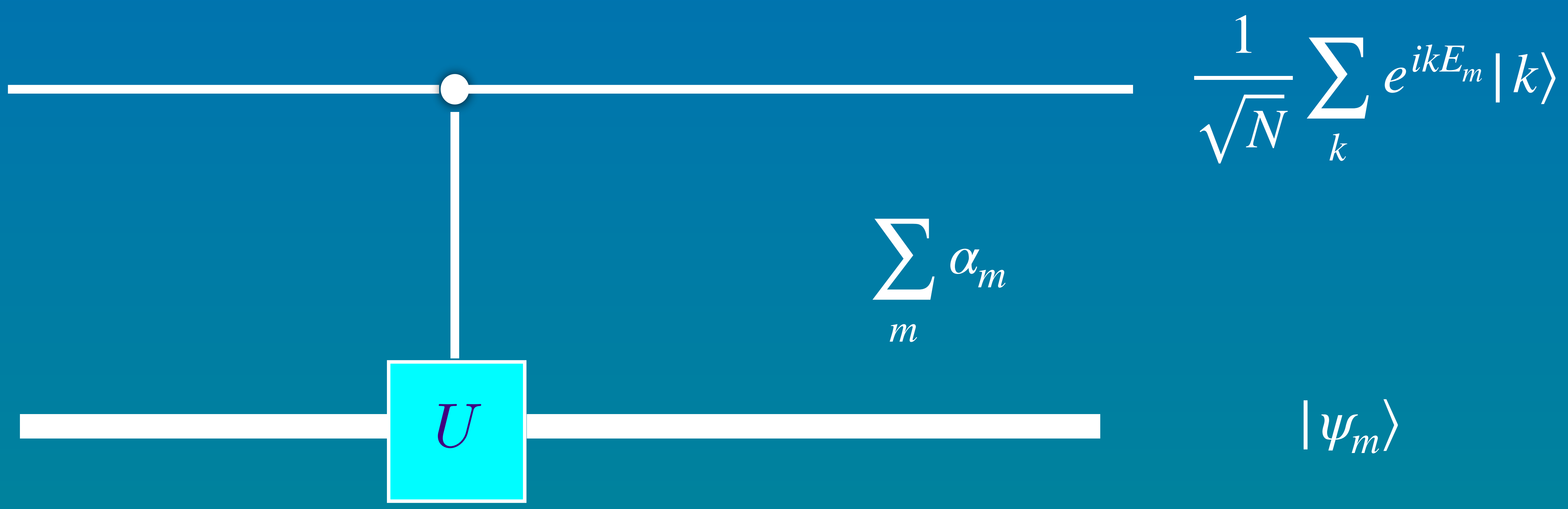
$$\frac{1}{\sqrt{N}}\sum_{k,m}\alpha_m|k\rangle\otimes e^{ikE_m}|\psi_m\rangle$$

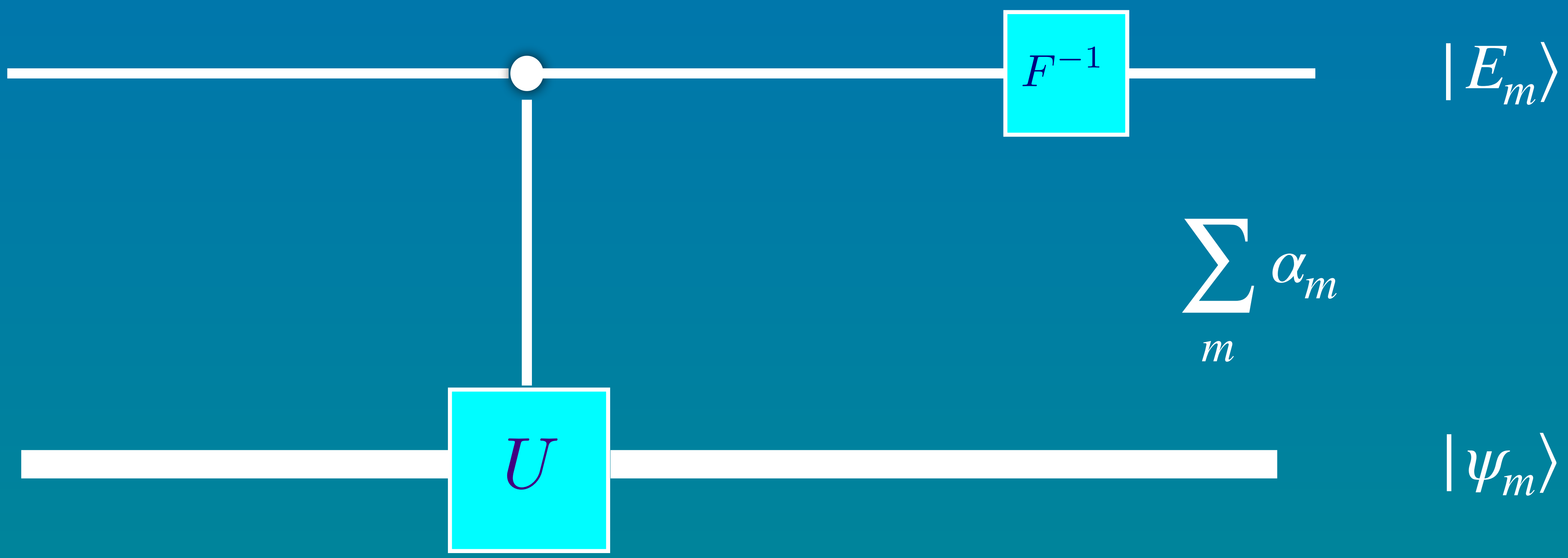
$$\frac{1}{\sqrt{N}}\sum_{k,m}\alpha_m|k\rangle\otimes e^{ikE_m}|\psi_m\rangle$$

$$=$$

$$\frac{1}{\sqrt{N}}\sum_{m}\alpha_m(\sum_{k}e^{ikE_m}|k\rangle)\otimes|\psi_m\rangle$$

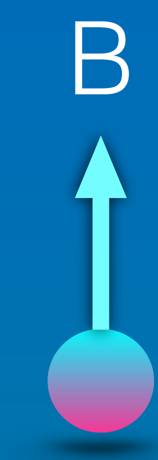
$$\frac{1}{\sqrt{N}} \sum_m \alpha_m \left(\sum_k e^{ikE_m} |k\rangle \right) \otimes |\psi_m\rangle$$

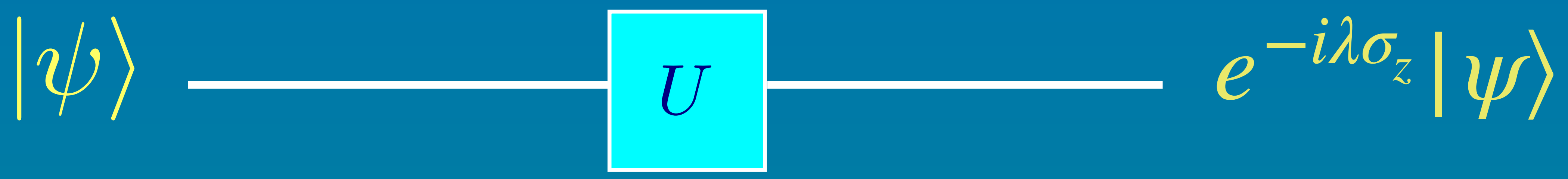



F^{-1}
$|E_m\rangle$
$\sum_m \alpha_m$
U
$|\psi_m\rangle$

A2-Digital Simulation of spin systems

a spin in a magnetic field

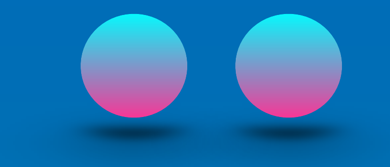




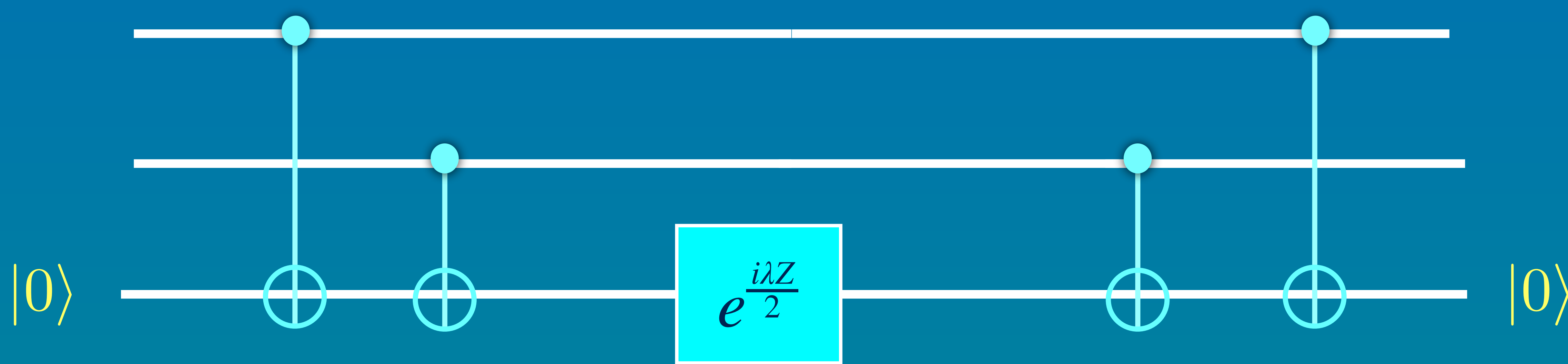
$$H = -\mu B \sigma_z$$

$$U = e^{-i\lambda\sigma_z}$$

Two interacting spins

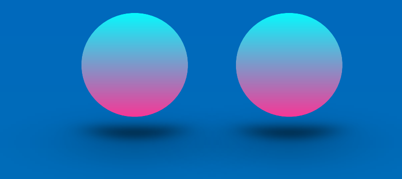


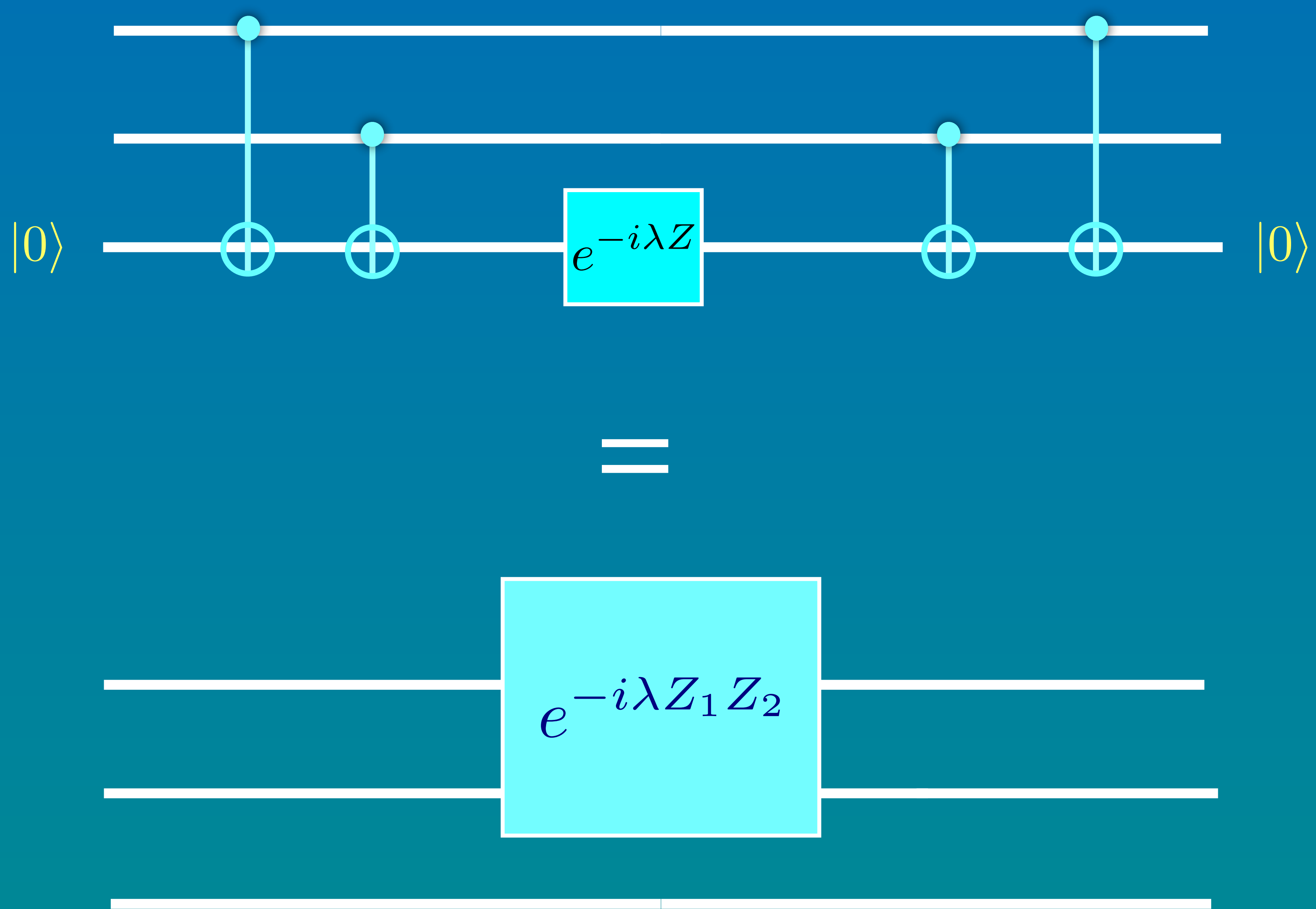
$$H = -J Z_1 Z_2$$



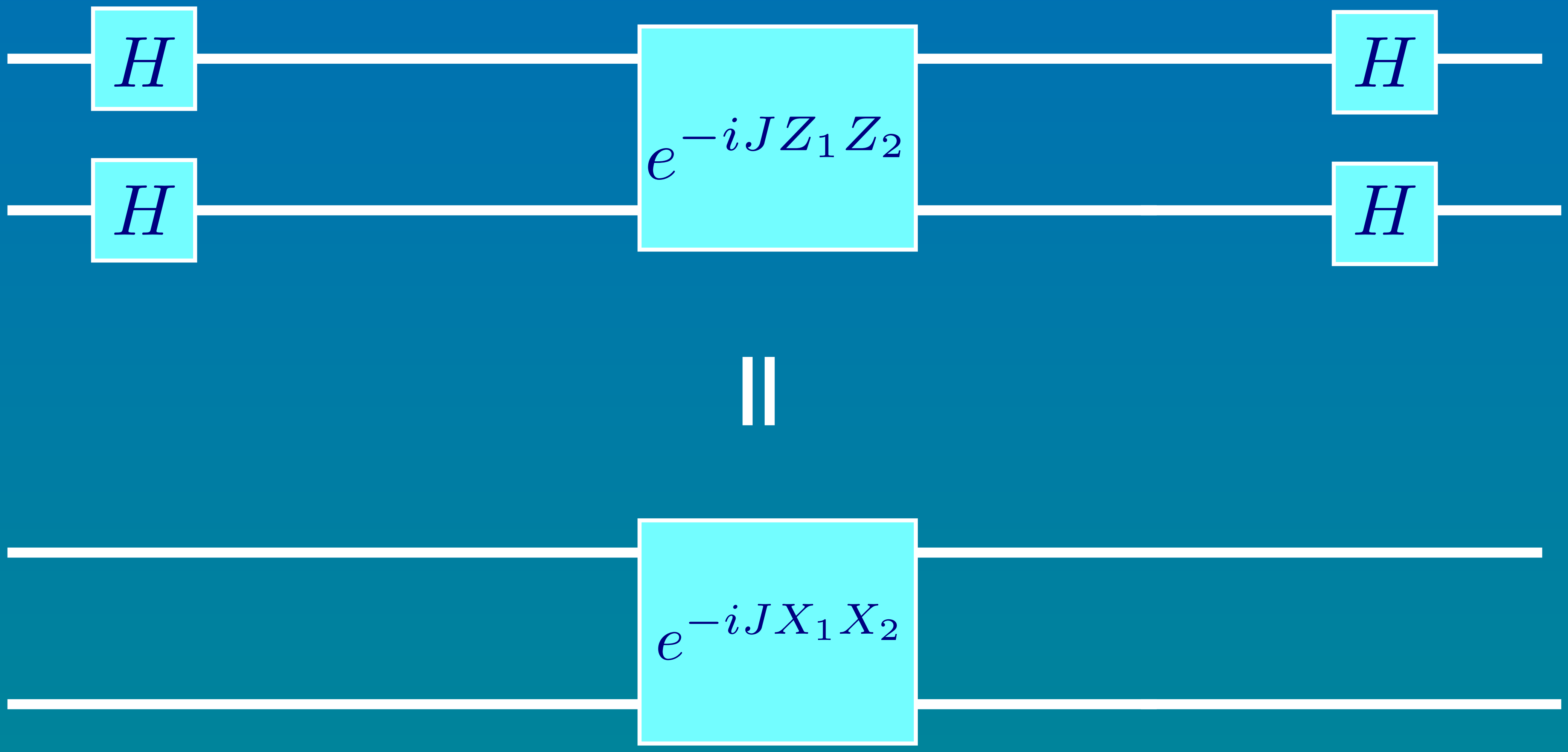
The clue → $m \oplus n = m + n - 2mn$

$$H = -JZ_1Z_2$$

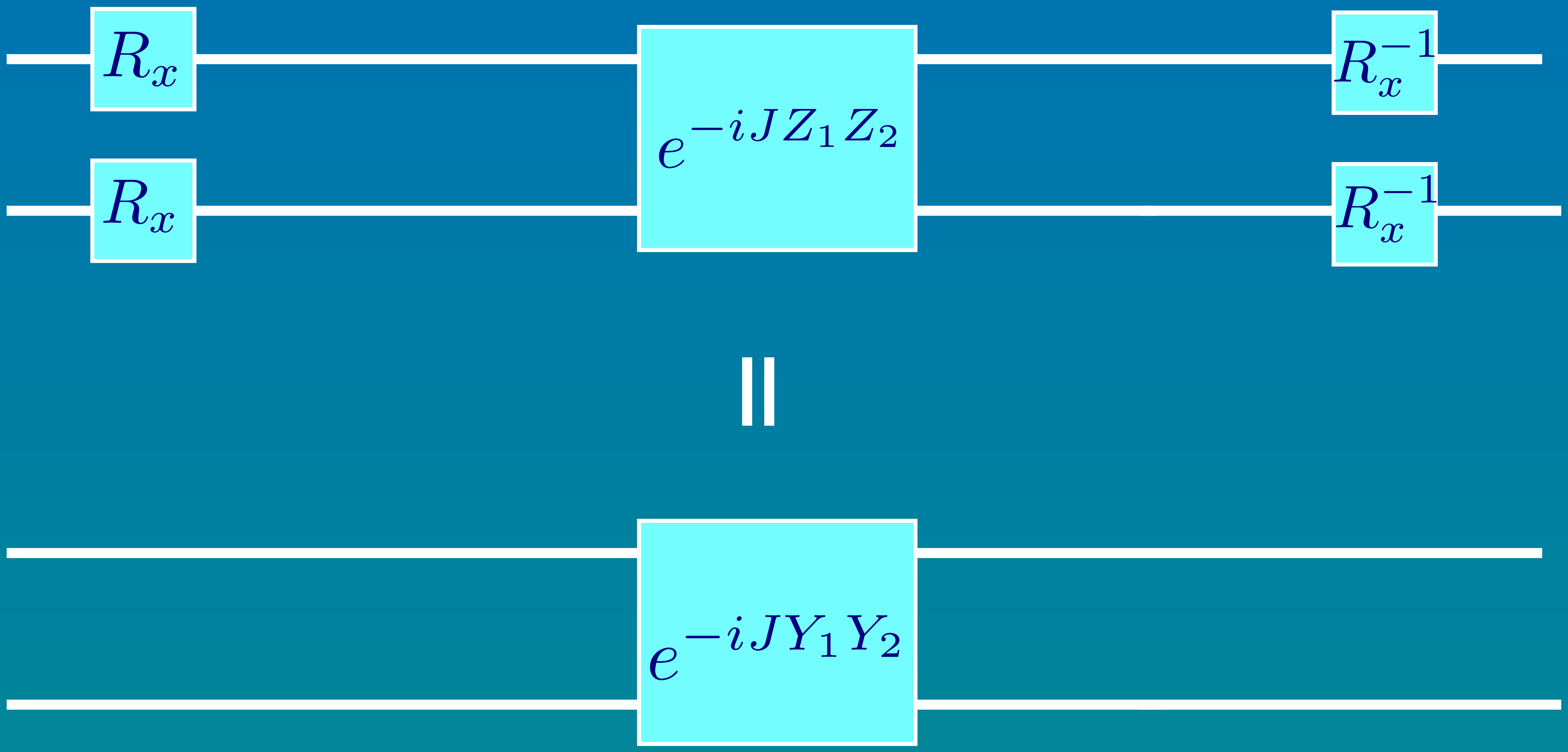




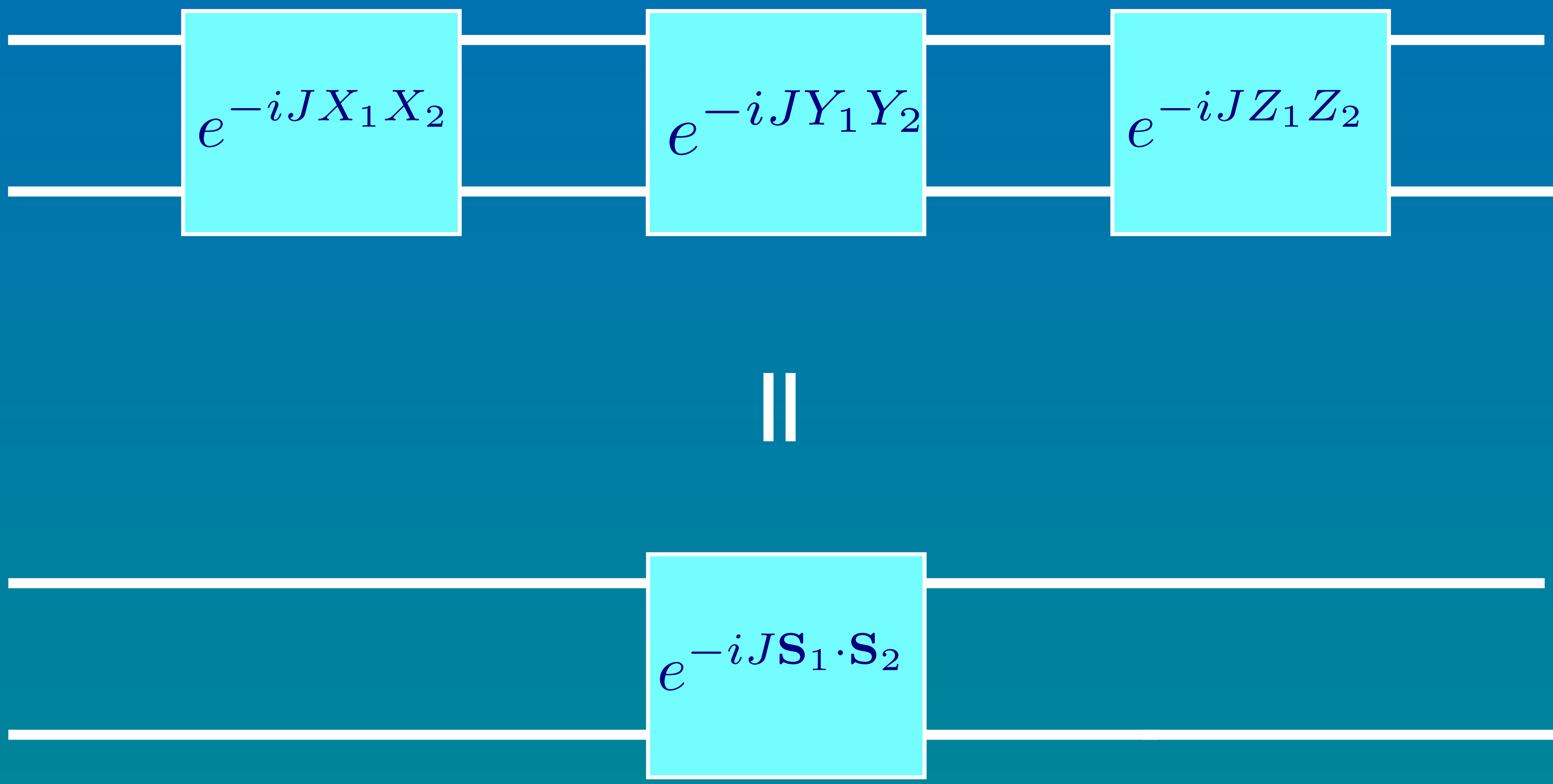
$$H = -JX_1X_2$$



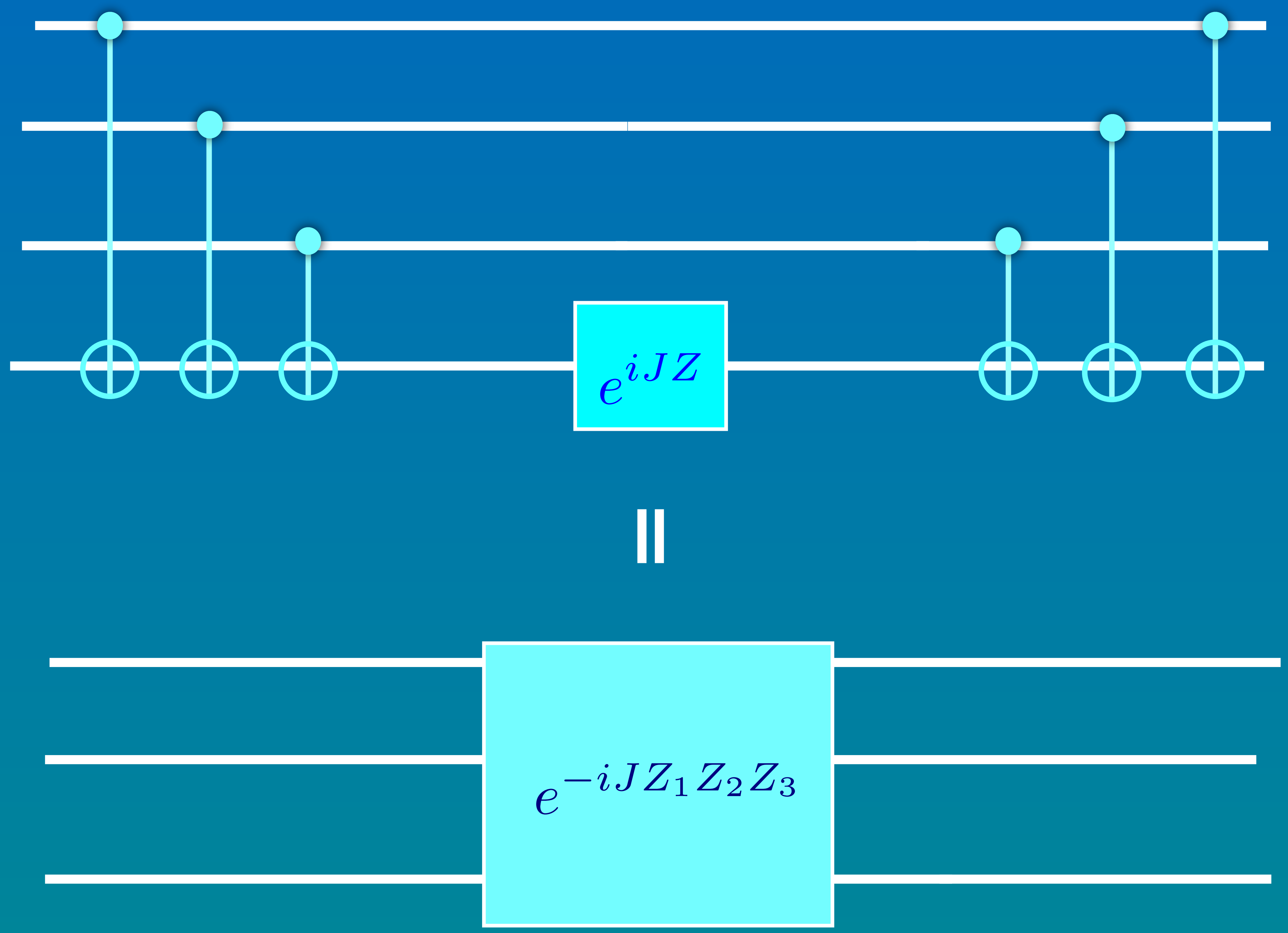
$$H = -JY_1Y_2$$



$$H = -J\mathbf{S}_1 \cdot \mathbf{S}_2$$

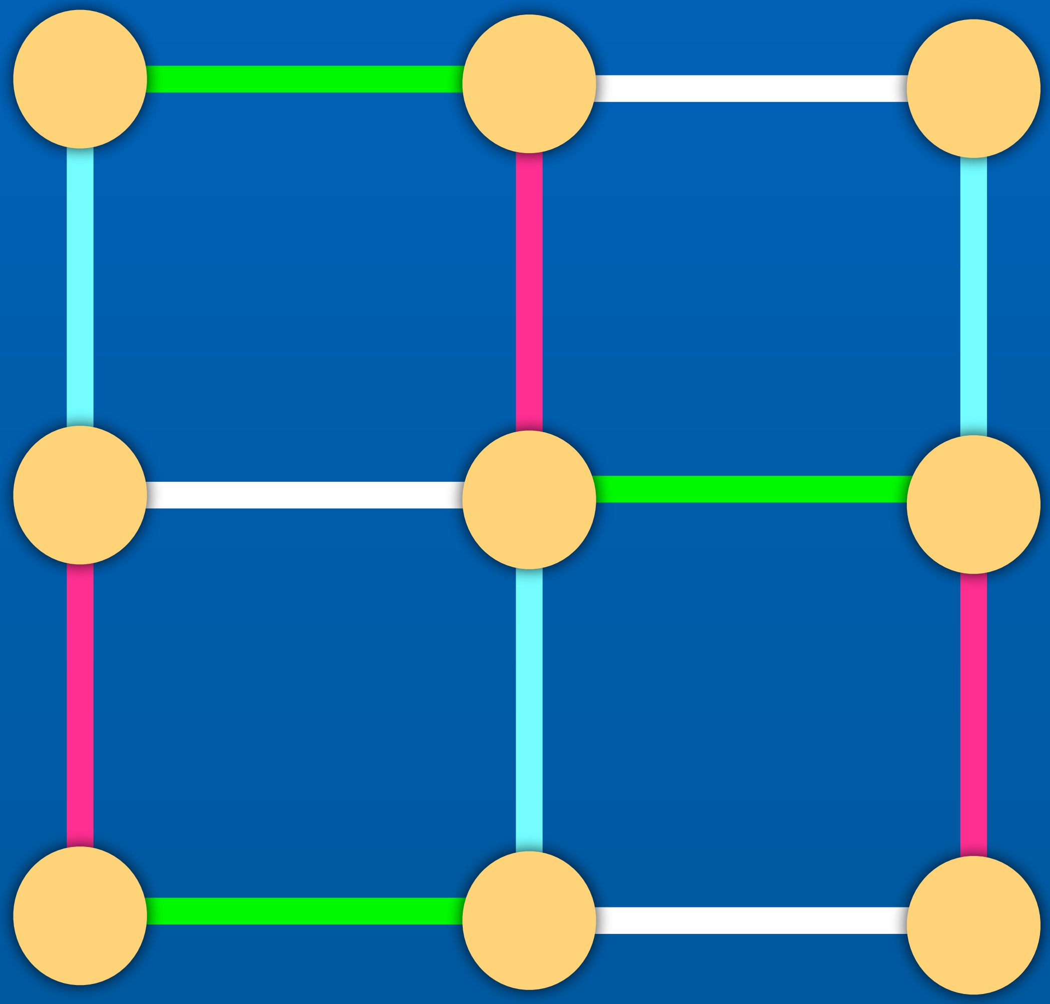


Three interacting spins and more!



Why do we need these types of gates?

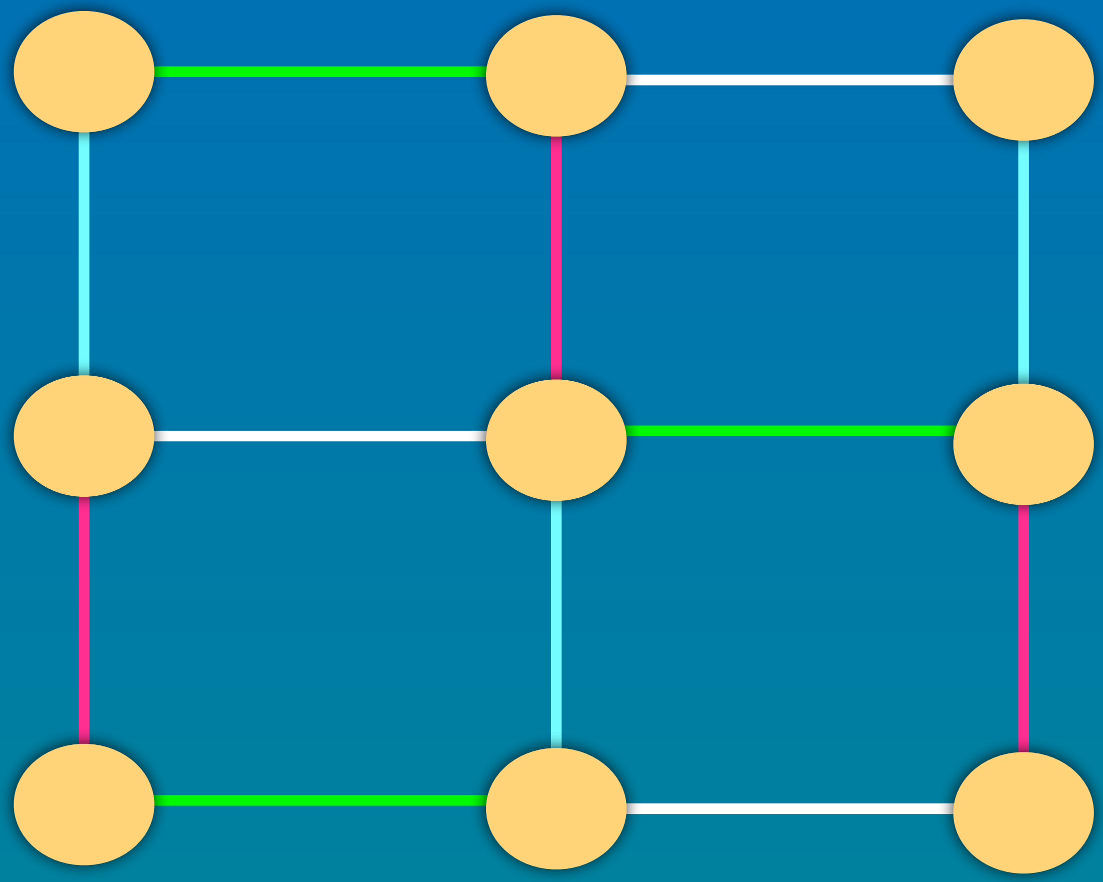
تجزیه هامیلتونی به جملاتی که با هم جابجا می شوند



$$H = H_1 + H_2 + H_3 + H_4$$

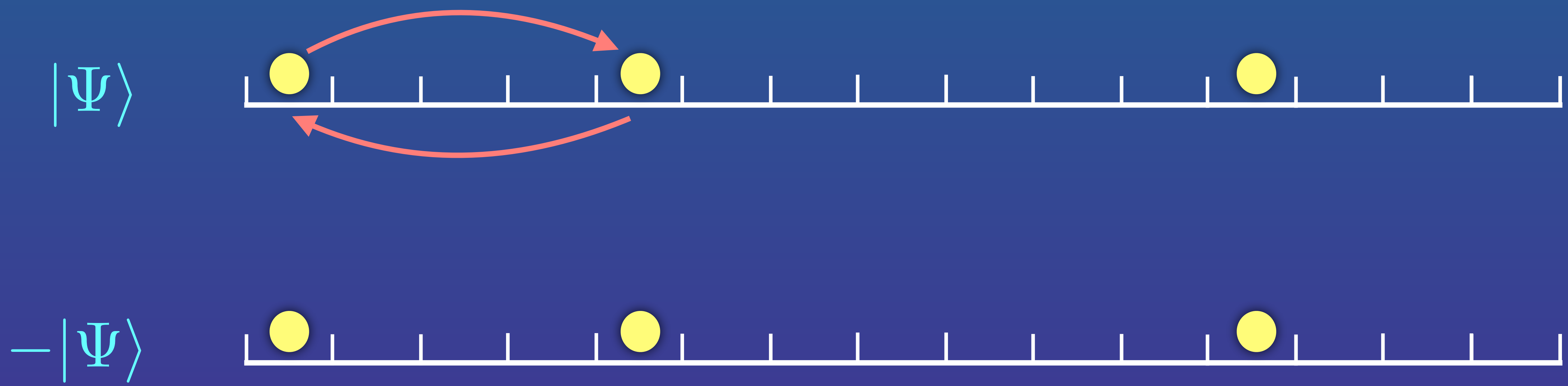
Suzuki-Trotter Formula

$$e^{A}e^{B} = e^{A+B+\frac{1}{2}\{A,B\}+\cdots}$$



$$e^{H_1+H_2} = \left(e^{\frac{H_1}{N}}e^{\frac{H_2}{N}}\right)^N$$

c-Digital Simulation of Fermions



$$\{c_i, c_j\} = 0 \qquad \{c_i^\dagger, c_j^\dagger\} = 0 \qquad \{c_i, c_j^\dagger\} = \delta_{i,j}$$

Hubbard Model

$$H = -t \sum_{i,\sigma} c^{\dagger}_{i,\sigma} c_{i+1,\sigma} + c^{\dagger}_{i+1,\sigma} c_{i,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i\downarrow} \qquad \sigma = \uparrow, \downarrow$$

$c^{\dagger}_{i+1,\sigma} c_{i,\sigma}$

$c^{\dagger}_{i,\sigma} c_{i+1,\sigma}$

Hopping terms

Jordan-Wigner Transformation

$$c_i = z_1 z_2 \cdots z_{i-1} \sigma_i^-$$

$$c_i^\dagger = z_1 z_2 \cdots z_{i-1} \sigma_i^+$$

$$c_i^\dagger |0\rangle$$

How to create a fermion?

$$e^{i\frac{\pi}{2}(c+c^\dagger)}$$

$$(c+c^\dagger)^2 = cc^\dagger + c^\dagger c = 1$$

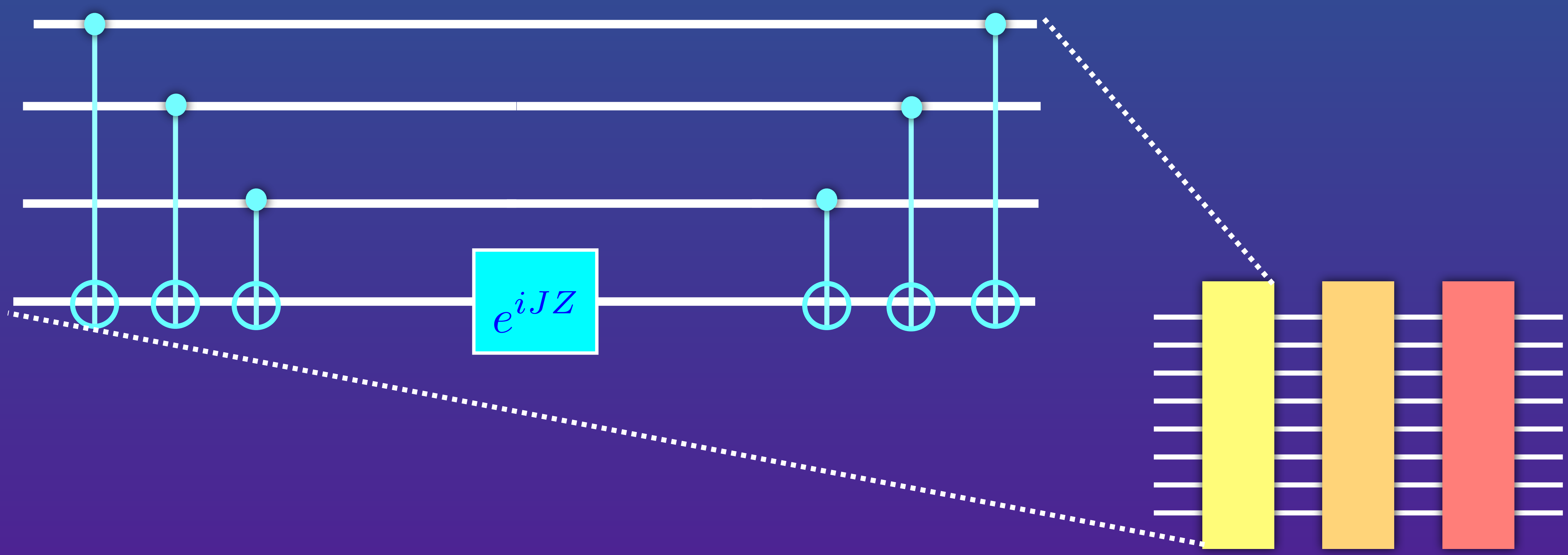
$$= \cos\frac{\pi}{2} I + i\sin\frac{\pi}{2}(c+c^\dagger) \;= i(c+c^\dagger)$$

$$e^{i\frac{\pi}{2}(c_j+c_j^\dagger)}|0\rangle \equiv c_j^\dagger|0\rangle$$

$$|\Psi\rangle = c^\dagger_{j_1} c^\dagger_{j_2} \cdots c^\dagger_{j_n} |0\rangle$$

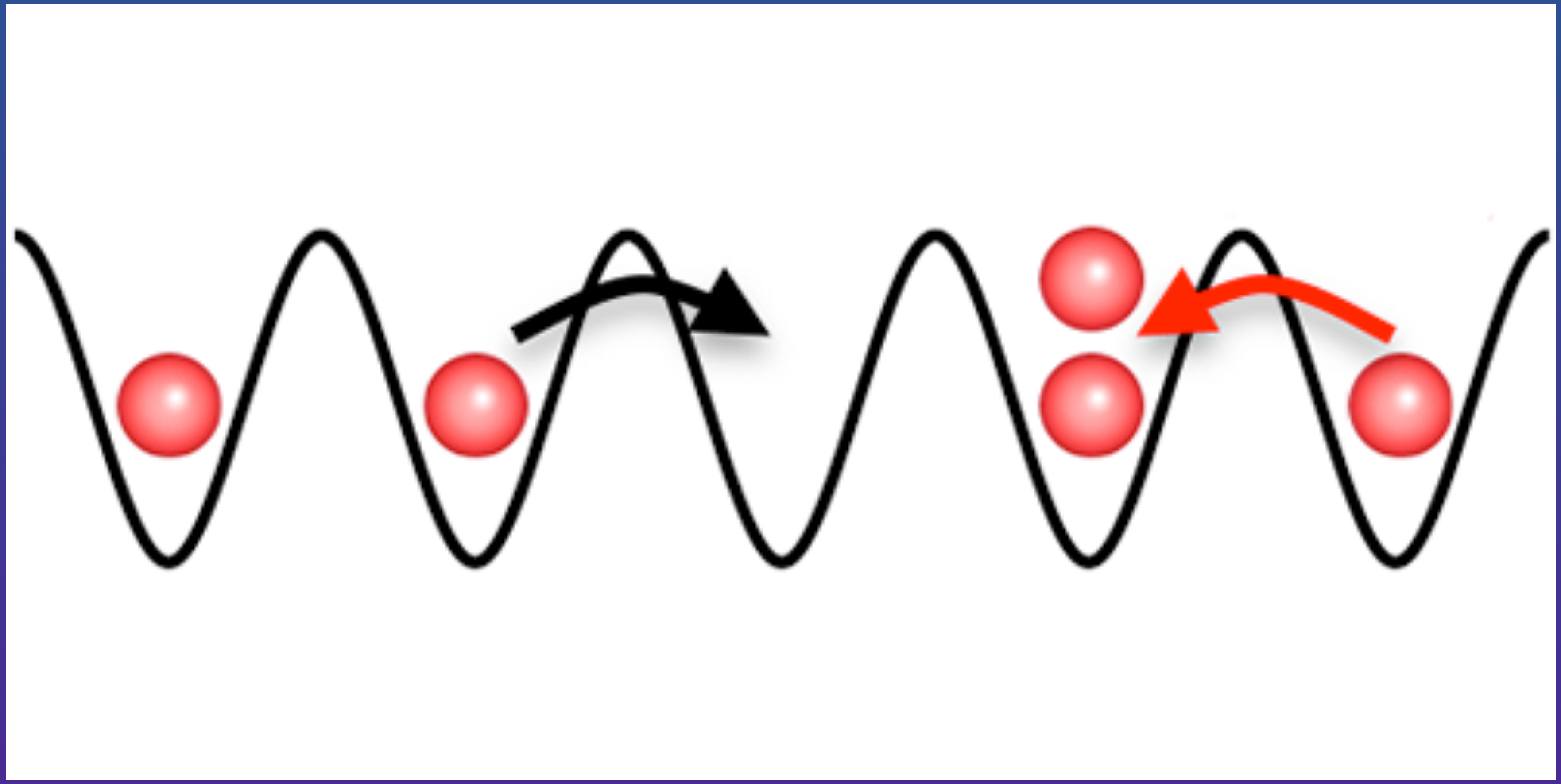
$$= e^{i\frac{\pi}{2}(c_{j_1}+c^\dagger_{j_1})} \ldots e^{i\frac{\pi}{2}(c_{j_n}+c^\dagger_{j_n})} |0\rangle$$

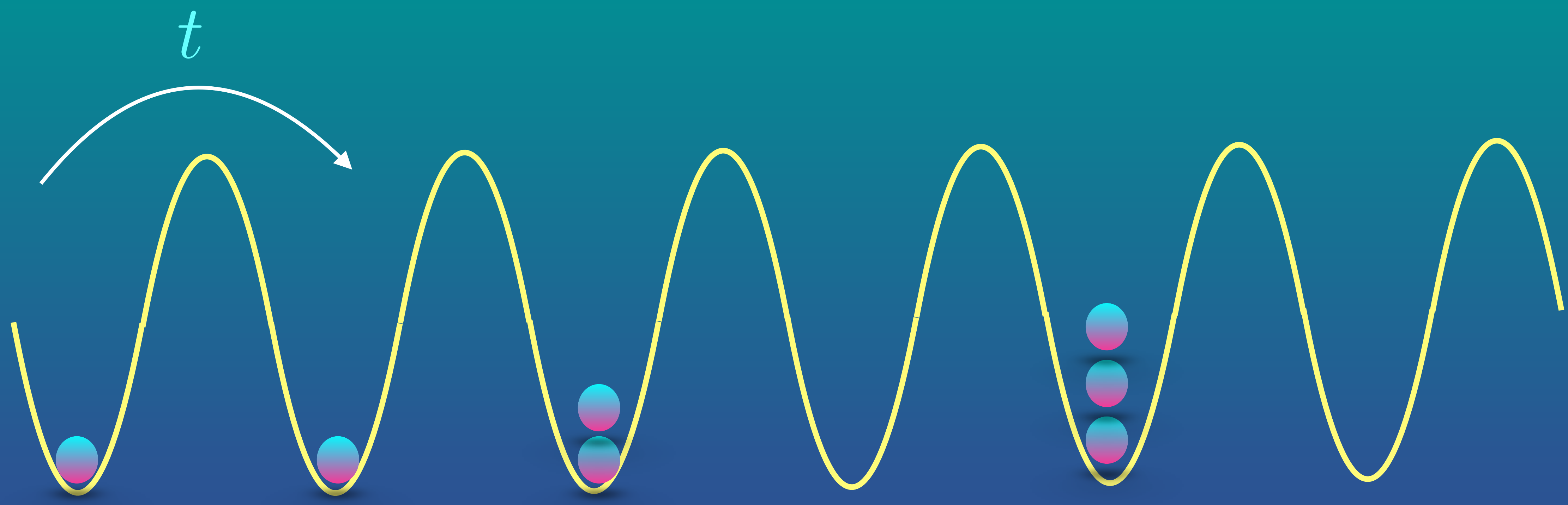
$$e^{i\frac{\pi}{2}(c_j+c^\dagger_j)} = e^{i\frac{\pi}{2} z_1 z_2 \cdots z_{j-1}\sigma_x}$$



d-Digital Simulation of Bosons

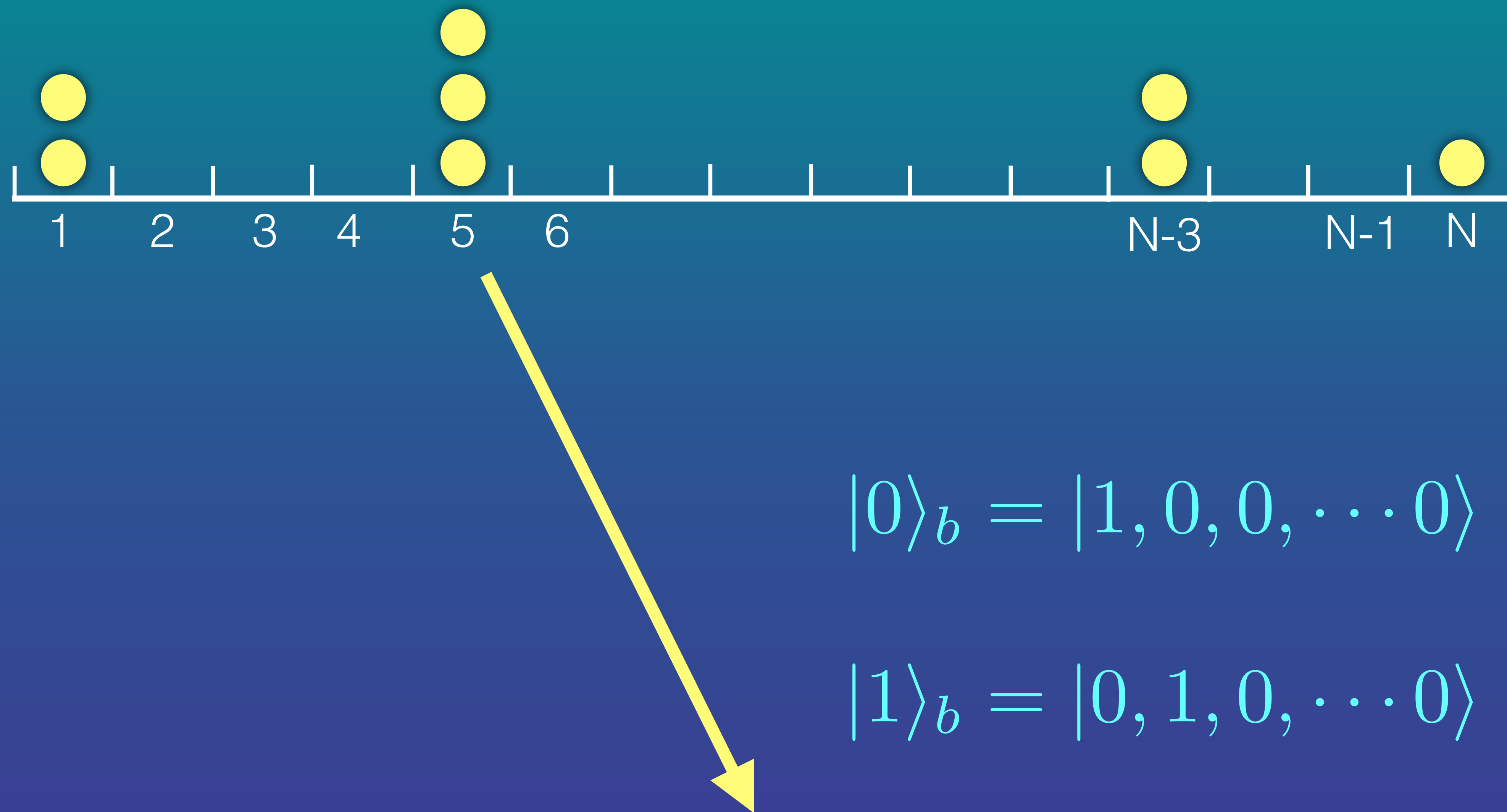
Bose-Hubbard Model,…





$$H = t\sum_{\langle i,j\rangle} b_i^\dagger b_j + \sum_i \epsilon_i n_i + \sum_i n_i(n_i - 1)$$

The Bose-Hubbard Hamiltonian



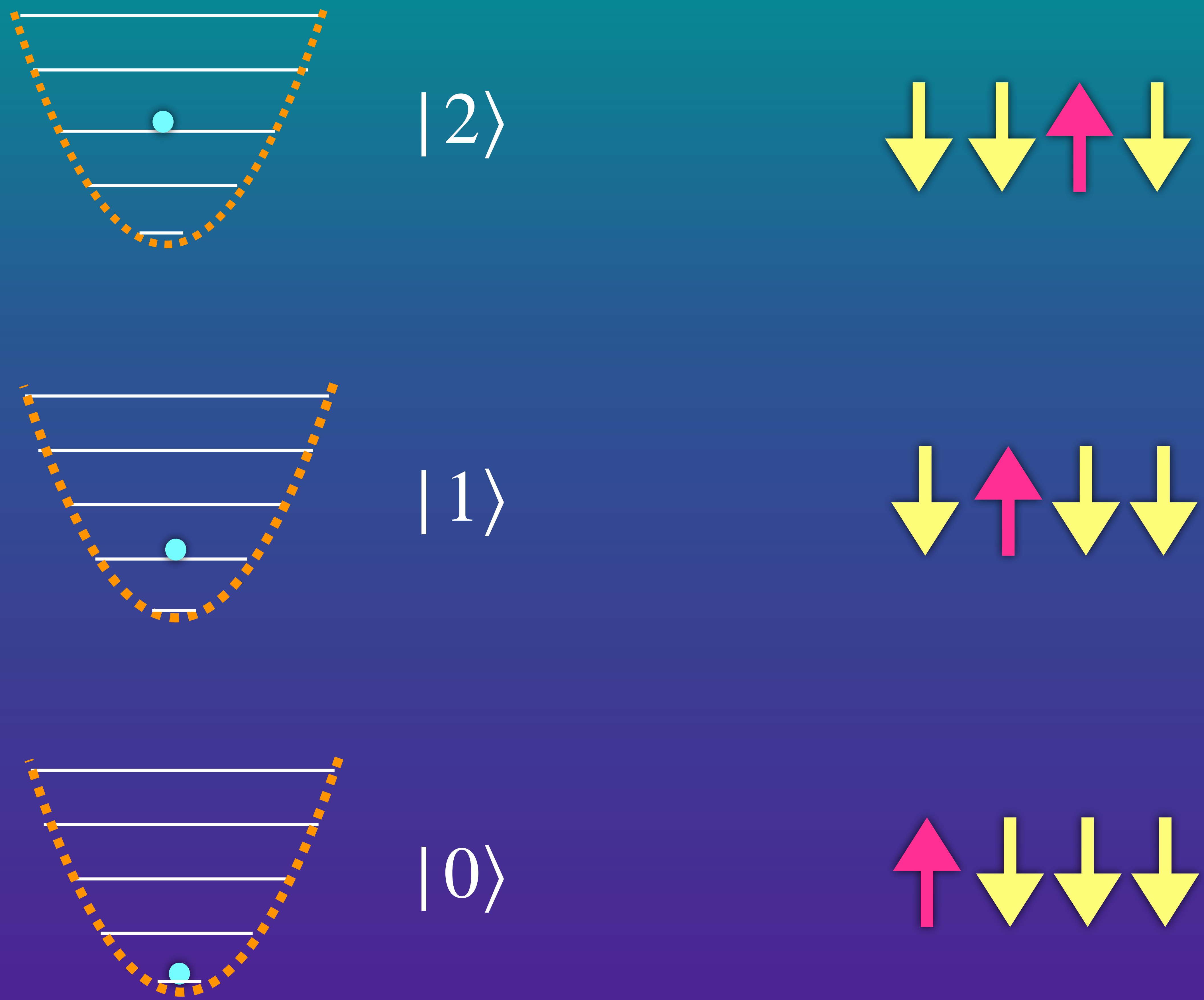
$$|0\rangle_b = |1, 0, 0, \cdots 0\rangle$$

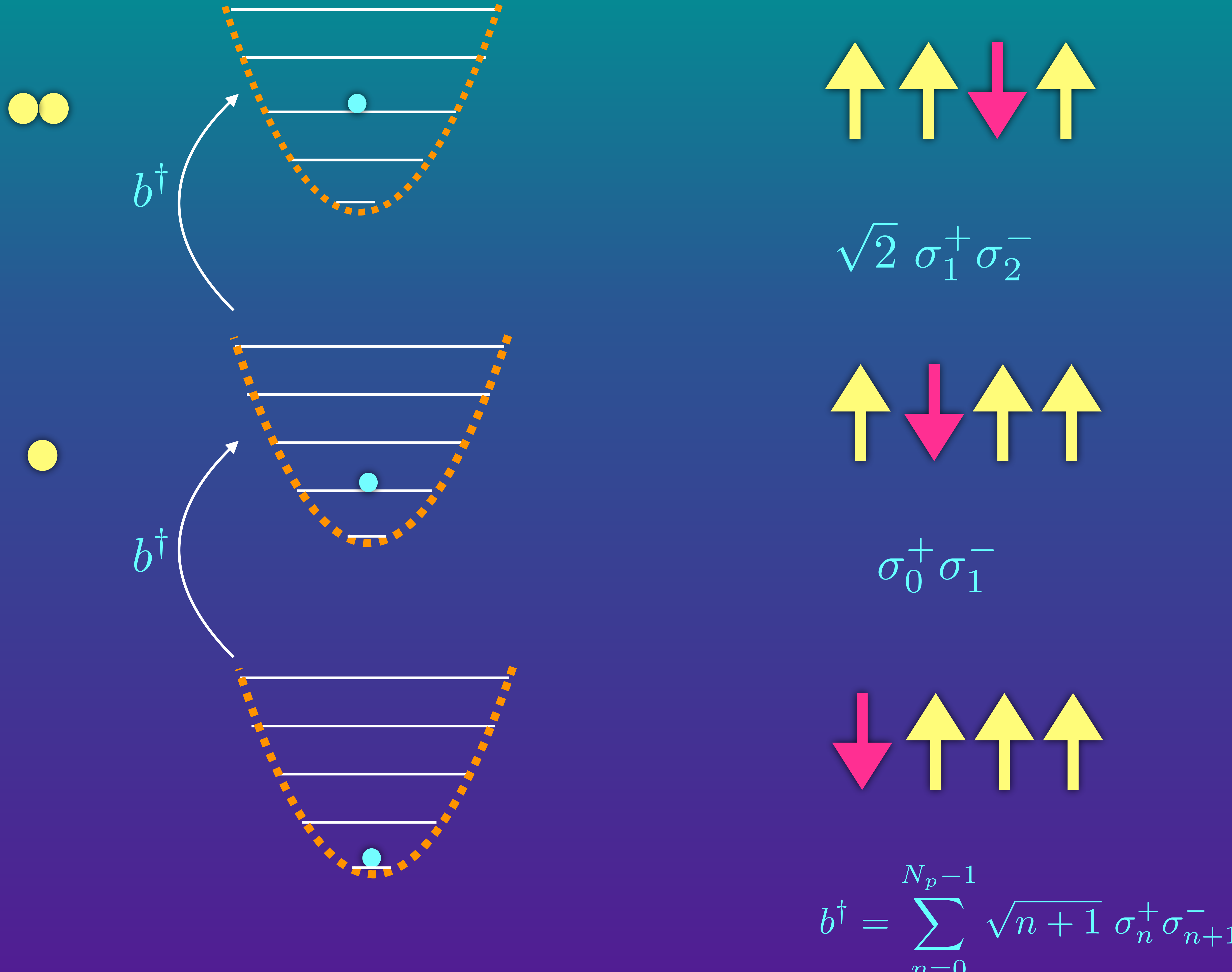
$$|1\rangle_b = |0, 1, 0, \cdots 0\rangle$$

$$|2\rangle_b = |0, 0, 1, \cdots 0\rangle$$

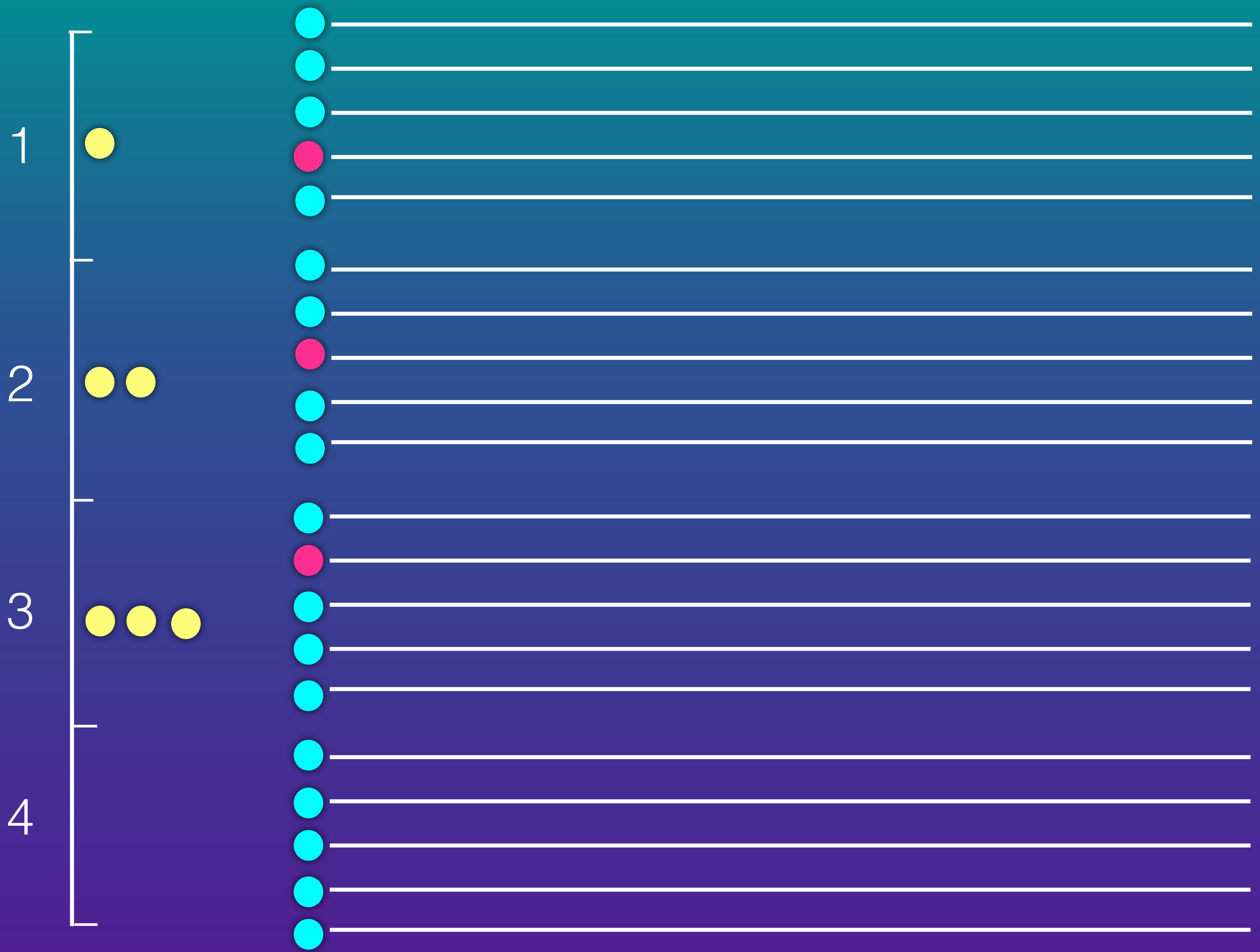
$$\cdots\cdots\cdots$$

$$|N\rangle_b = |0, 0, 0, \cdots 1\rangle$$


$|2\rangle$
$|1\rangle$
$|0\rangle$

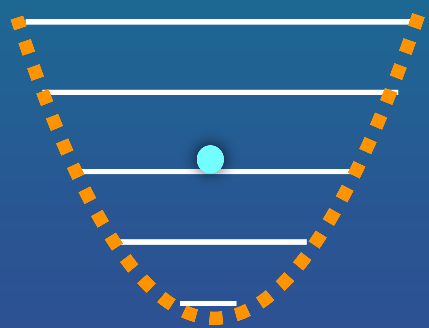


$b^\dagger$
$b^\dagger$
$\sqrt{2}\,\sigma_1^+\sigma_2^-$
$\sigma_0^+\sigma_1^-$
$b^\dagger = \sum_{n=0}^{N_p-1} \sqrt{n+1}\,\sigma_n^+\sigma_{n+1}^-$



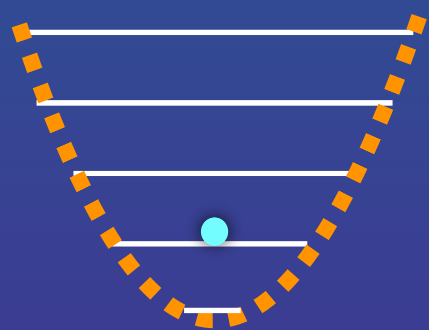
1
2
3
4

How to simulate the number operator?



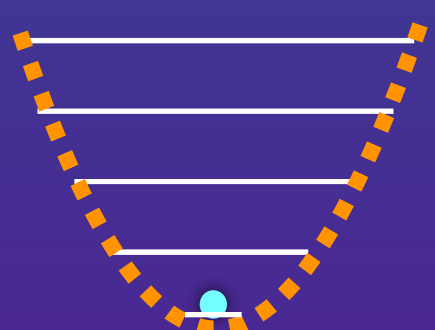
$|2\rangle$

$\hat{n}|2\rangle = 2|2\rangle$

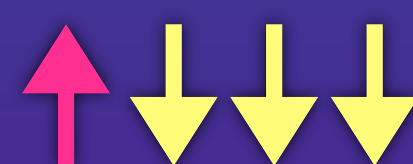


$|1\rangle$

$\hat{n}|1\rangle = |1\rangle$



$|0\rangle$

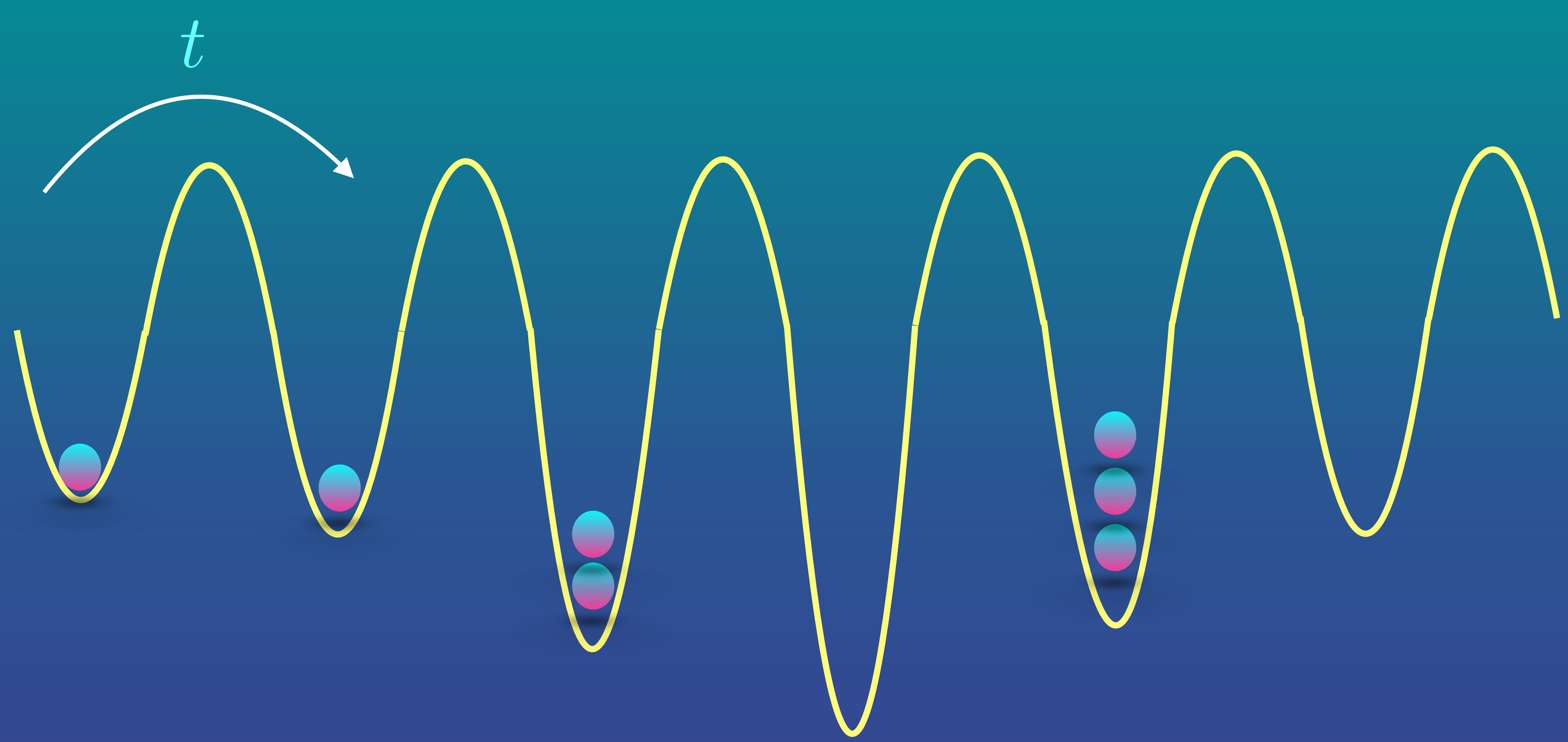


$\hat{n}|0\rangle = 0$

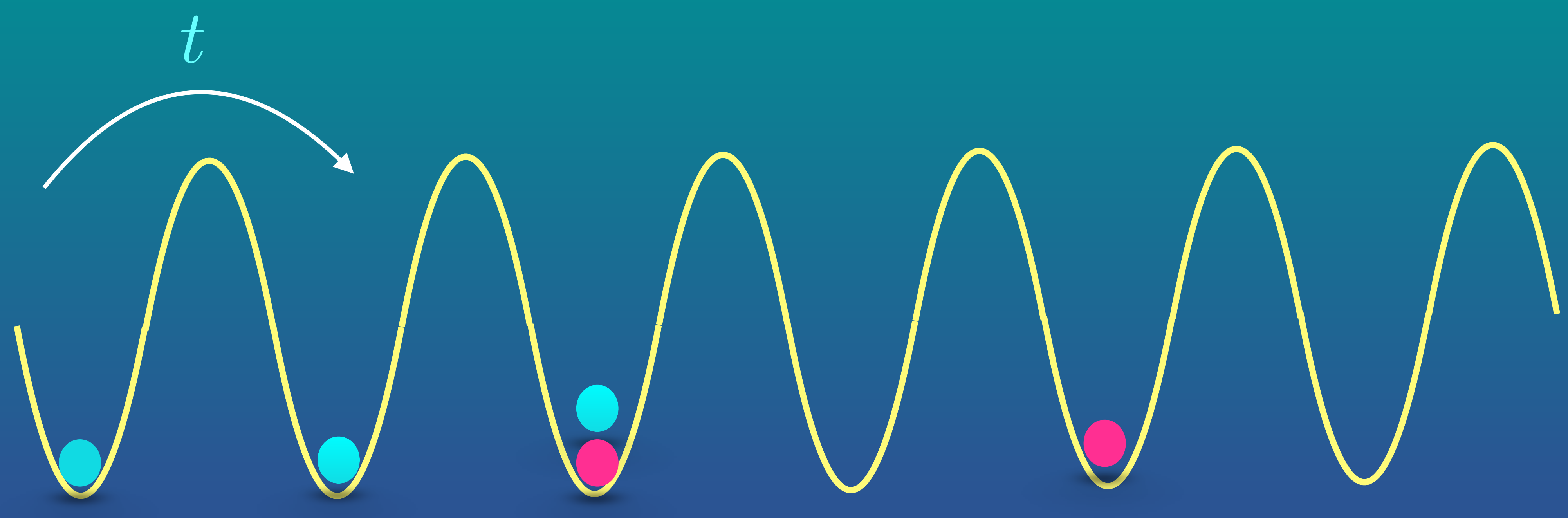
How to simulate the number operator?

$$Z|\downarrow\rangle = -|\downarrow\rangle \qquad Z|\uparrow\rangle = |\uparrow\rangle$$

$$\hat{n} = \sum_{k=0}^{l} k \, \frac{1 + Z_k}{2}$$

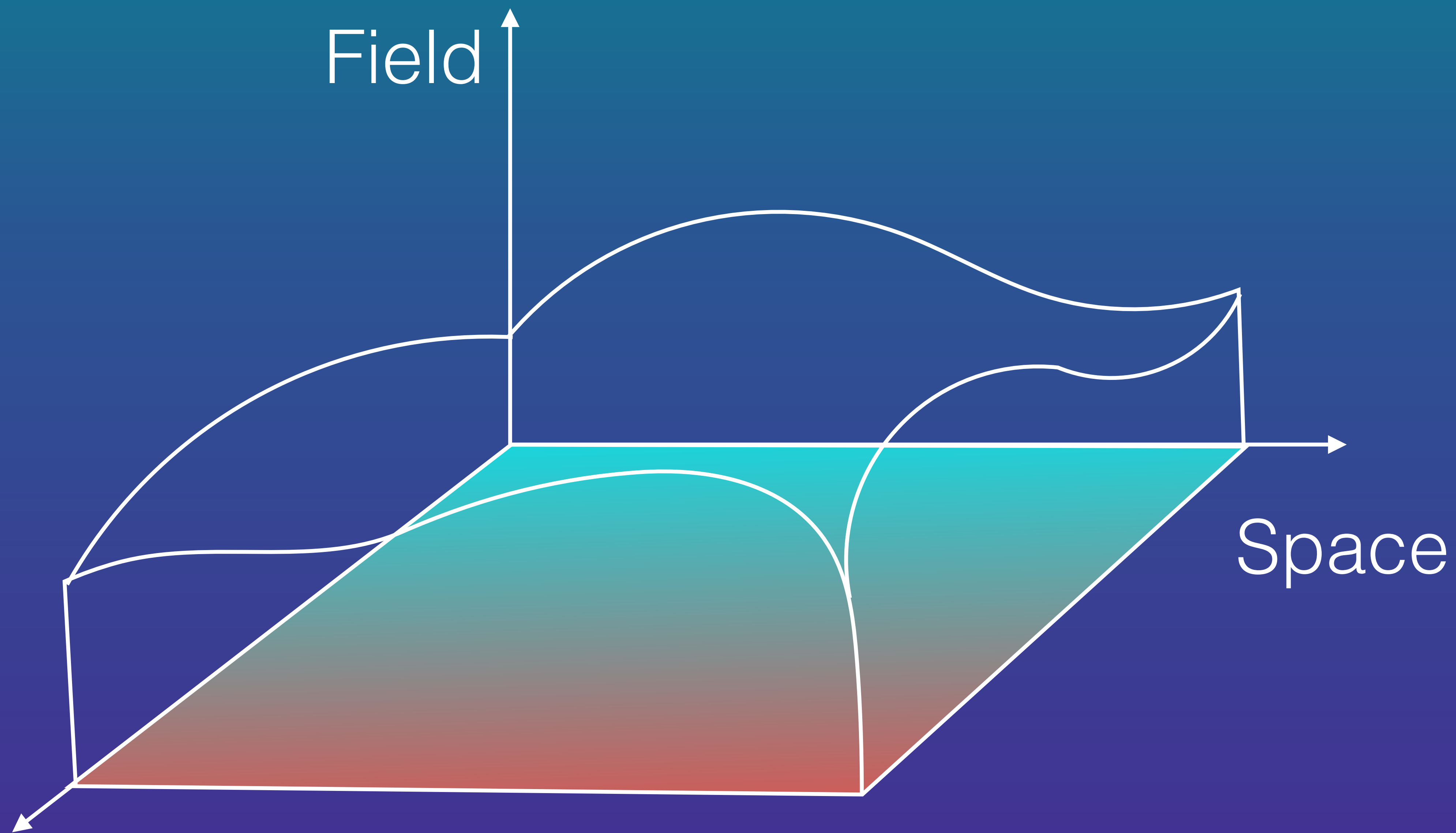


$$H = \sum_{\langle i,j \rangle} b_i^\dagger b_j + \sum_i \epsilon_i n_i + \sum_i n_i(n_i - 1)$$



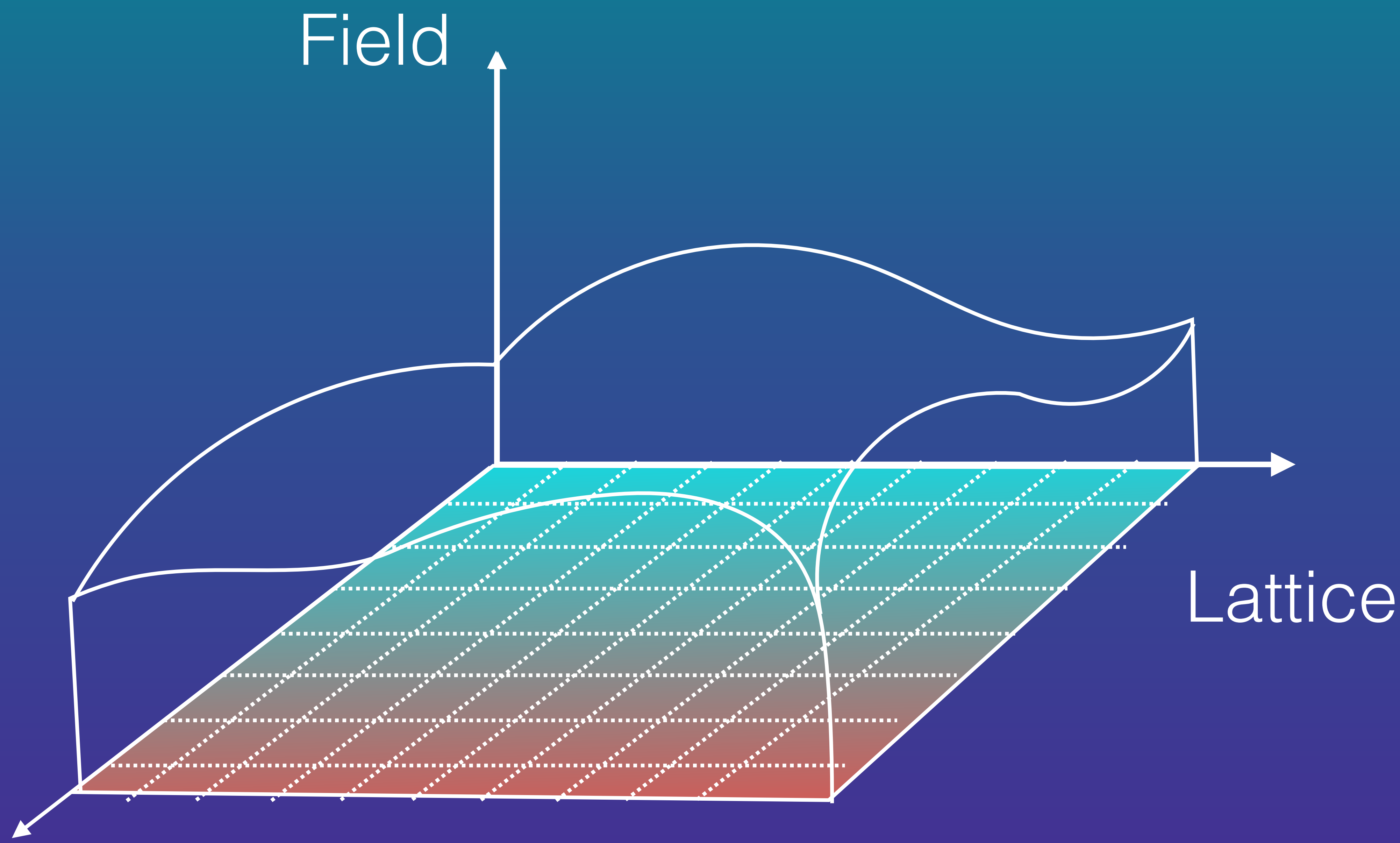
$$H = t \sum_{\langle i,j,\sigma \rangle} c^\dagger_{i,\sigma} c_{j,\sigma} + \sum_i \epsilon_{i,\sigma} n_{i,\sigma} + U \sum_{i,\sigma} n_{i,\sigma} n_{i,\overline{\sigma}}$$

e-Quantum simulation of field theories



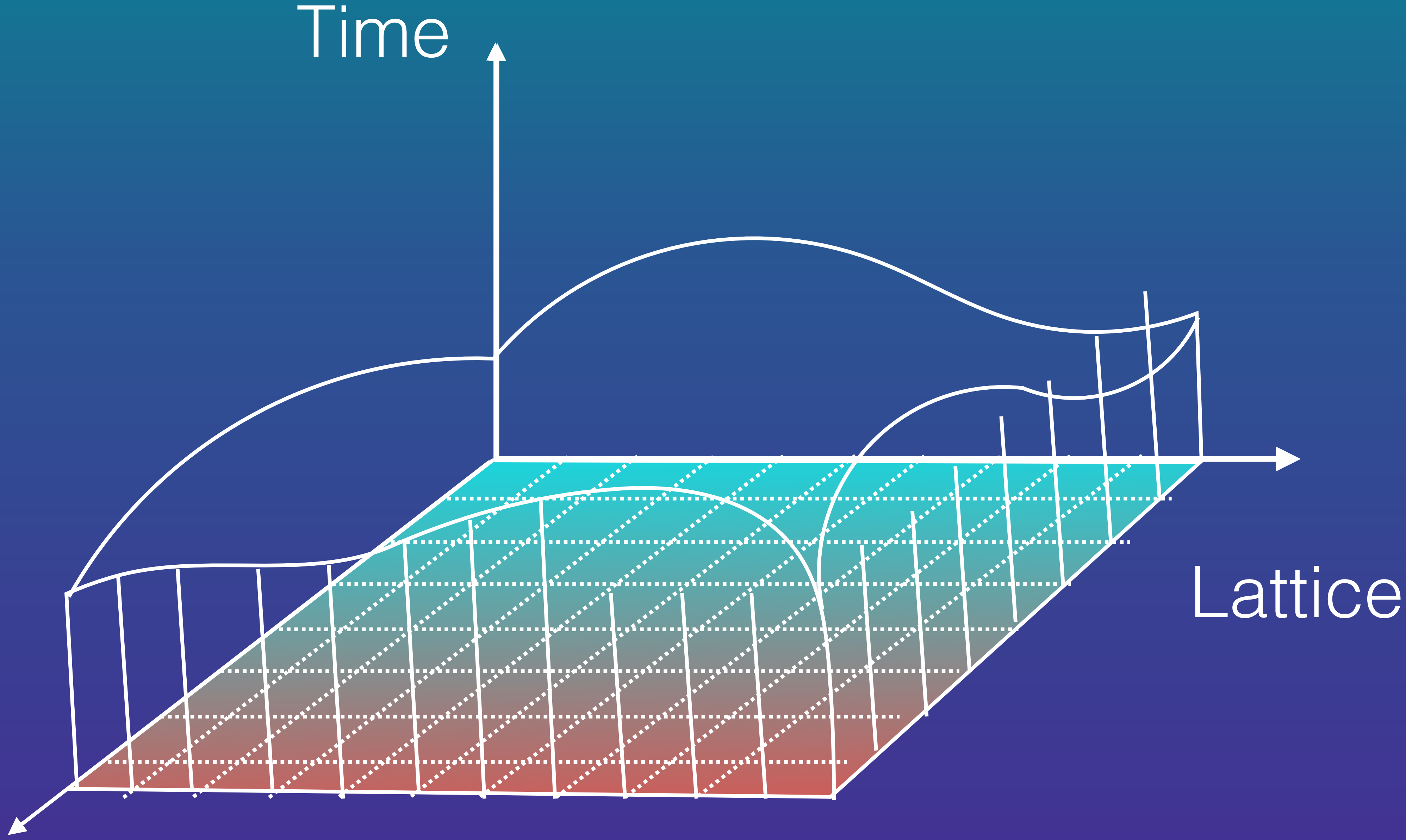
$$H = \int d^D x \left[\frac{1}{2}\pi(x)^2 + \frac{1}{2}(\nabla\phi)^2(x) + \frac{1}{2}m^2\phi(x)^2 + \frac{\lambda}{4}\phi(x)^4\right]$$

Discretize the space



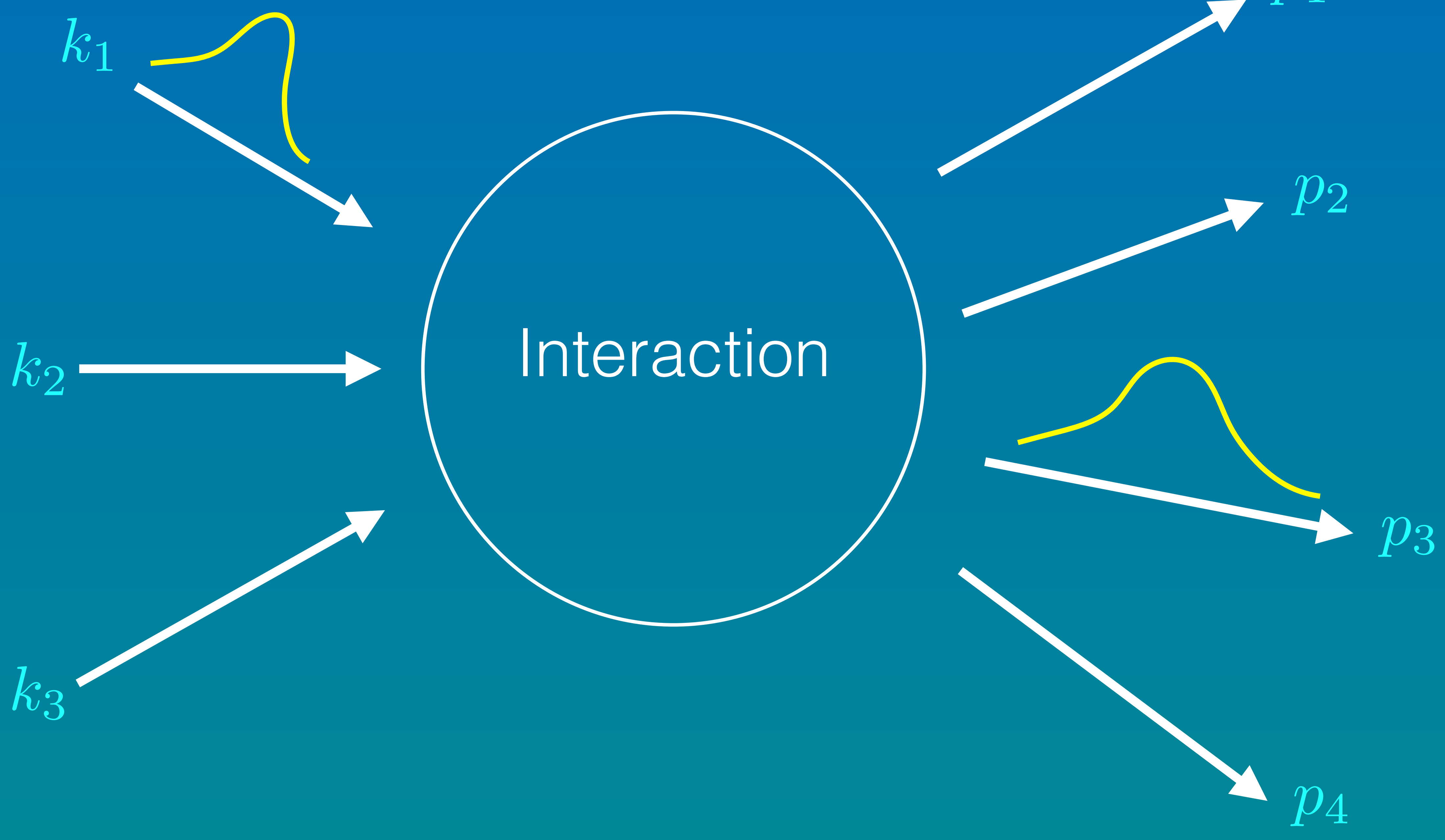
$$H = a^D \sum_{\mathbf{n}} [\frac{1}{2}\pi(\mathbf{n})^{\mathbf{2}} + \frac{\mathbf{1}}{\mathbf{2}}(\nabla\phi)^{\mathbf{2}}(\mathbf{n}) + \frac{\mathbf{1}}{\mathbf{2}}\mathbf{m}^{\mathbf{2}}\phi(\mathbf{n})^{\mathbf{2}} + \frac{\lambda}{\mathbf{4}}\phi(\mathbf{n})^{\mathbf{4}}]$$

Discretize the field



$$H = a^D \sum_{\mathbf{n}} [\frac{1}{2}\pi(\mathbf{n})^{\mathbf{2}} + \frac{\mathbf{1}}{\mathbf{2}}(\nabla\phi)^{\mathbf{2}}(\mathbf{n}) + \frac{\mathbf{1}}{\mathbf{2}}\mathbf{m^2}\phi(\mathbf{n})^{\mathbf{2}} + \frac{\lambda}{\mathbf{4}}\phi(\mathbf{n})^{\mathbf{4}}]$$

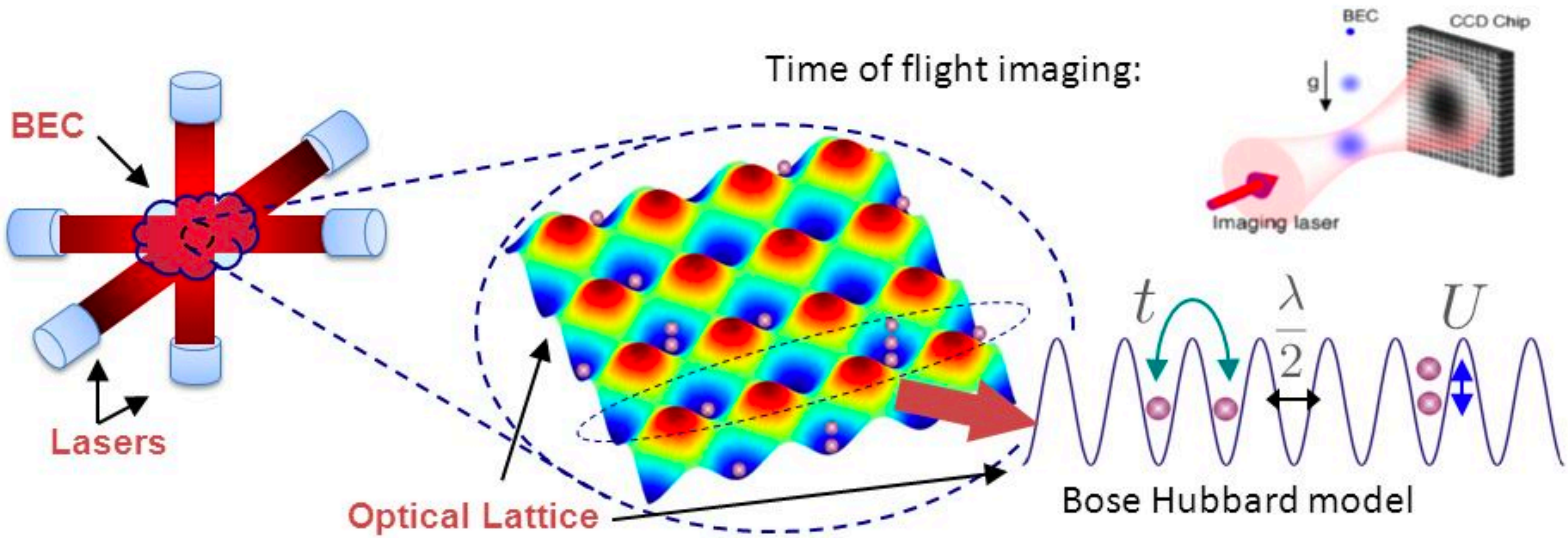
Scattering



B-Analog Quantum Simulation

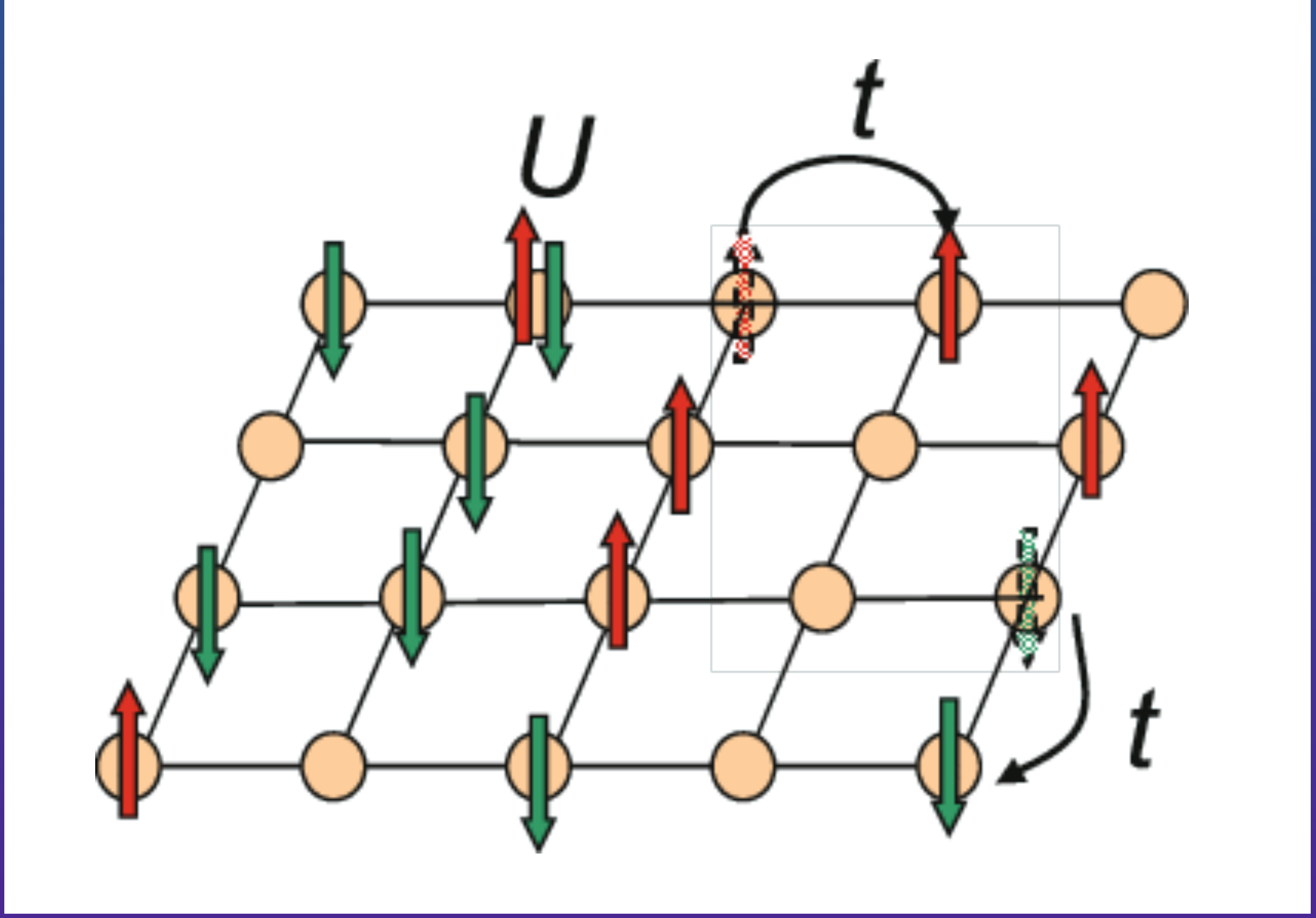
Analogue quantum simulation

Such model Hamiltonian are now accurately realisable with cold atoms:



Fermionic Systems

Electron Gas, Hubbard Model, Superconductivity…



Chemistry and material science

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Simulating Chemistry Using Quantum Computers

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and Alán Aspuru-Guzik

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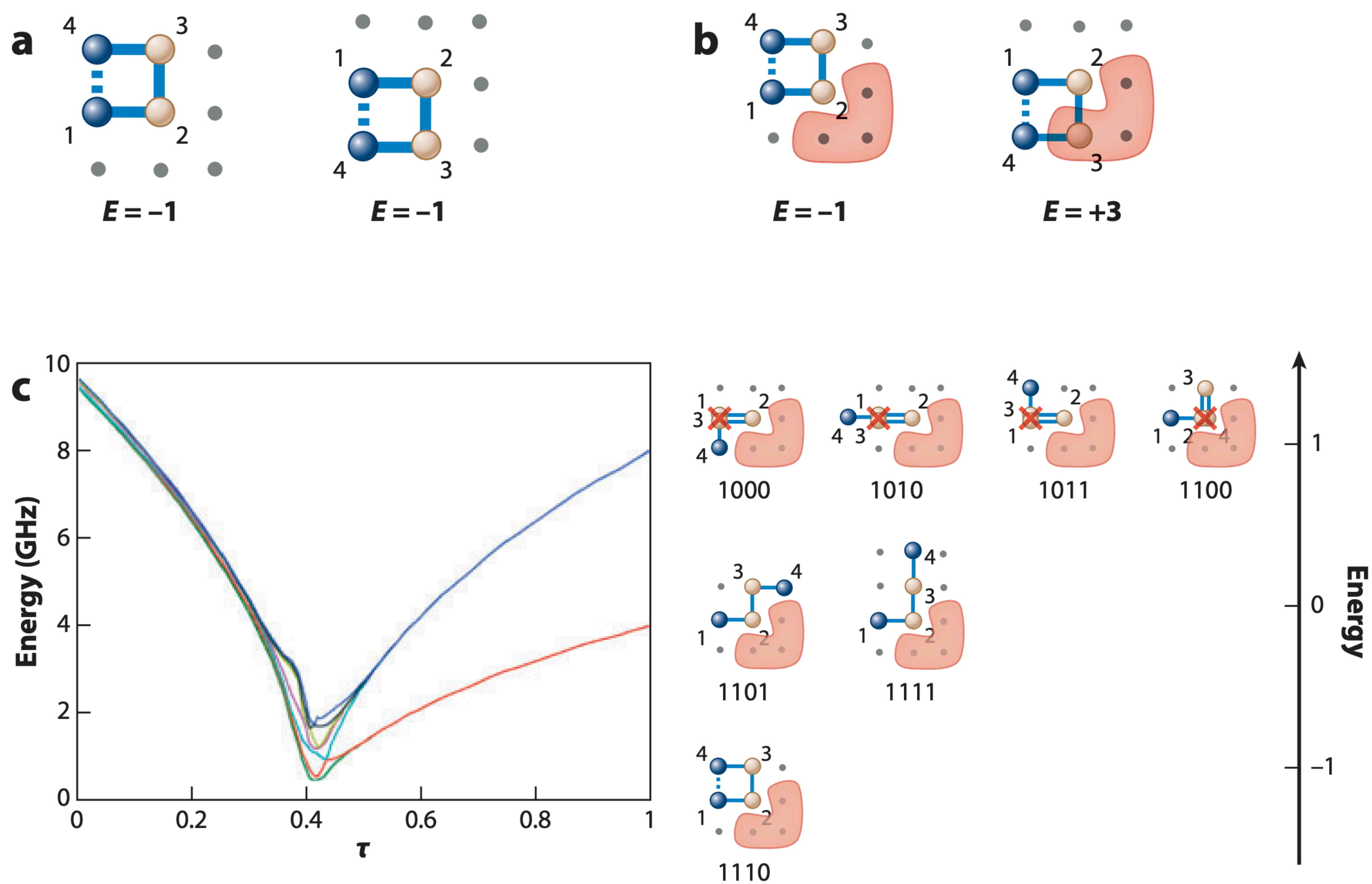

a
E = −1
E = −1
b
E = −1
E = +3
c
Energy (GHz)
τ
1000
1010
1011
1100
1101
1111
1110
Energy

Opportunities in quantum simulation

- Impact on the society

Chemistry, Materials, Energy production, agriculture, sustainability of our planet

A- The problem should be so hard to be solvable only by quantum computers,

B- It should be of real scientific value with application

Difficulties in quantum simulation

Currently, simulating ground states of materials by classical computers is progressing fast for two reasons:

A- Faster computers,

B-Better algorithms

Difficulties in quantum simulation

The states of most materials is not highly entangled,
so the quantum advantage for these materials is not exponential,
but polynomial (147).

Moreover, these methods are heuristic and not rigorous, since
if we want accurate results in an efficient way, the initial
state should have a high overlap with the target state,
which is a difficult problem.

A window in quantum simulation

Exponential speed up is expected in dynamics,
when an initial state evolves to a highly entangled state,
i.e. scattering in field theory (148).