Sharif Quantum Information Group

Quantum Simulation by Quantum Computers

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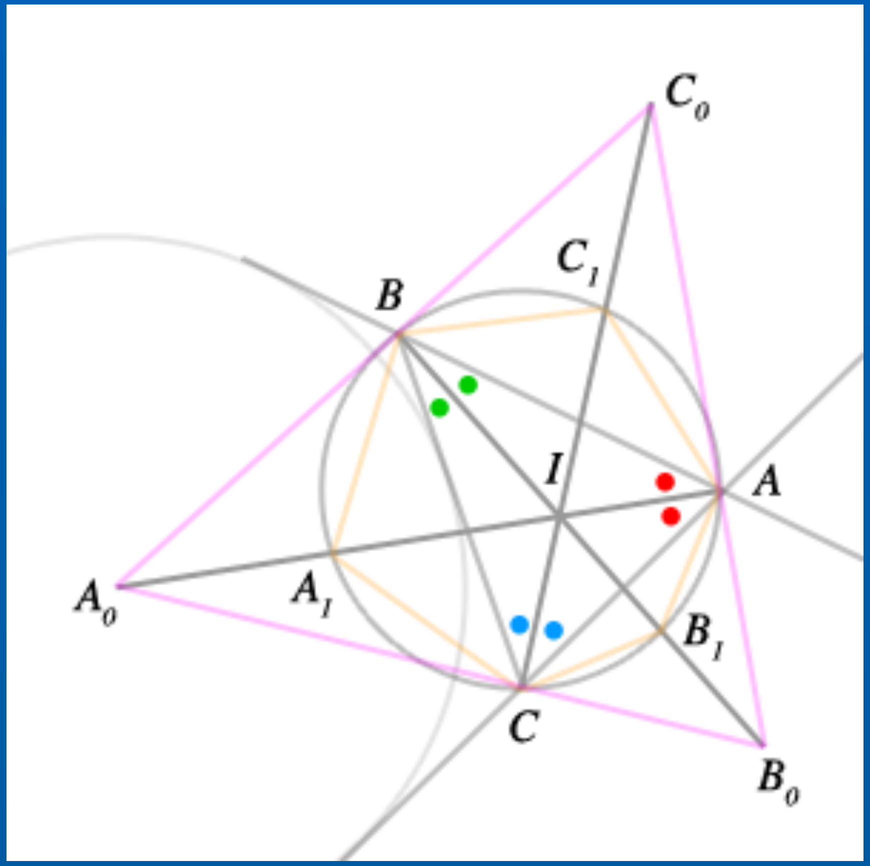
Great Transitions in Science

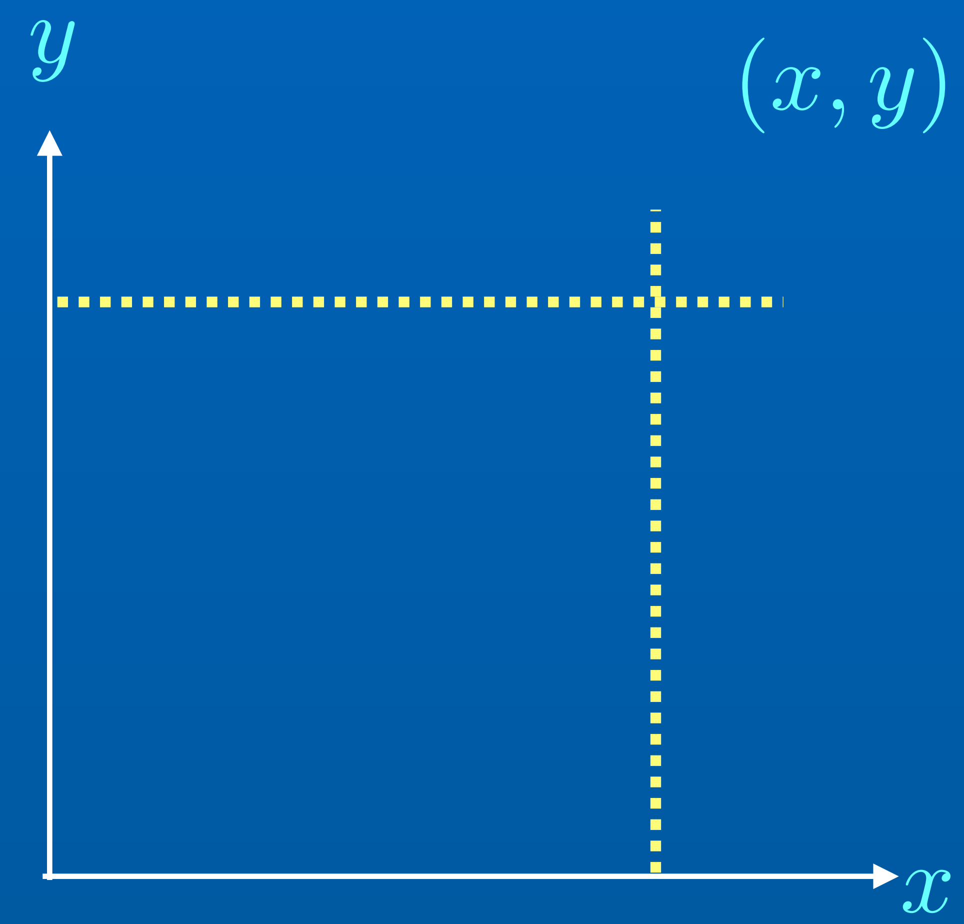
Or

The way we do Science

The old Geometry

Analytic Geometry





Creativity → Algebraic Calculations

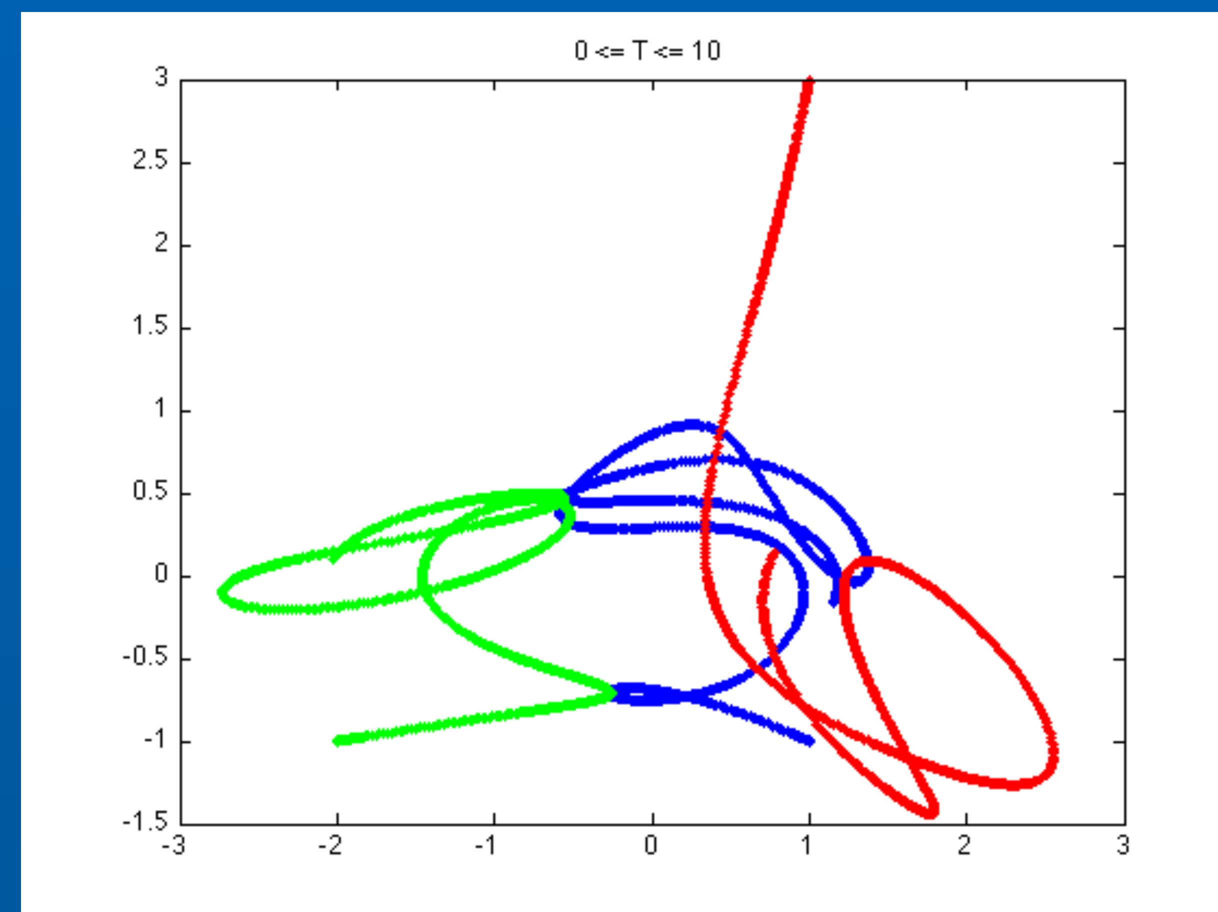
Analytical Solutions

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

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

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

Numerical Solutions



Mathematical Physics

Computer Simulation

$$-32 z m^3 \frac{\partial^2 \vartheta_c(z|m)}{\partial m^2} \frac{\partial \vartheta_c(z|m)}{\partial z} - 24(m-1)^2 m^2 \left(\frac{\partial \vartheta_c(z|m)}{\partial m}\right)^2 -$$

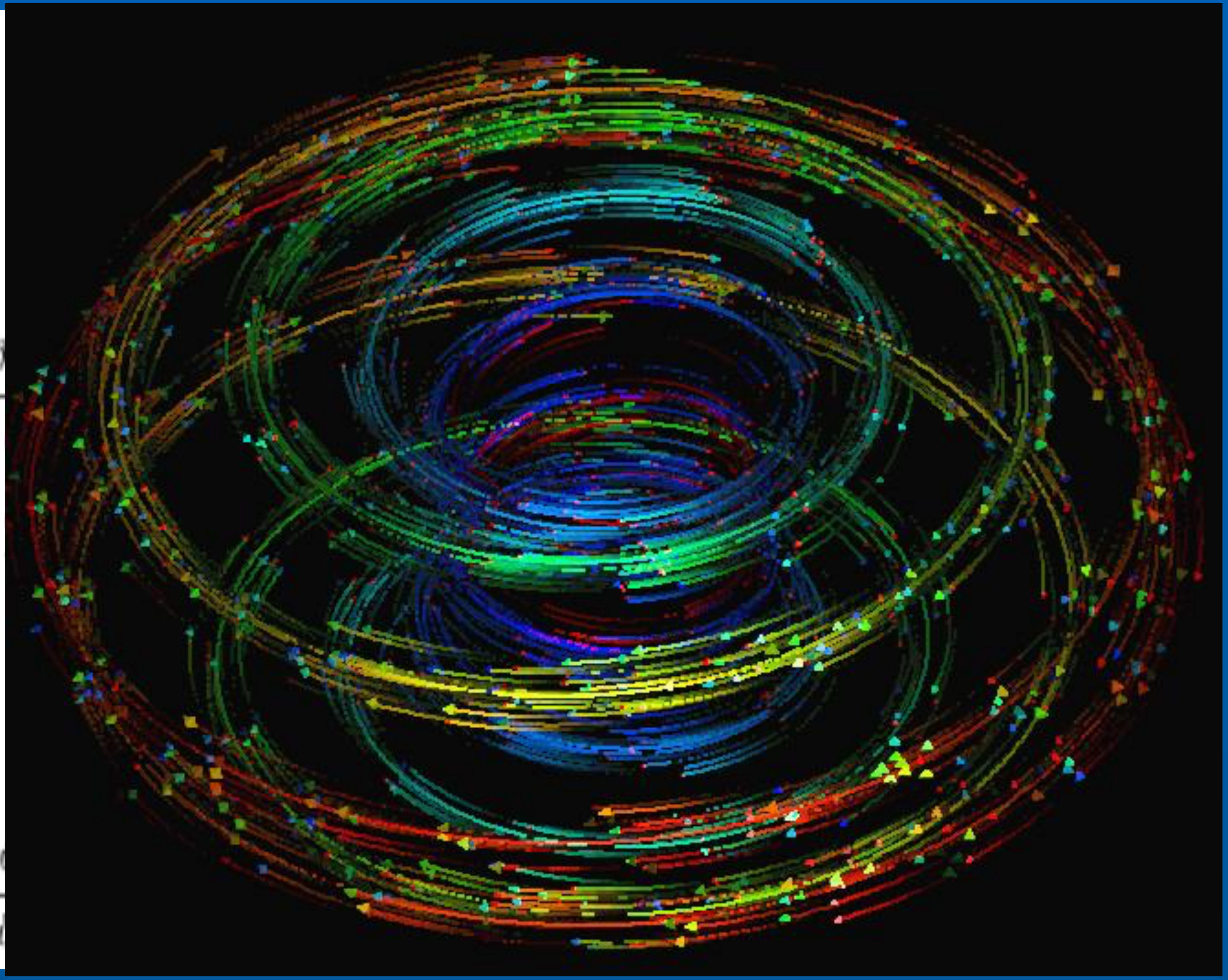
$$4 z^2 m^2 \left(\frac{\partial \vartheta_c(z|m)}{\partial z}\right)^2 + 16\left(m^2+1\right) z m^2 \frac{\partial \vartheta_c(z|m)}{\partial z} \frac{\partial^2 \vartheta_c(z|m)}{\partial m^2} +$$

$$4 z m^2 \frac{\partial^2 \vartheta_c(z|m)}{\partial z^2} \frac{\partial^2 \vartheta_c(z|m)}{\partial z \partial m} + 4 z^2 m \left(\frac{\partial \vartheta_c(z|m)}{\partial z}\right)^2 - 4 z m \frac{\partial^2 \vartheta_c(z|m)}{\partial z \partial m} \partial^2 \vartheta$$

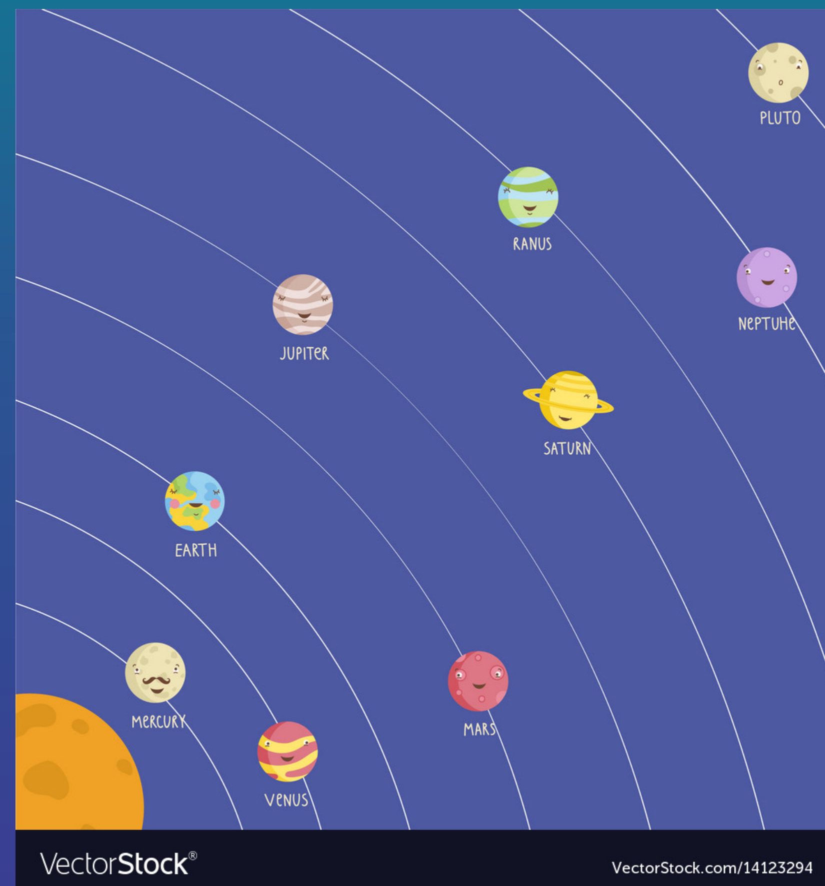
$$2(m-1) m \frac{\partial \vartheta_c(z|m)}{\partial m} \left(5 \frac{\partial^2 \vartheta_c(z|m)}{\partial z^2} + 2 z \left((9m-5) \frac{\partial \vartheta_c(z|m)}{\partial z} - 4(m-1) m\right.\right.$$

$$4(m-1) z m \frac{\partial \vartheta_c(z|m)}{\partial z} \frac{\partial^3 \vartheta_c(z|m)}{\partial z^2 \partial m} - \left(\frac{\partial^2 \vartheta_c(z|m)}{\partial z^2}\right)^2 + (m-1) \vartheta_c(z|m)^2 +$$

$$2(m-1)\left(\frac{\partial^2 \vartheta_c(z|m)}{\partial z^2} + m\left(4 m \frac{\partial \vartheta_c(z|m)}{\partial m} + 2(m-1)\left(2 m \frac{\partial^2 \vartheta_c(z|m)}{\partial m^2} - z\right.\right.\right.$$



Simulation of the solar system



Number of variables= $6 \times N$

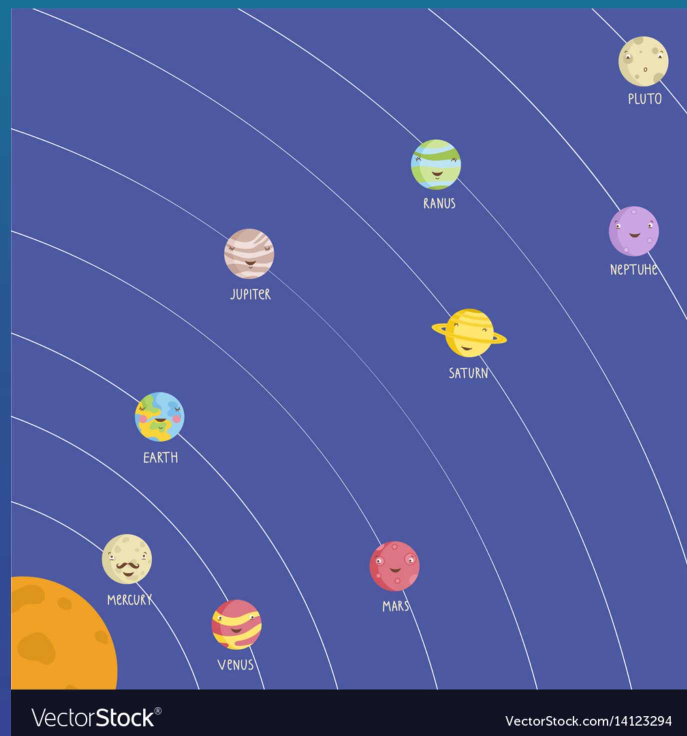
$$\frac{d}{dt} x_i = f_i(x_1, \cdots x_{6N})$$

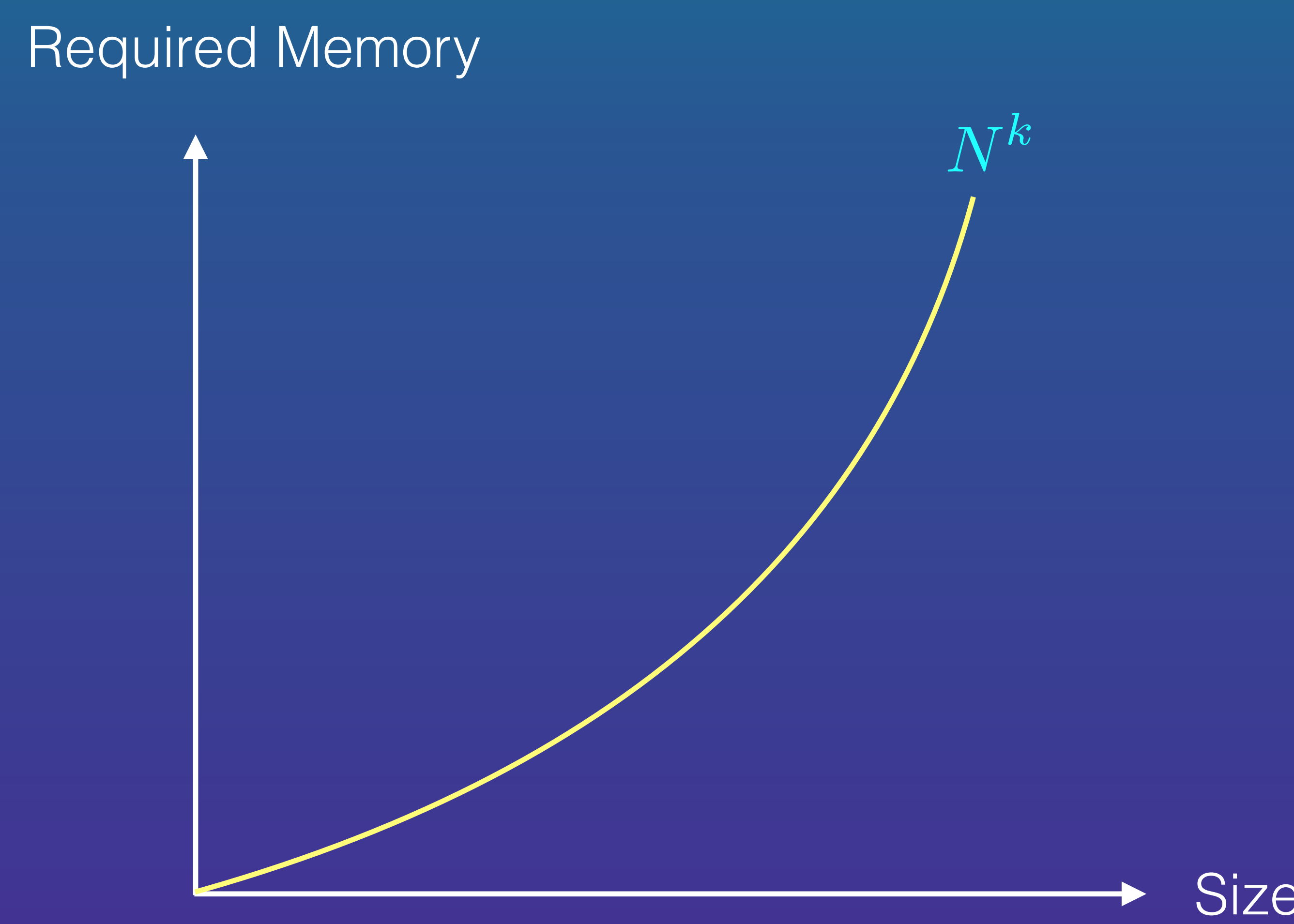
Simulation of a Globular Cluster

Number of variables= $6 \times N$

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

Easy problems!





Simulation of a Complex Process: A Flight

There is no plane, no land, no pilot….on your screen.

Simulation of a Very Simple Quantum Mechanical System

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

$$|\Psi\rangle = \begin{pmatrix} \psi(\uparrow, \uparrow, \uparrow, \cdots \uparrow) \\ \psi(\downarrow, \uparrow, \uparrow, \cdots \uparrow) \\ \cdots \\ \cdots \\ \cdots \\ \psi(\downarrow, \downarrow, \downarrow, \cdots \downarrow) \end{pmatrix}$$

How many variables should we store?

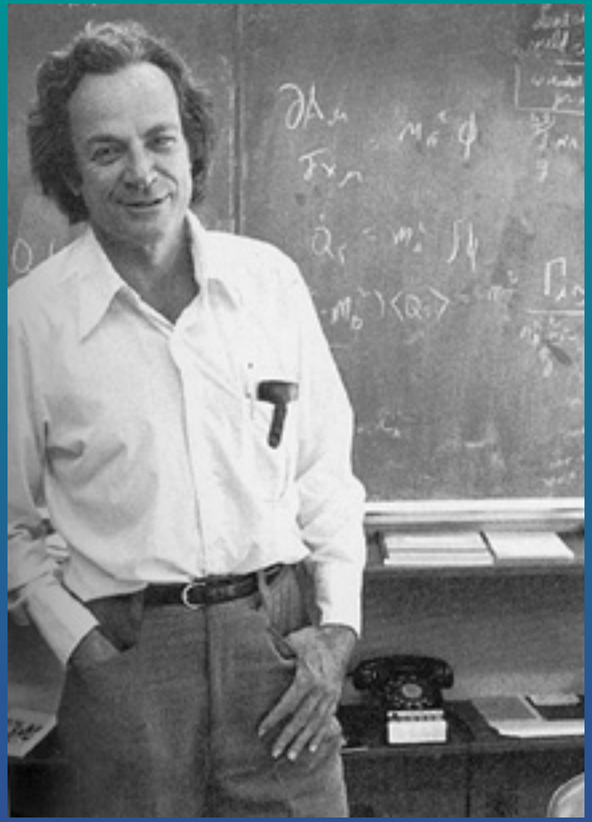
For 10 spins $2^{10} = 1024$ Bytes

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

We cannot simulate even a very

simple quantum system

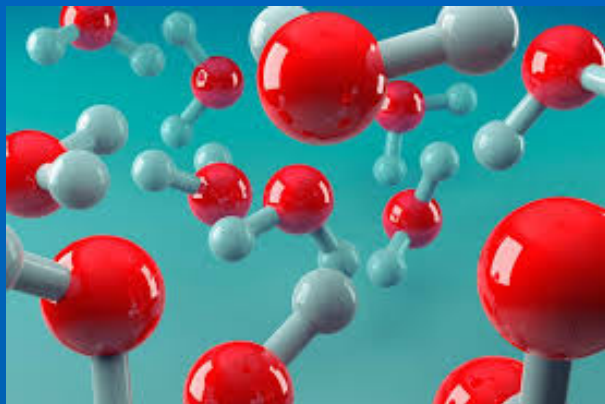
on a classical computer.



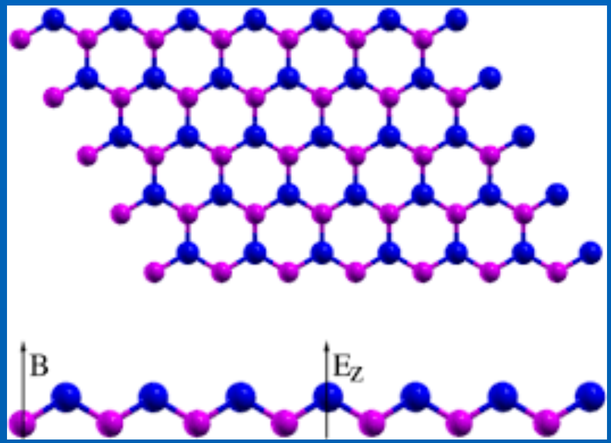
Quantum Simulation

Use a simple quantum system
simulate another quantum system

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

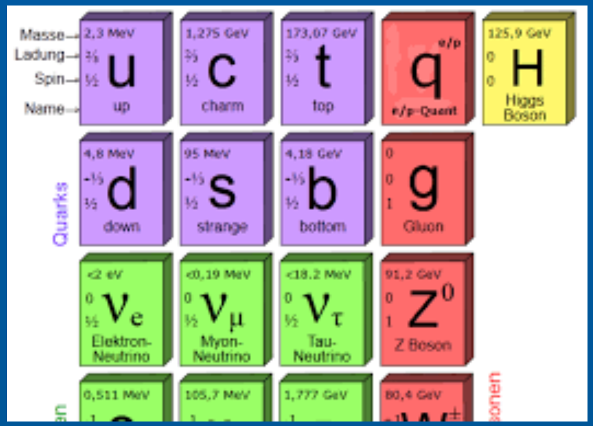


Molecules

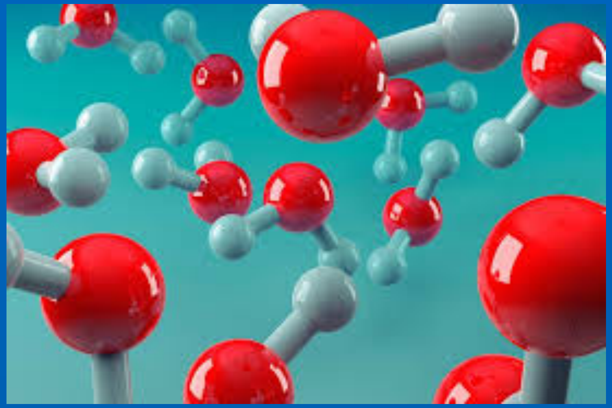


Solids

A Universal Quantum Simulator



Elementary Particles

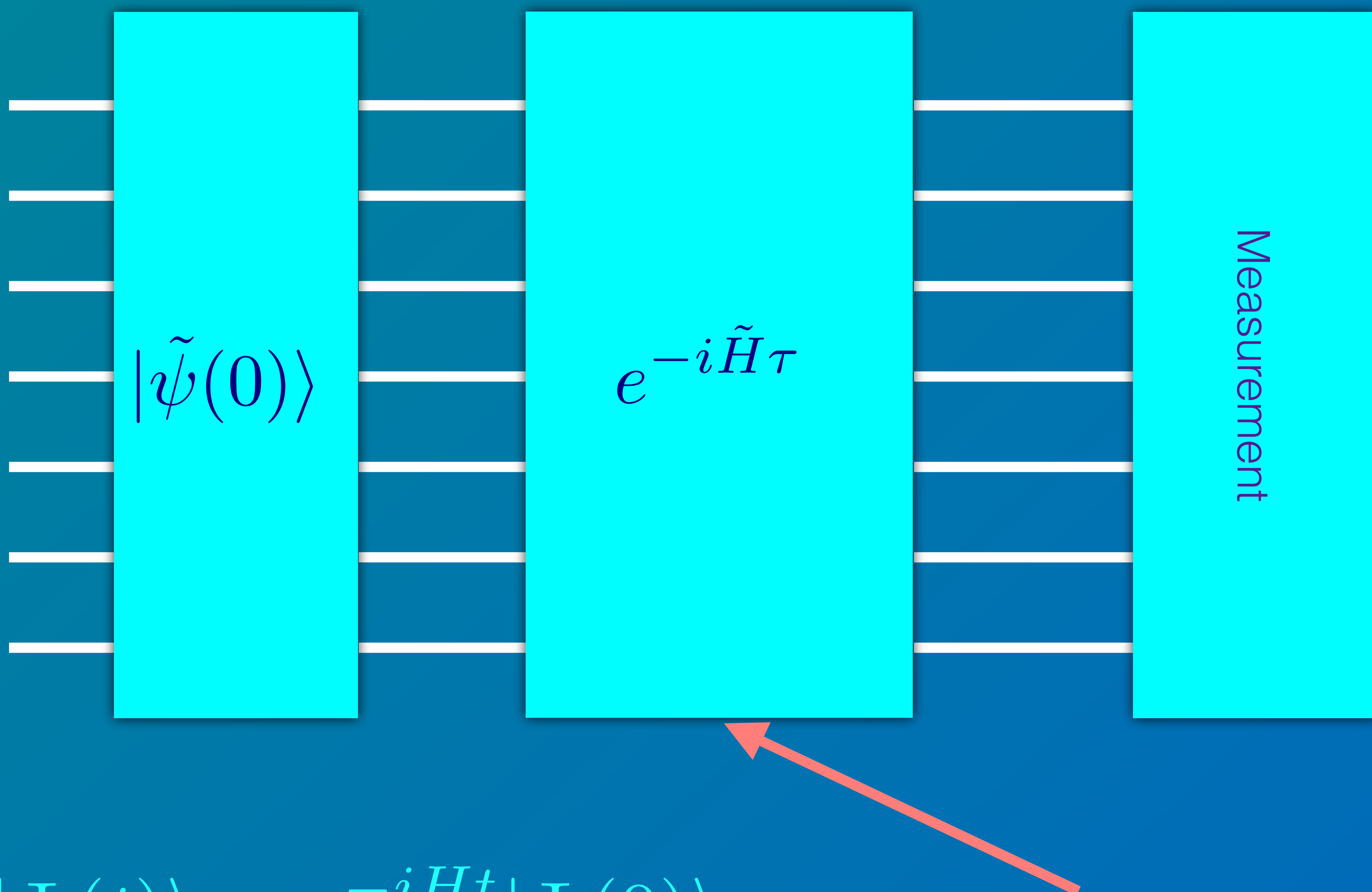


Molecules

A Quantum Simulator

A- Digital Quantum Simulation

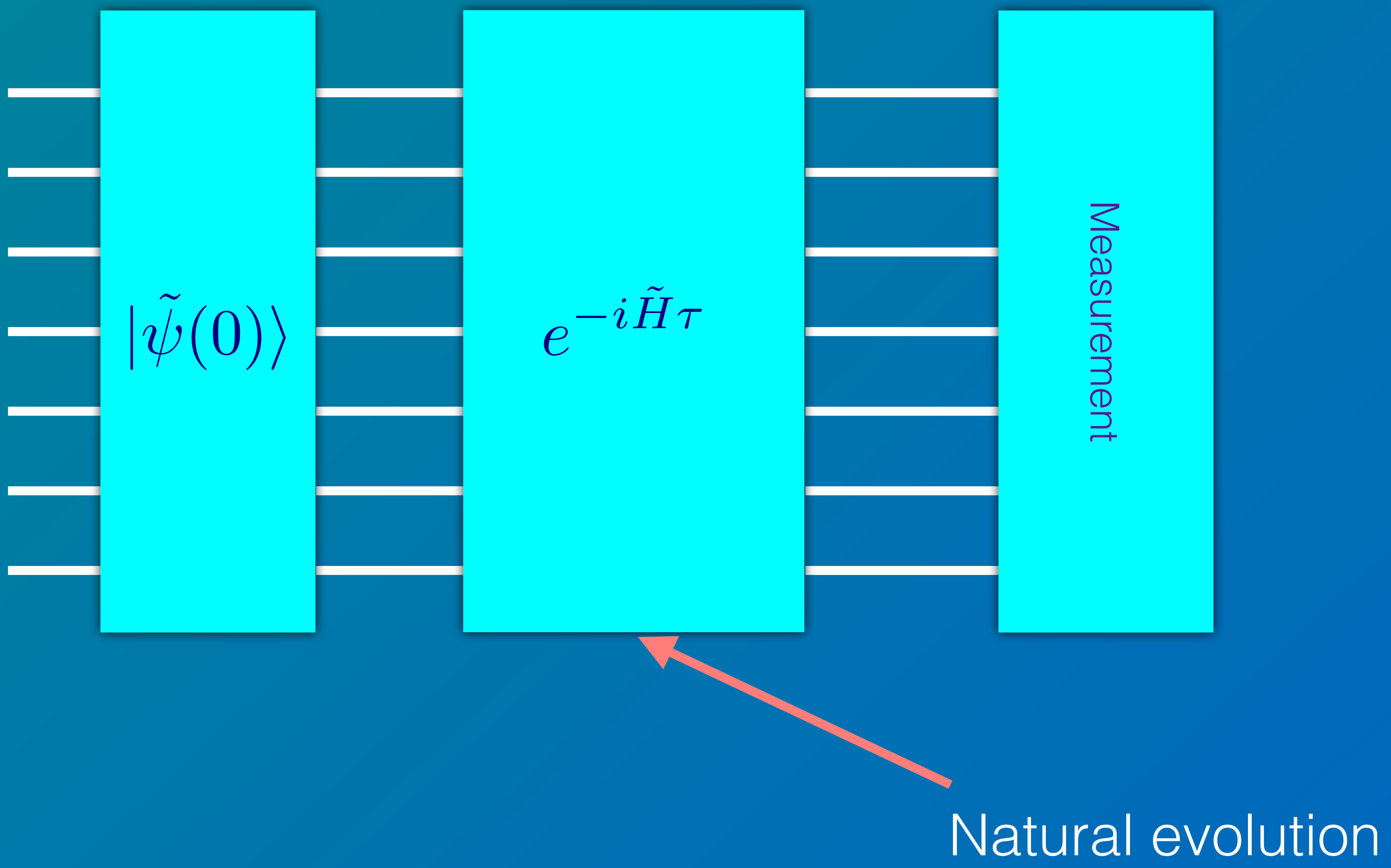
$$|\tilde{\psi}\rangle = e^{-i\tilde{H}\tau}|\tilde{\psi}(0)\rangle$$



$$|\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle$$

Quantum Circuit (gates)

B- Analog Quantum Simulation



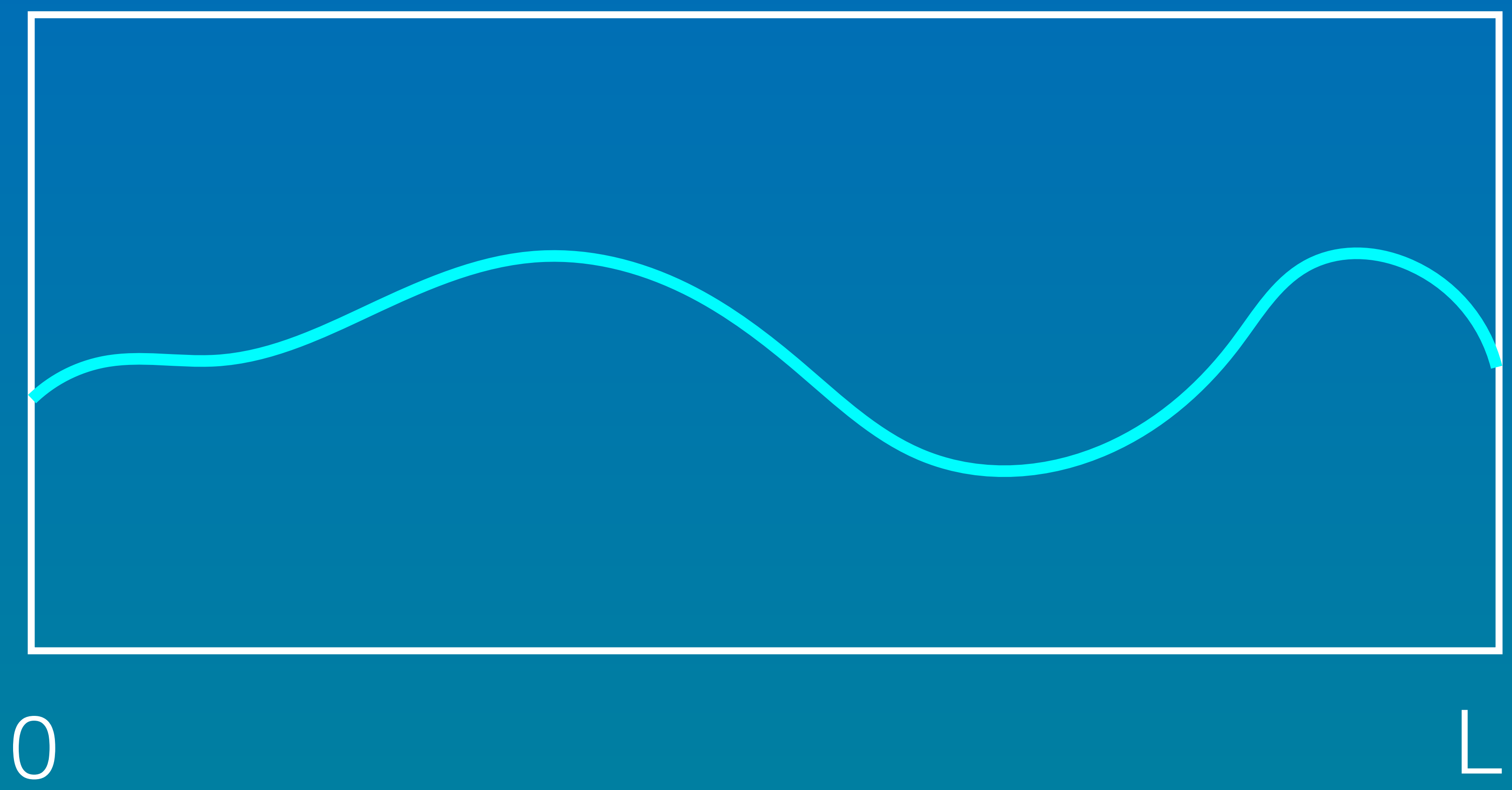
A TOY MODEL

Solving the Schrodinger Equation

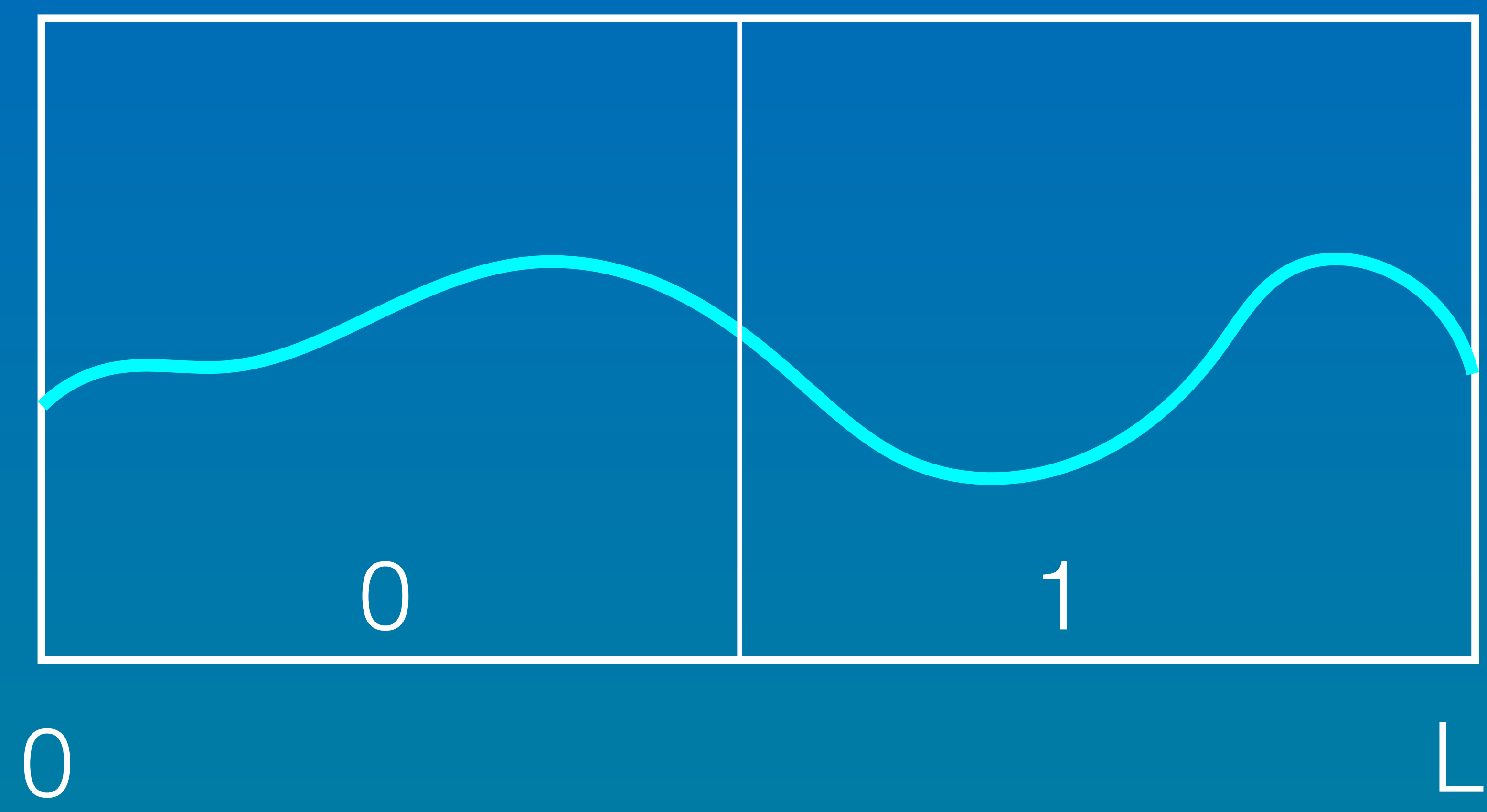
For a single particle

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

1-Preparation of the initial state



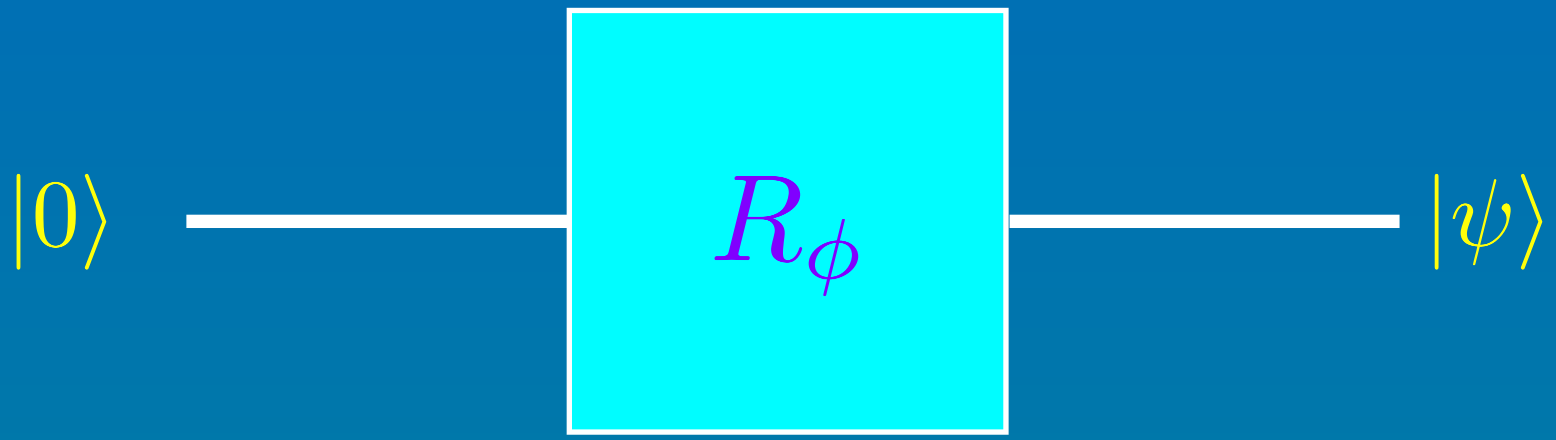
$$|\psi\rangle = \int_0^L \psi(x)|x\rangle$$



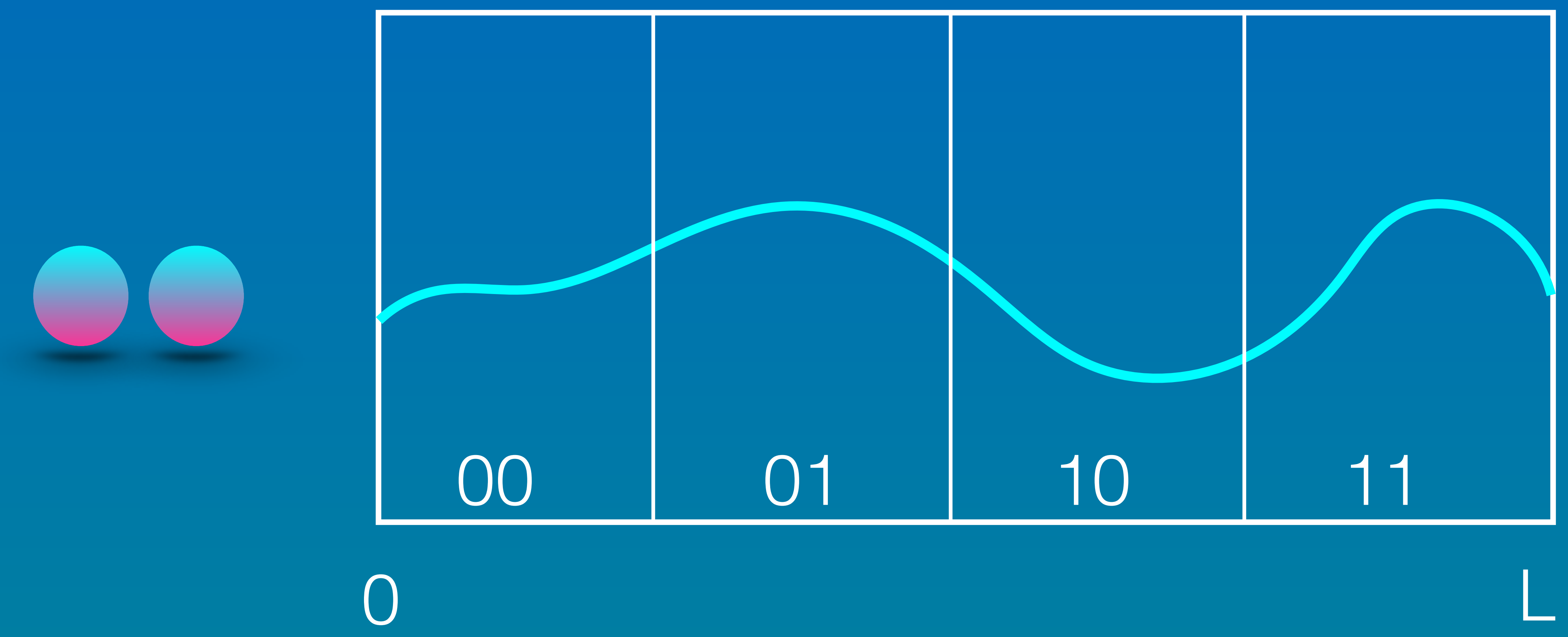
$$|\psi\rangle = \cos\phi|0\rangle + \sin\phi|1\rangle$$

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

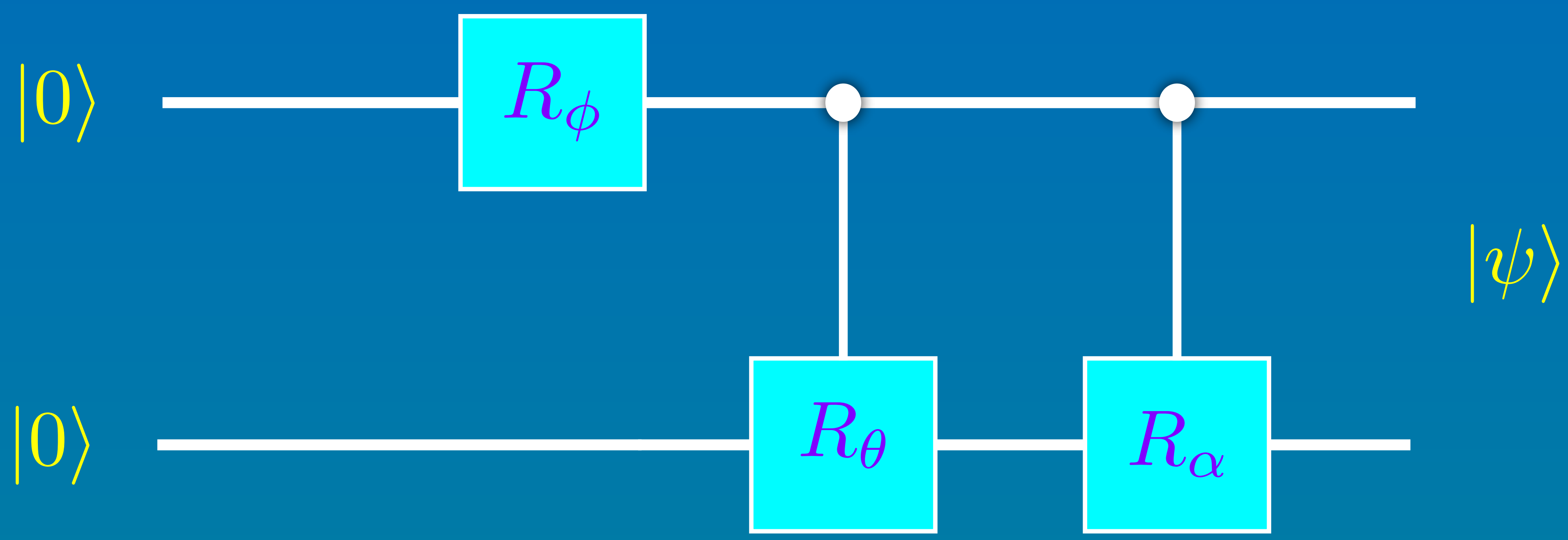
$$\sin^2\phi = \int_{\frac{L}{2}}^{L} |\psi(x)|^2 dx$$



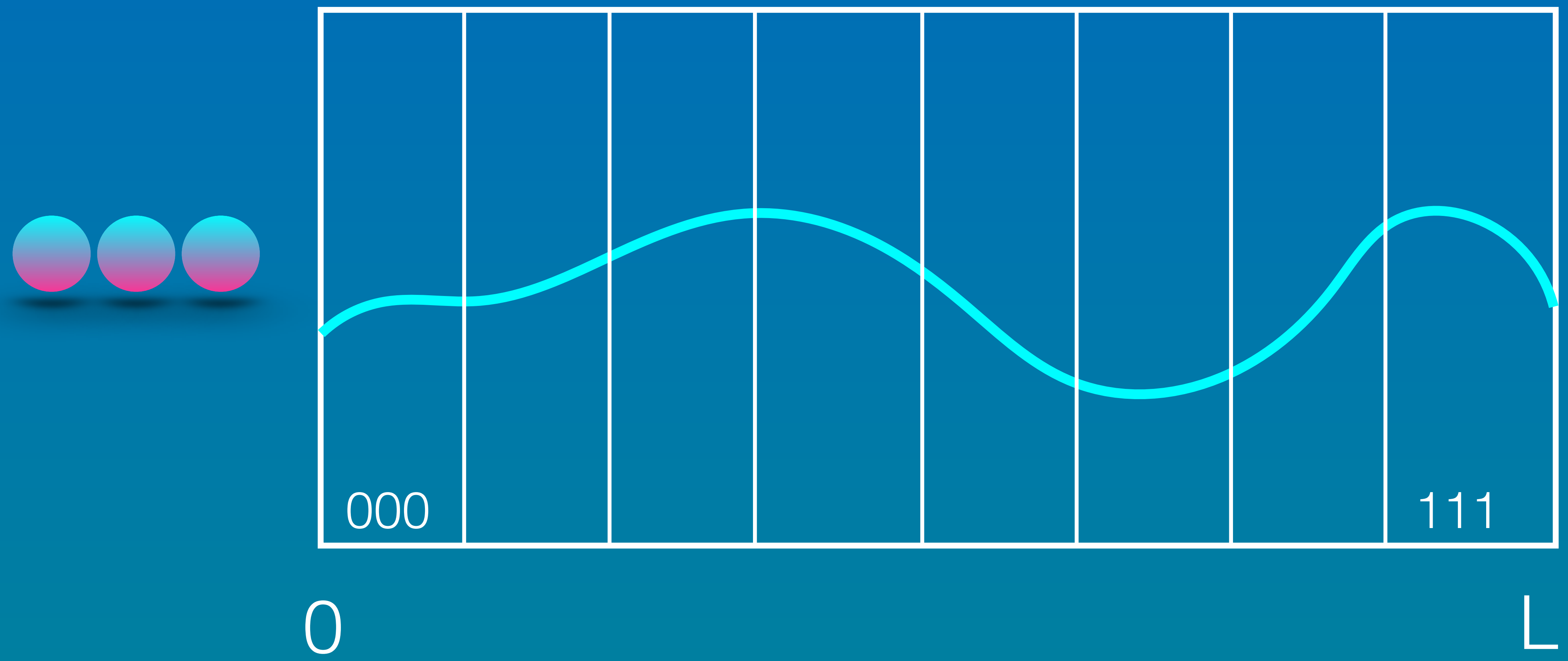
$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad R_\phi = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \qquad \begin{pmatrix} \cos\phi \\ \sin\phi \end{pmatrix}$$



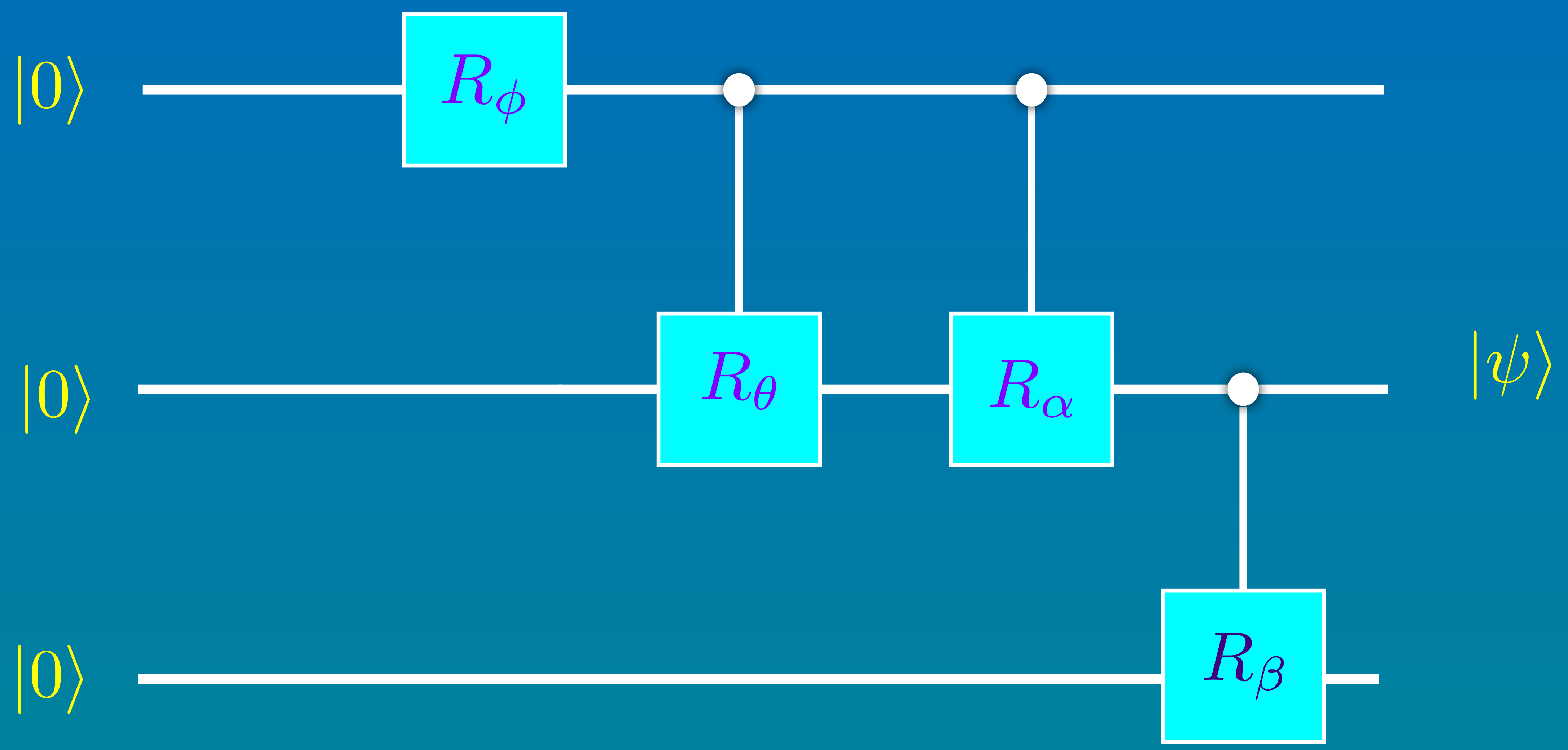
$$|\psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$$

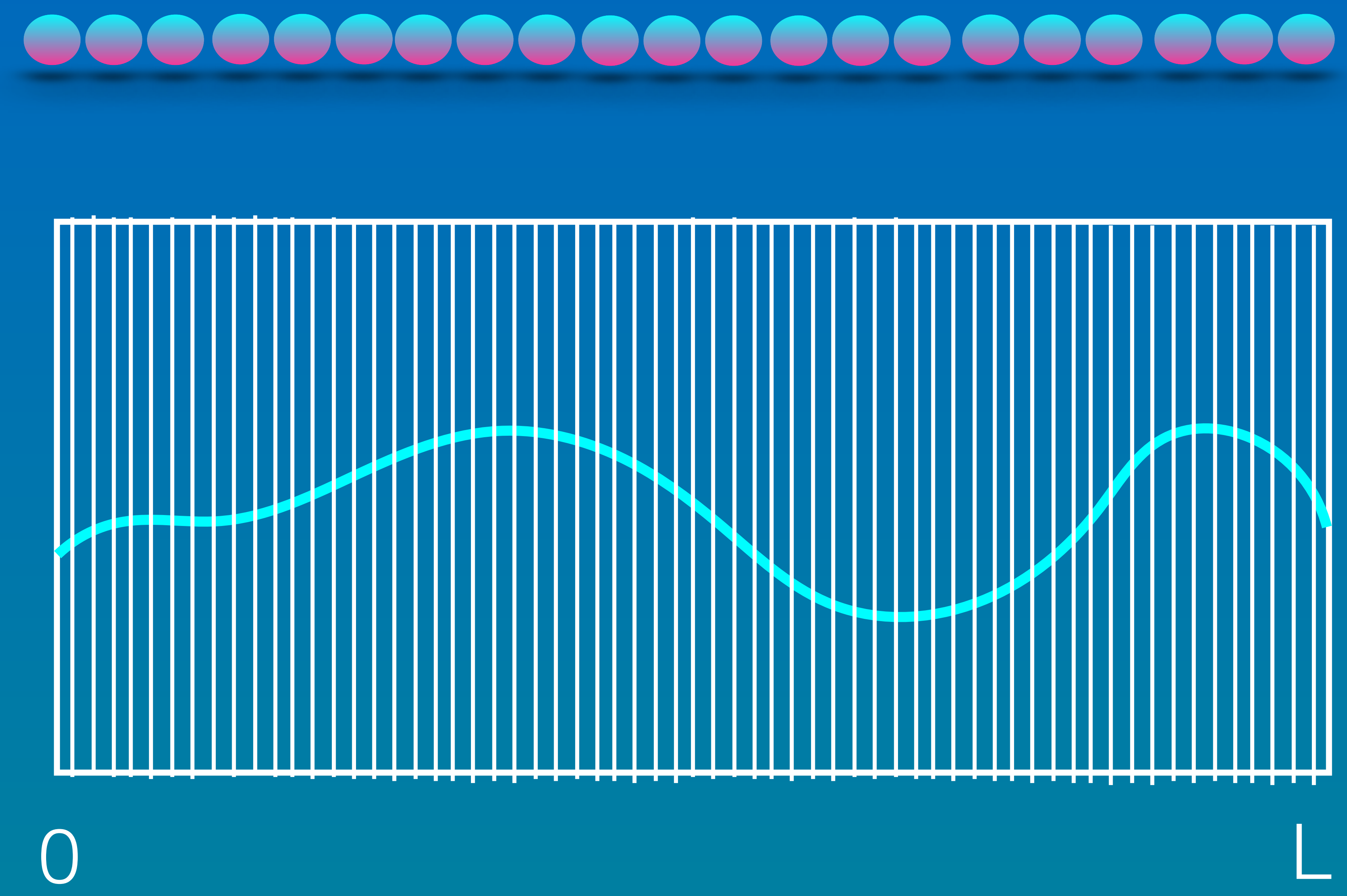


$$|\psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$$



With 3 qubits

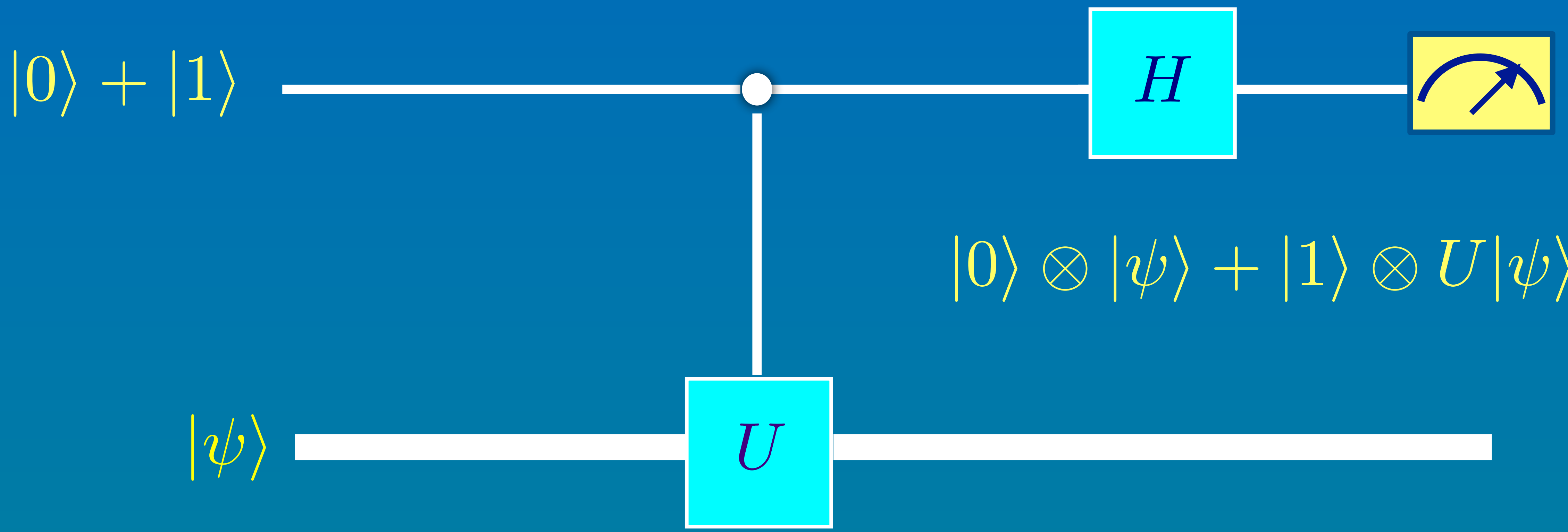

|0⟩
|0⟩
|0⟩
R_ϕ
R_θ
R_α
R_β
|ψ⟩



With only 20 qubits

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

Expectation Values

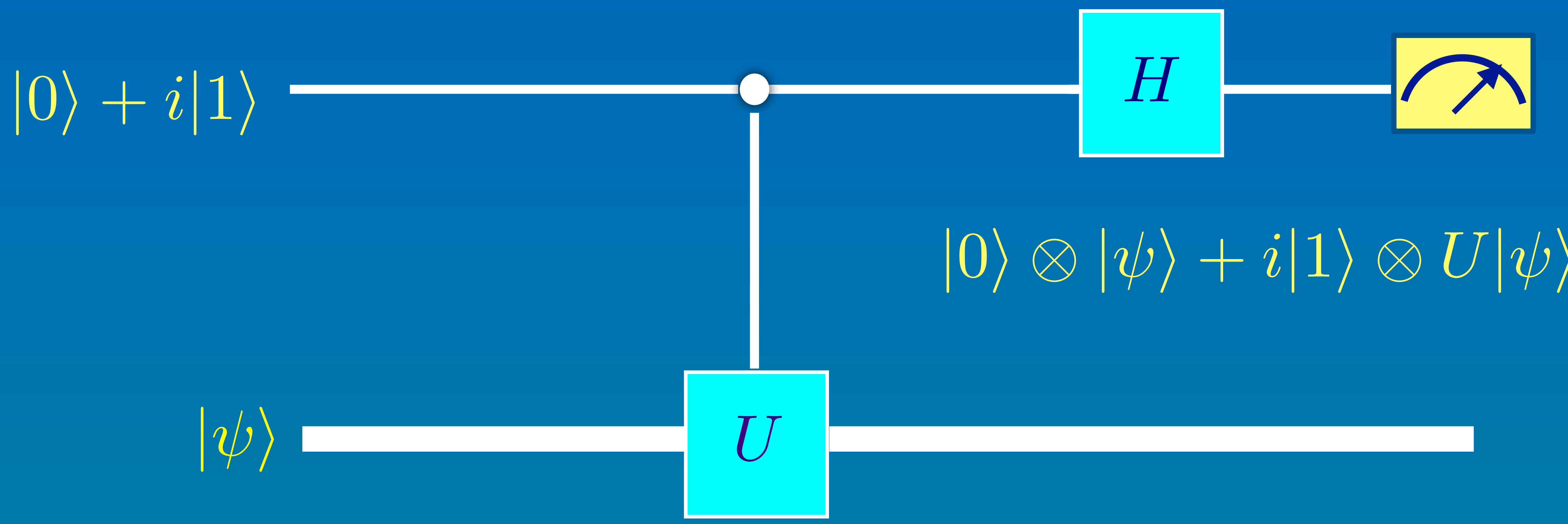


$$P(0) = \frac{1}{4}||(I + U)|\psi\rangle||$$

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

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

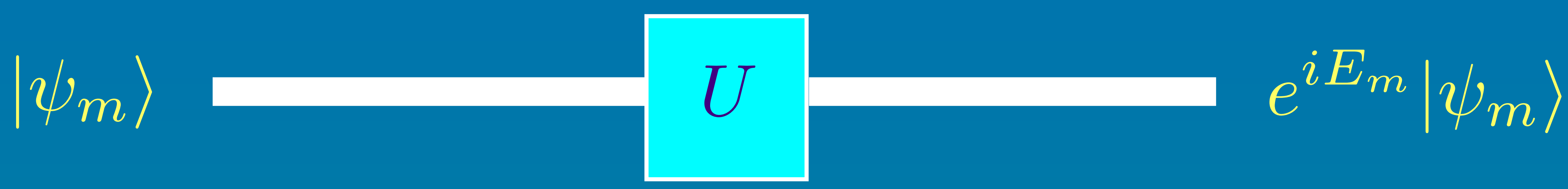
$$P(1) = \frac{1}{2}(1 - Re\langle\psi|U|\psi\rangle)$$



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

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

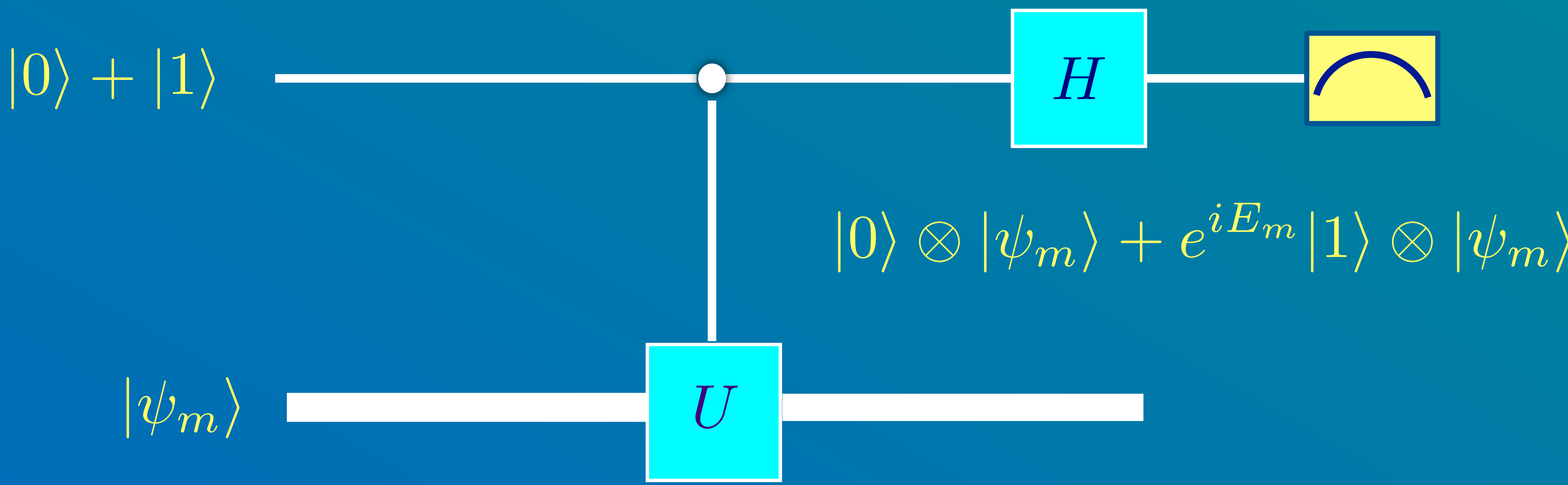
Finding the Spectrum of the Hamiltonian



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

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

Finding the Spectrum of the Hamiltonian

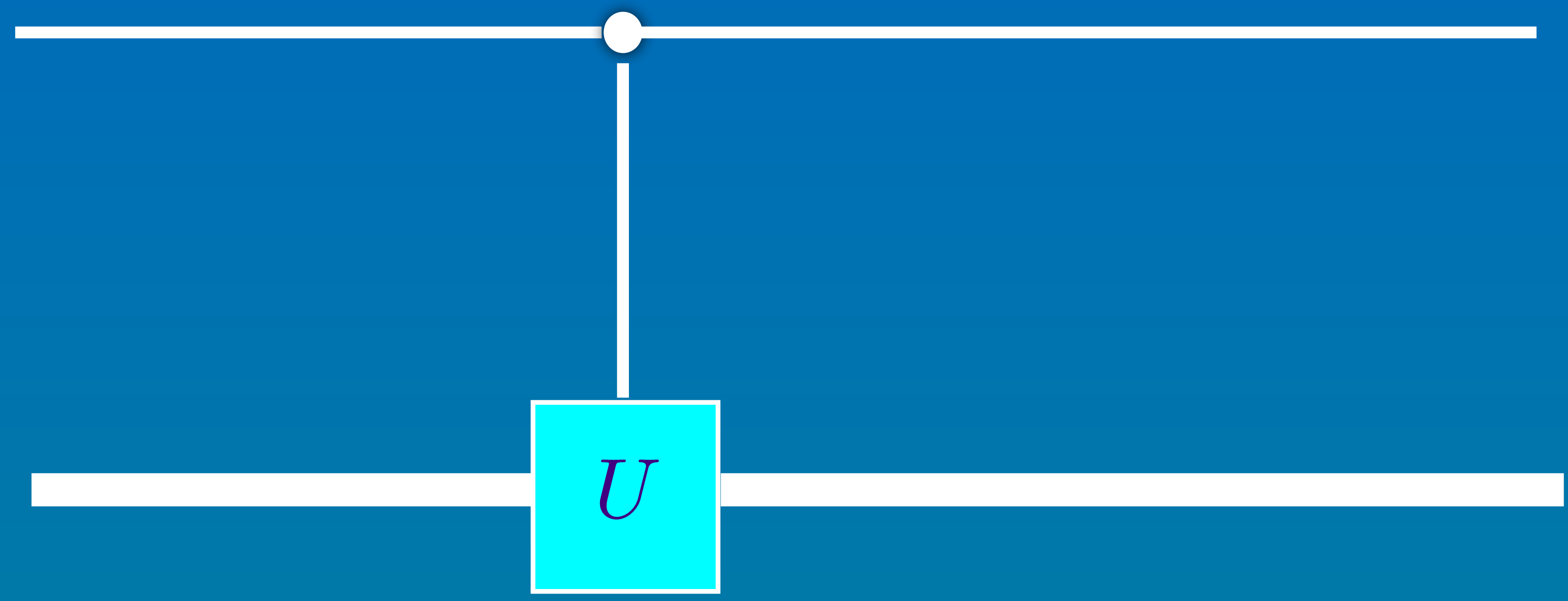


$$P(0) = \frac{1}{2}(1 + \cos E_m)$$

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

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

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

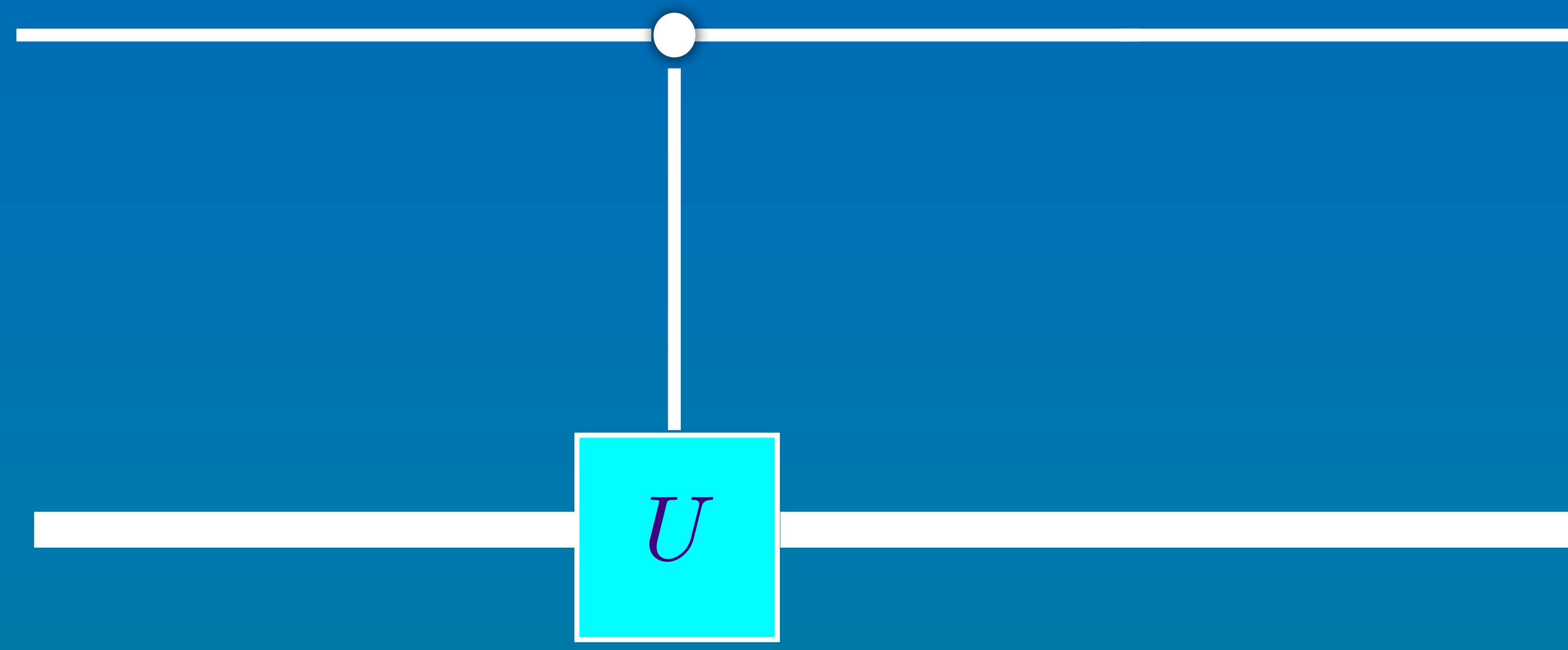


$$\sum_{m,k} \alpha_m |k\rangle \otimes U^k |\psi_m\rangle$$

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

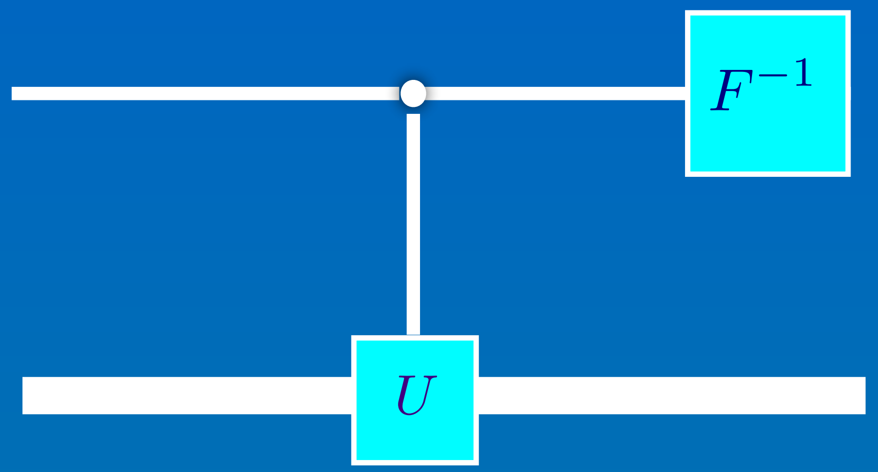
$$\frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}|k\rangle$$

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



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

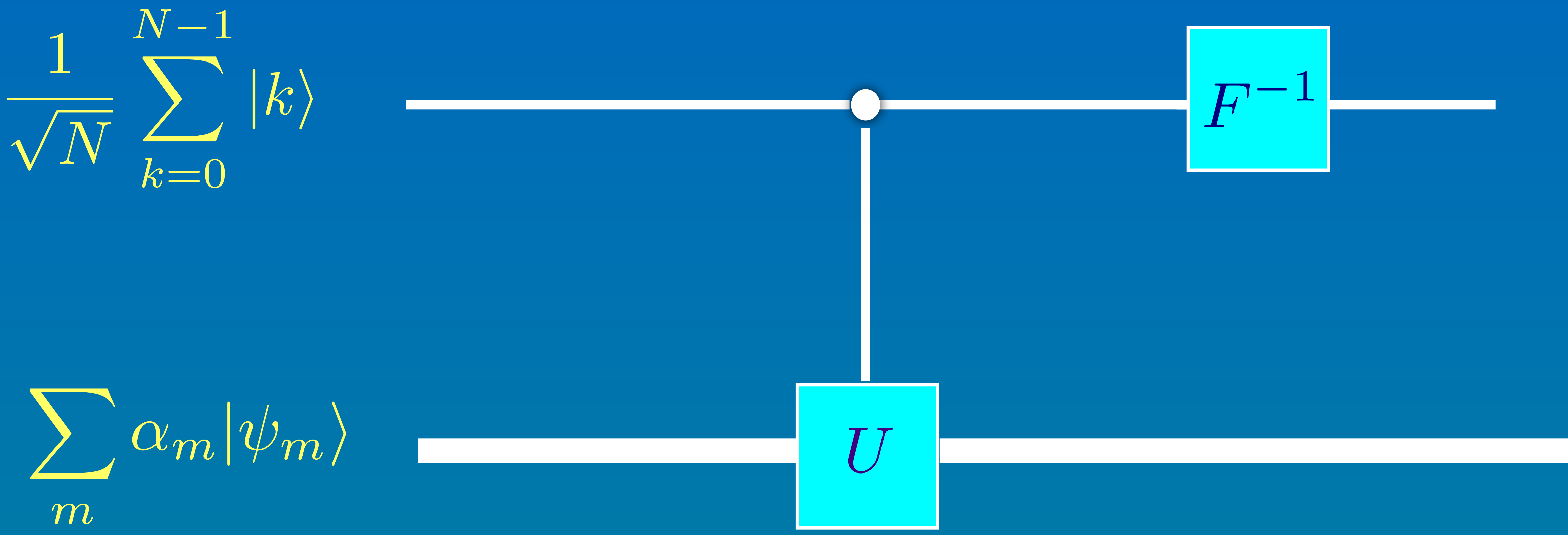
$$\frac{1}{\sqrt{N}}\sum_{k,m}\alpha_m|k\rangle\otimes e^{ikE_m}|\psi_m\rangle$$

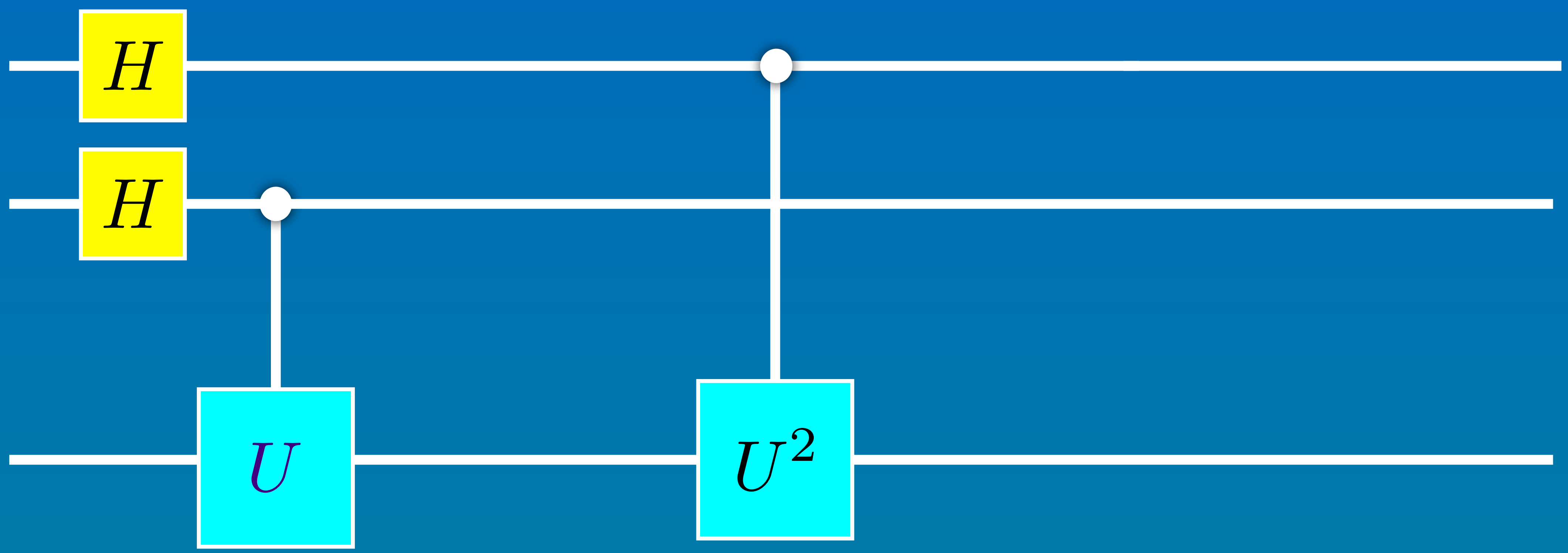


$$\frac{1}{\sqrt{N}} \sum_{k,m} \alpha_m |k\rangle \otimes e^{ikE_m} |\psi_m\rangle$$

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

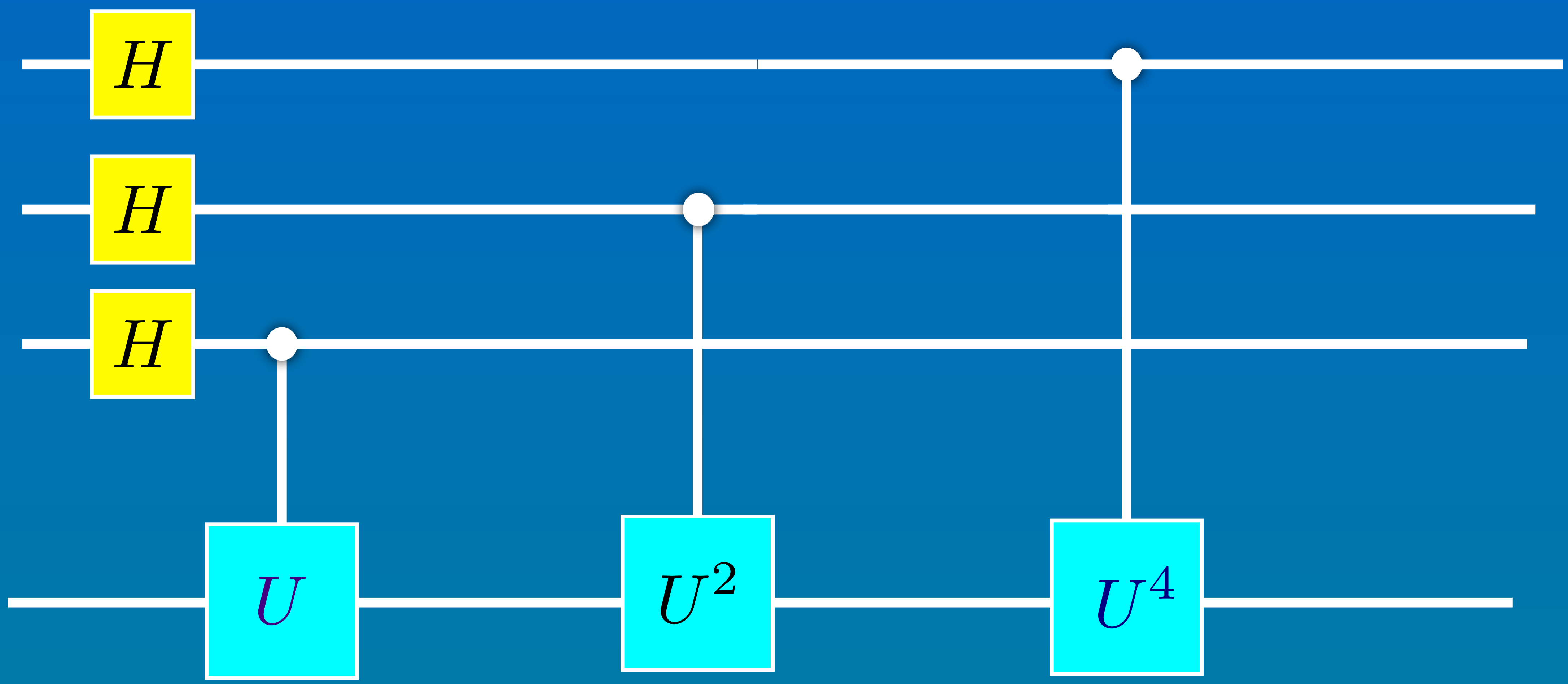
$$F|E_m\rangle = \frac{1}{\sqrt{N}} \sum_{k} e^{ikE_m} |k\rangle \qquad \sum_{m} \alpha_m |E_m\rangle \otimes |\psi_m\rangle$$


$\frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}|k\rangle$
$\sum_m \alpha_m|\psi_m\rangle$
U
F^{-1}



$$(|00\rangle + |01\rangle + |10\rangle + |11\rangle)|\psi\rangle$$

$$|00\rangle|\psi\rangle + |01\rangle U|\psi\rangle + |10\rangle U^2|\psi\rangle + |11\rangle U^3|\psi\rangle$$



$$|000\rangle|\psi\rangle + |001\rangle U|\psi\rangle + |010\rangle U^2|\psi\rangle + |011\rangle U^3|\psi\rangle +$$

$$|100\rangle U^4|\psi\rangle + |101\rangle U^5|\psi\rangle + |110\rangle U^6|\psi\rangle + |111\rangle U^7|\psi\rangle$$

Simulation of many body systems

A- Spin systems

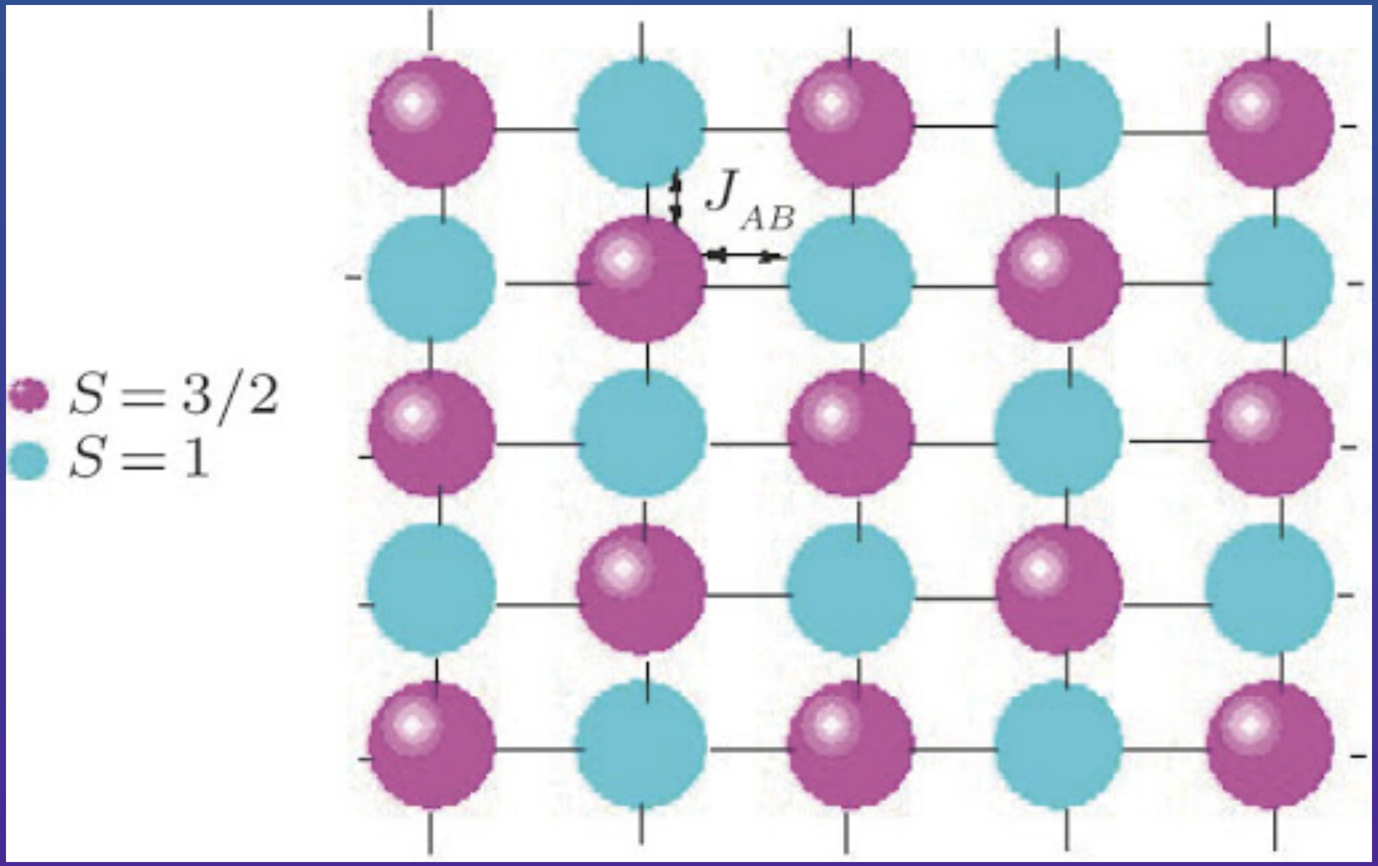
B- Bosonic systems

C- Fermionic systems

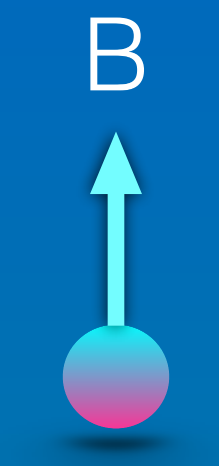
D- Field Theories

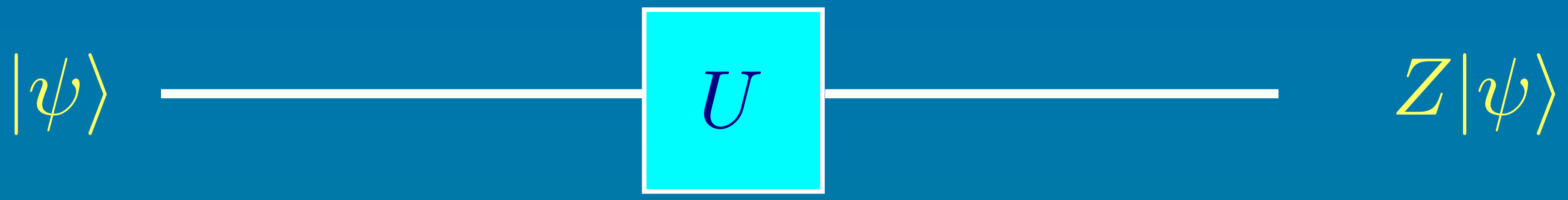
A-Spin Systems

Magnetic Systems



A single spin in a magnetic field

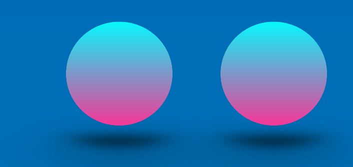




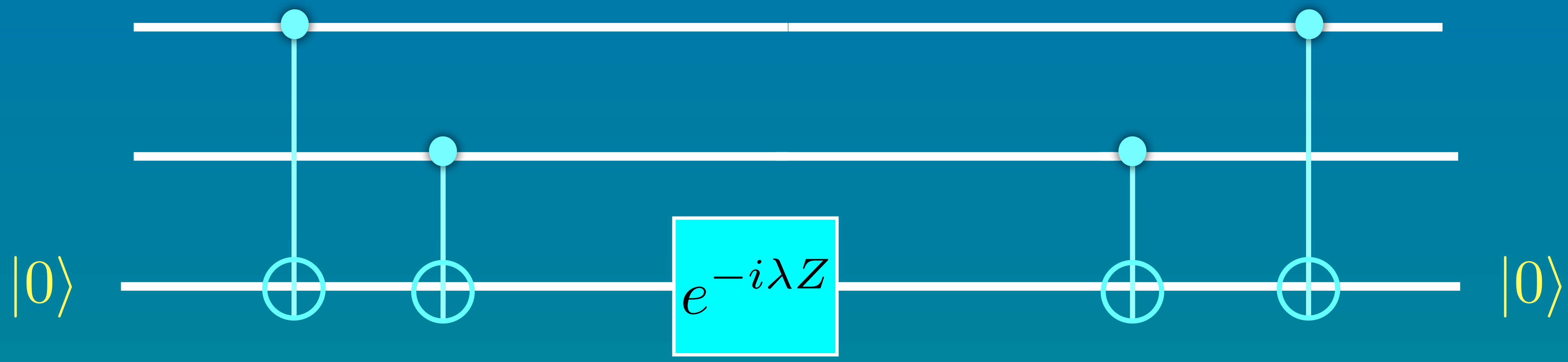
$$H = -\mu B \sigma_z$$

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

Two interacting spins

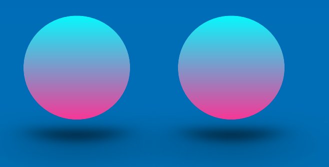


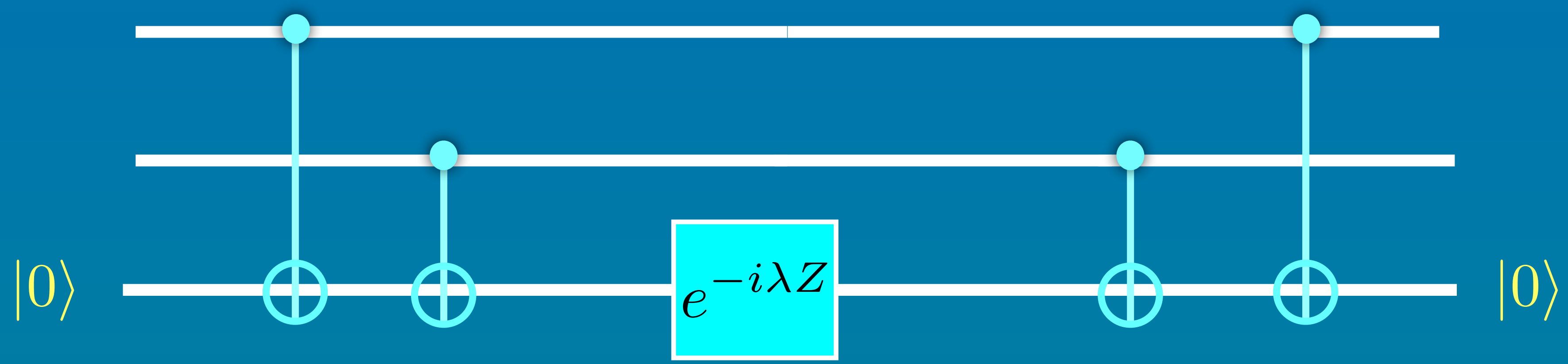
$$H = -JZ_1Z_2$$

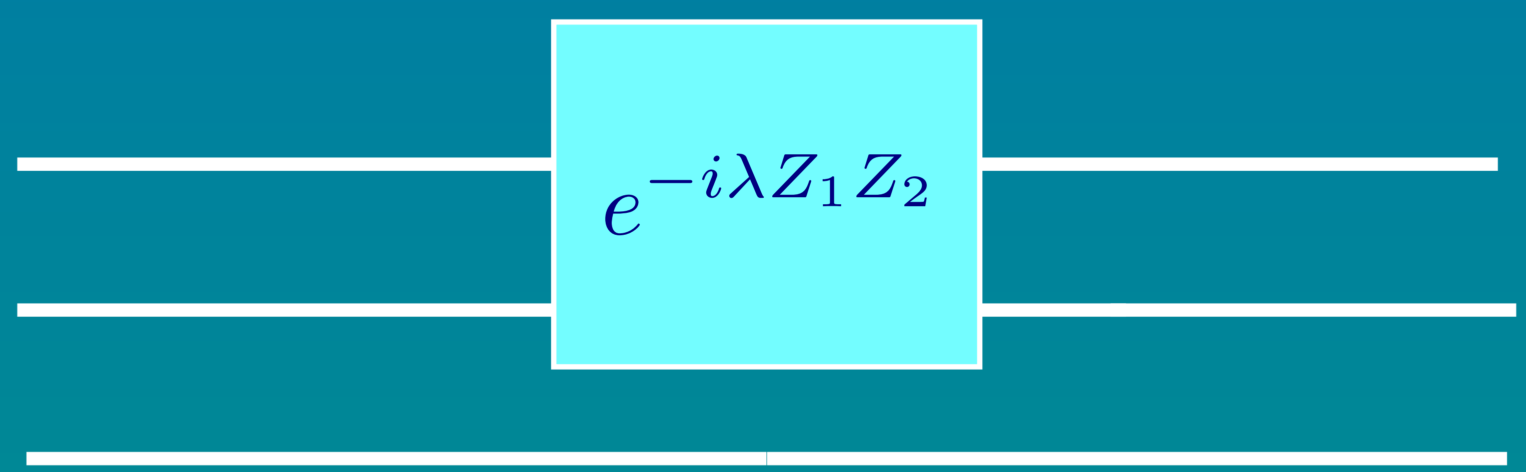


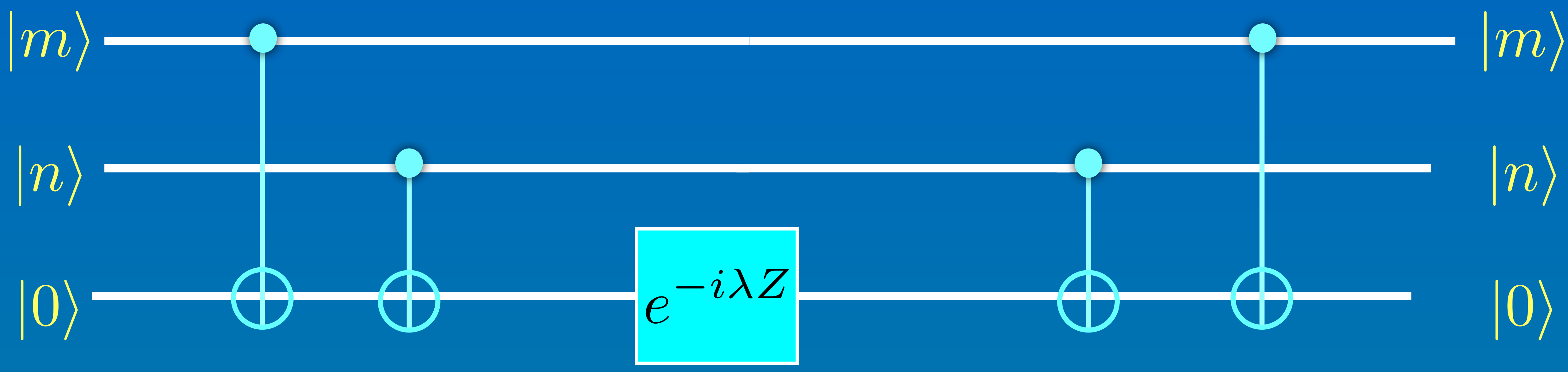
Two interacting spins

$$H = -JZ_1Z_2$$



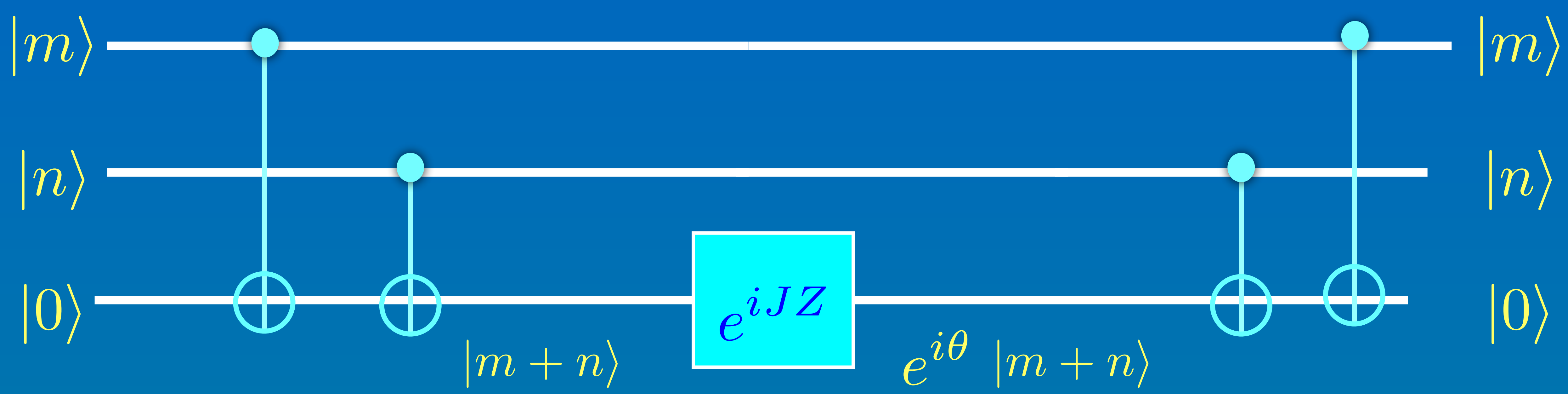






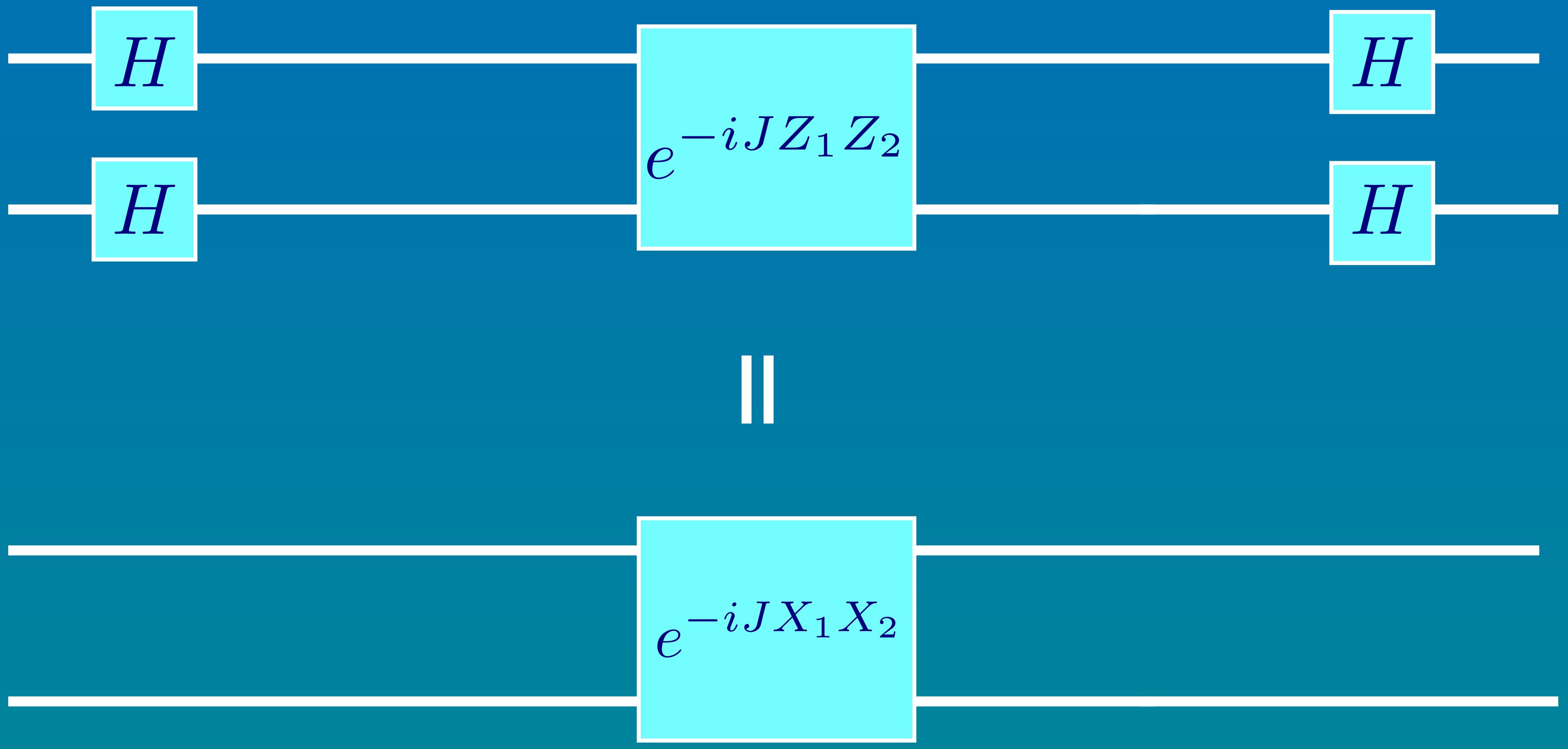
$$Z_1 Z_2 = Z \otimes Z = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix} \begin{matrix} 00 \\ 01 \\ 10 \\ 11 \end{matrix}$$

$$U = e^{-iH} = e^{iJZ_1Z_2} = \begin{pmatrix} e^{iJ} & & & \\ & e^{-iJ} & & \\ & & e^{-iJ} & \\ & & & e^{iJ} \end{pmatrix}$$



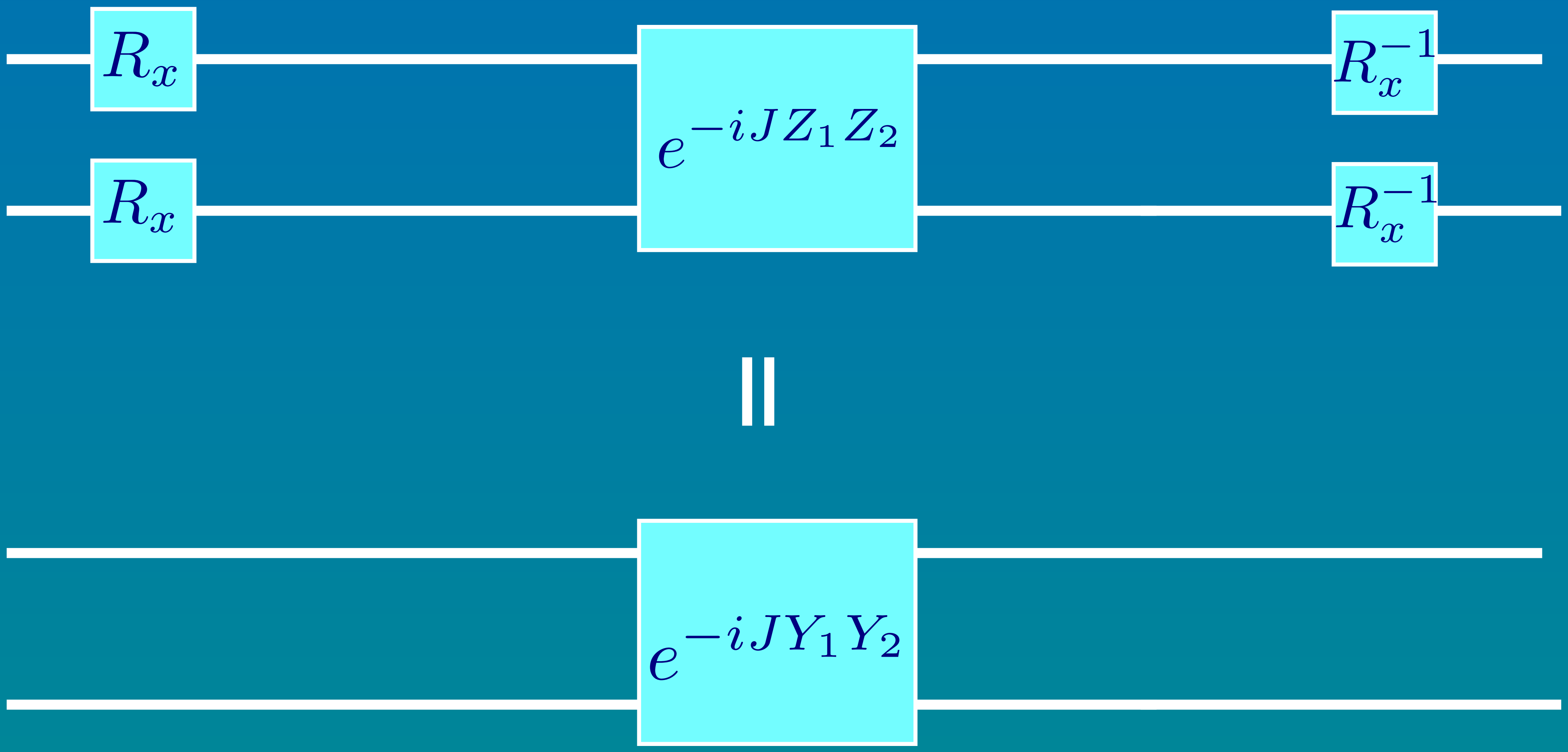
$$U = e^{-iH} = e^{iJZ_1Z_2} = \begin{pmatrix} e^{iJ} & & & \\ & e^{-iJ} & & \\ & & e^{-iJ} & \\ & & & e^{iJ} \end{pmatrix} \begin{matrix} 00 \\ 01 \\ 10 \\ 11 \end{matrix}$$

$$H = -JX_1X_2$$

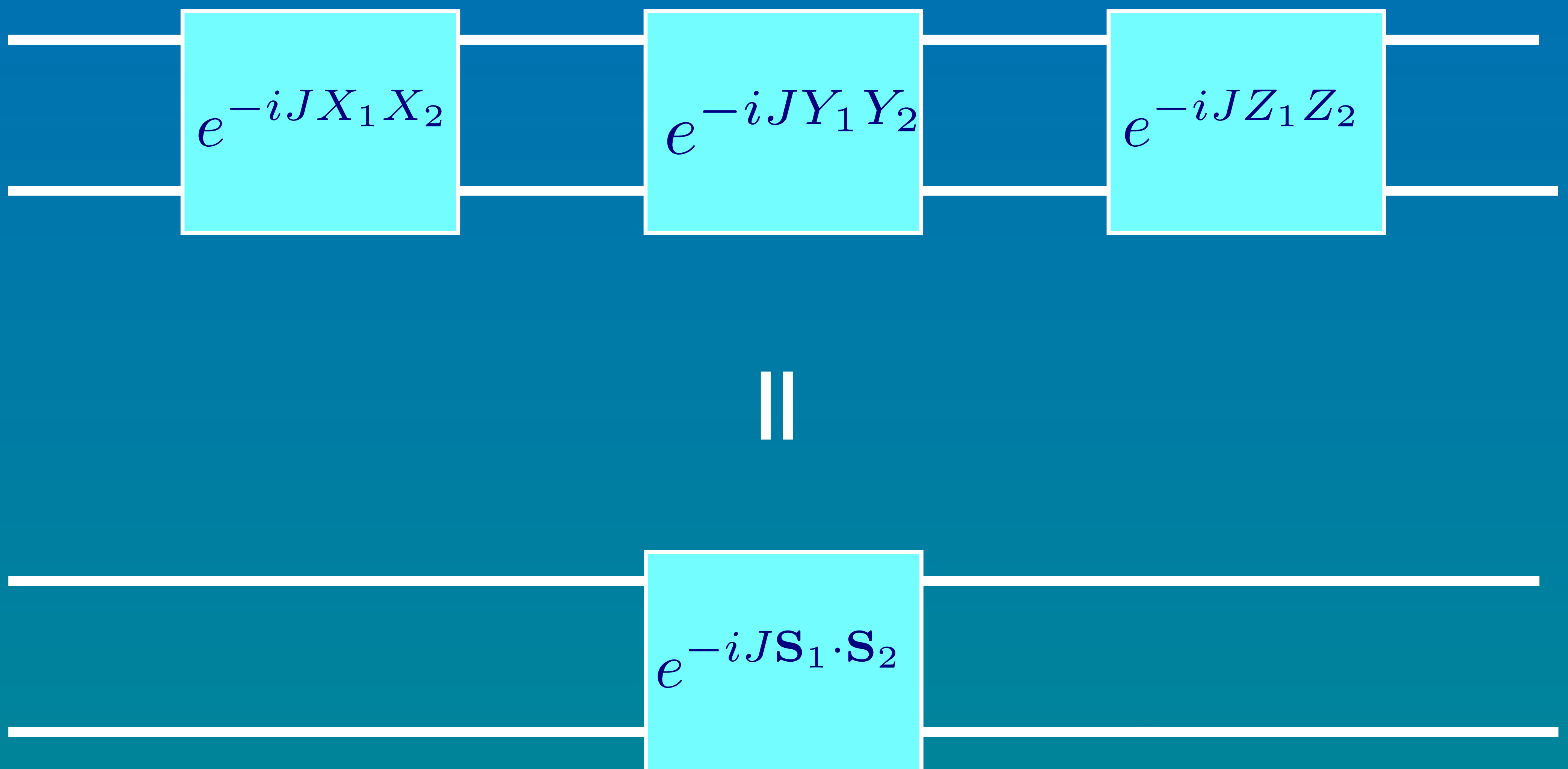


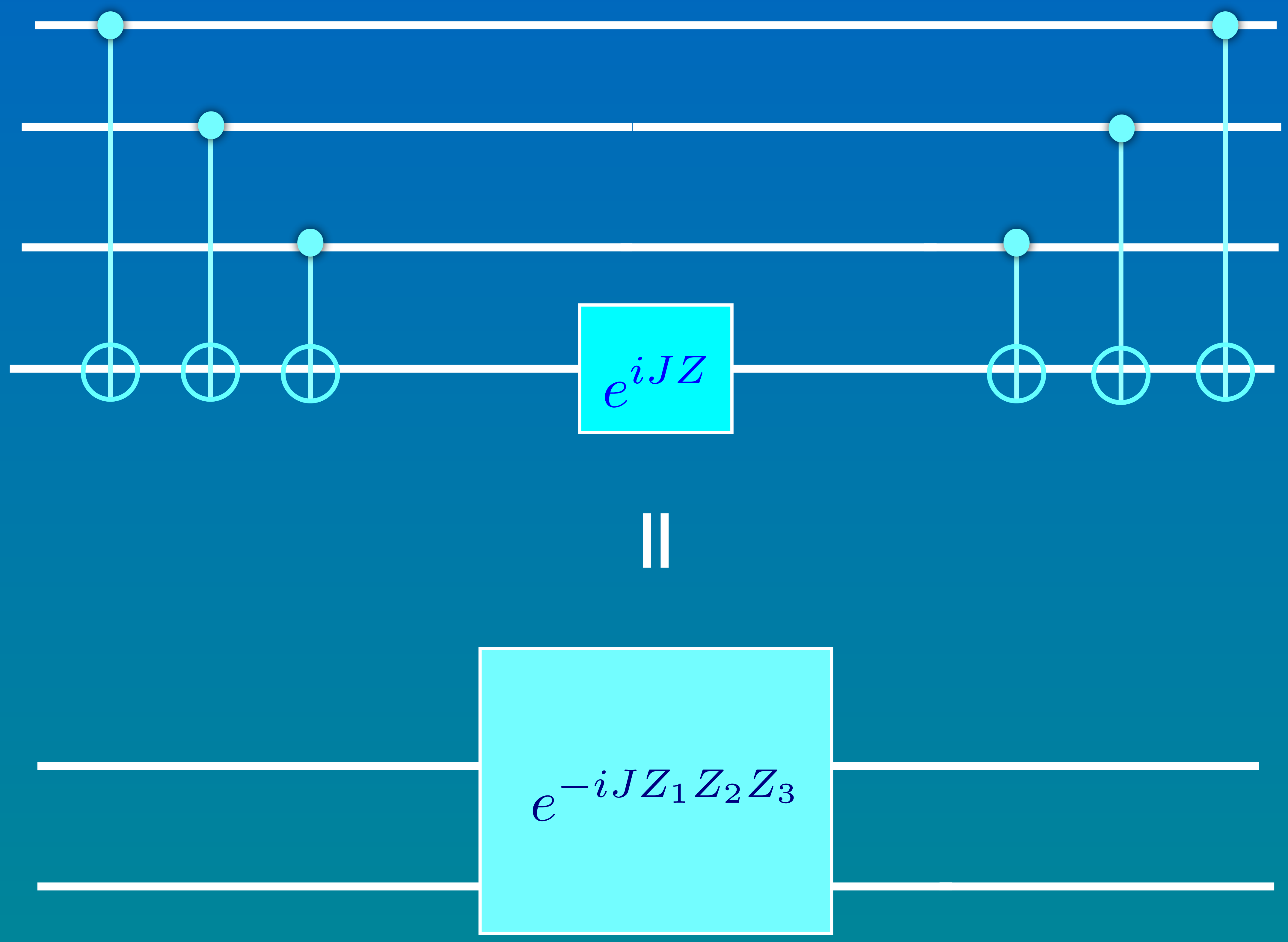
$$H = -JY_1Y_2$$

x

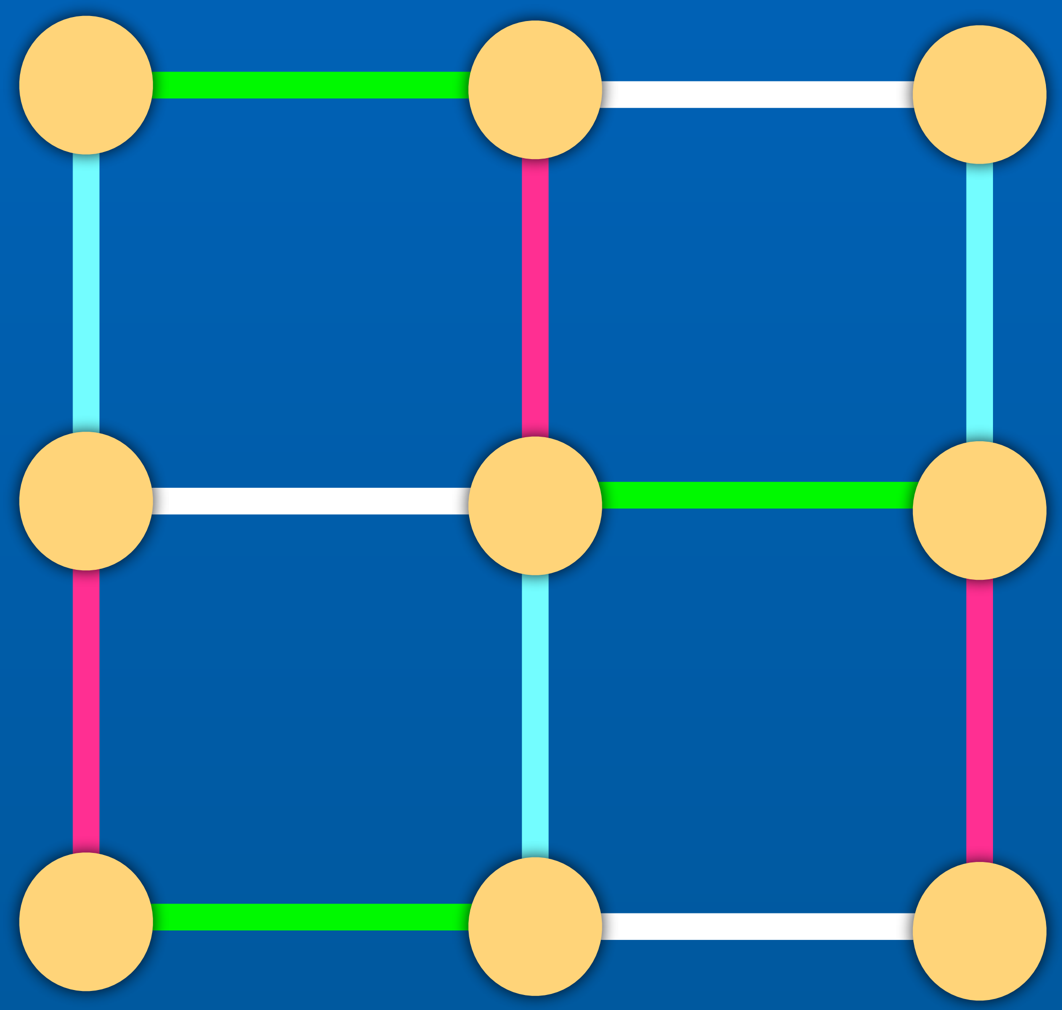


$$H = -J Z_1 Z_2 Z_3 \cdots Z_N$$




e^{iJZ}
=
$e^{-iJZ_1Z_2Z_3}$

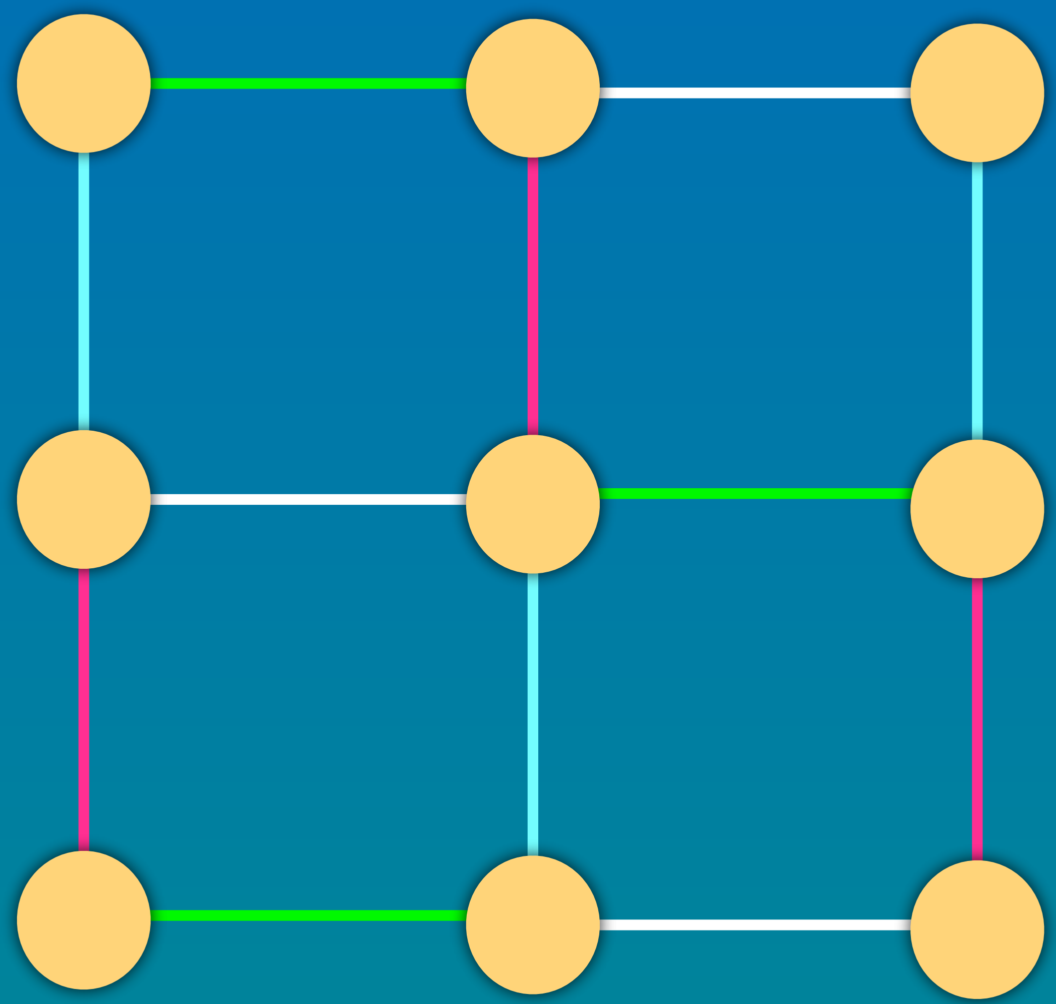
Non-Commuting Terms



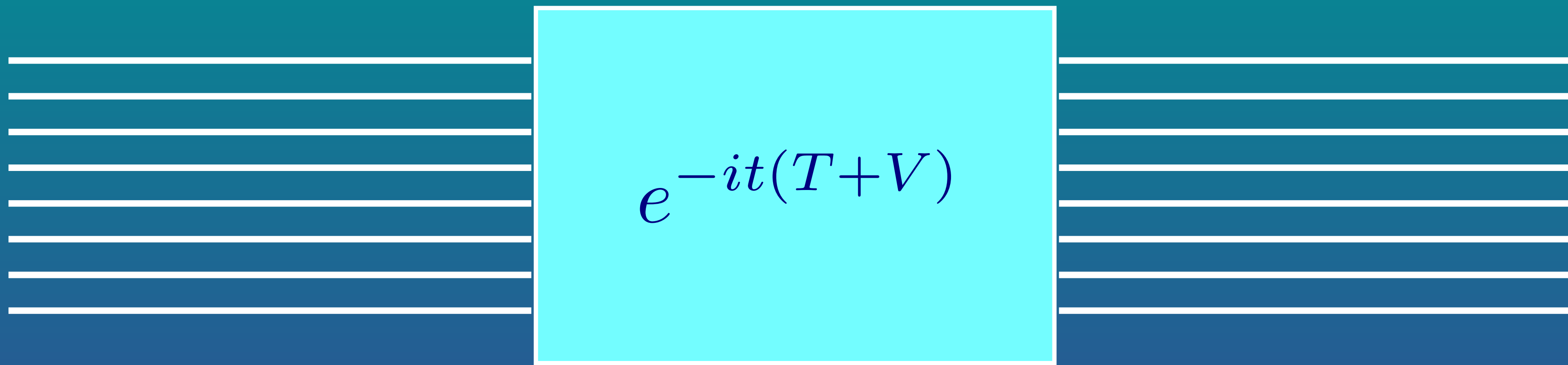
$$H = H_1 + H_2 + H_3 + H_4$$

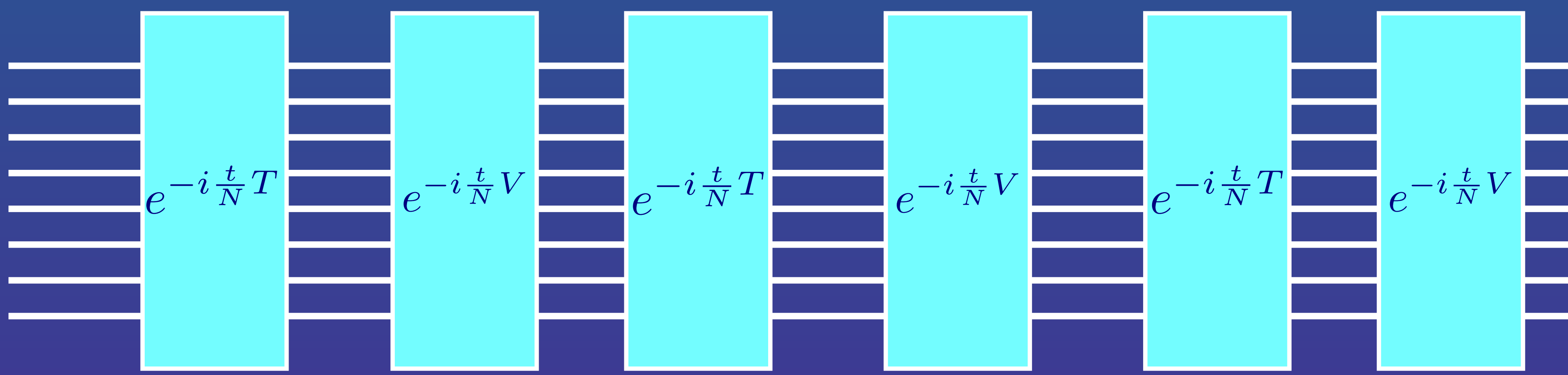
Suzuki-Trotter Formula

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



$$e^{-iHt}a \approx \left[e^{\frac{it}{N}H_1}e^{\frac{it}{N}H_2}e^{\frac{it}{N}H_3}e^{\frac{it}{N}H_4}\right]^N$$



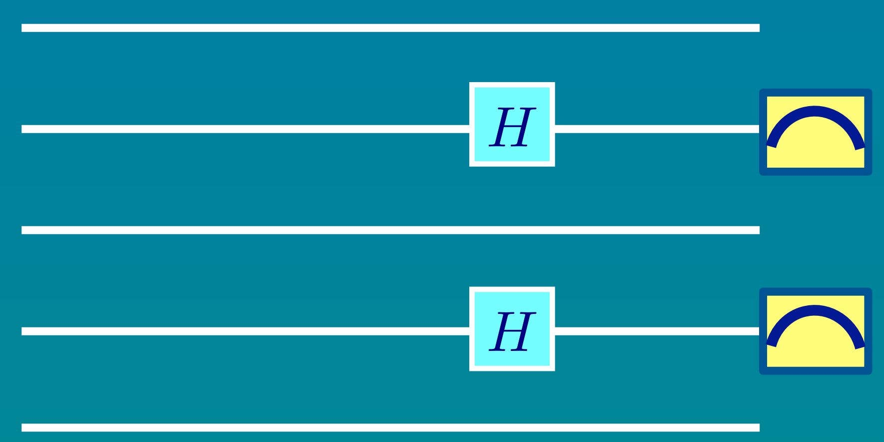


$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i,j} V(\mathbf{r}_i - \mathbf{r}_j)$$

Measurement

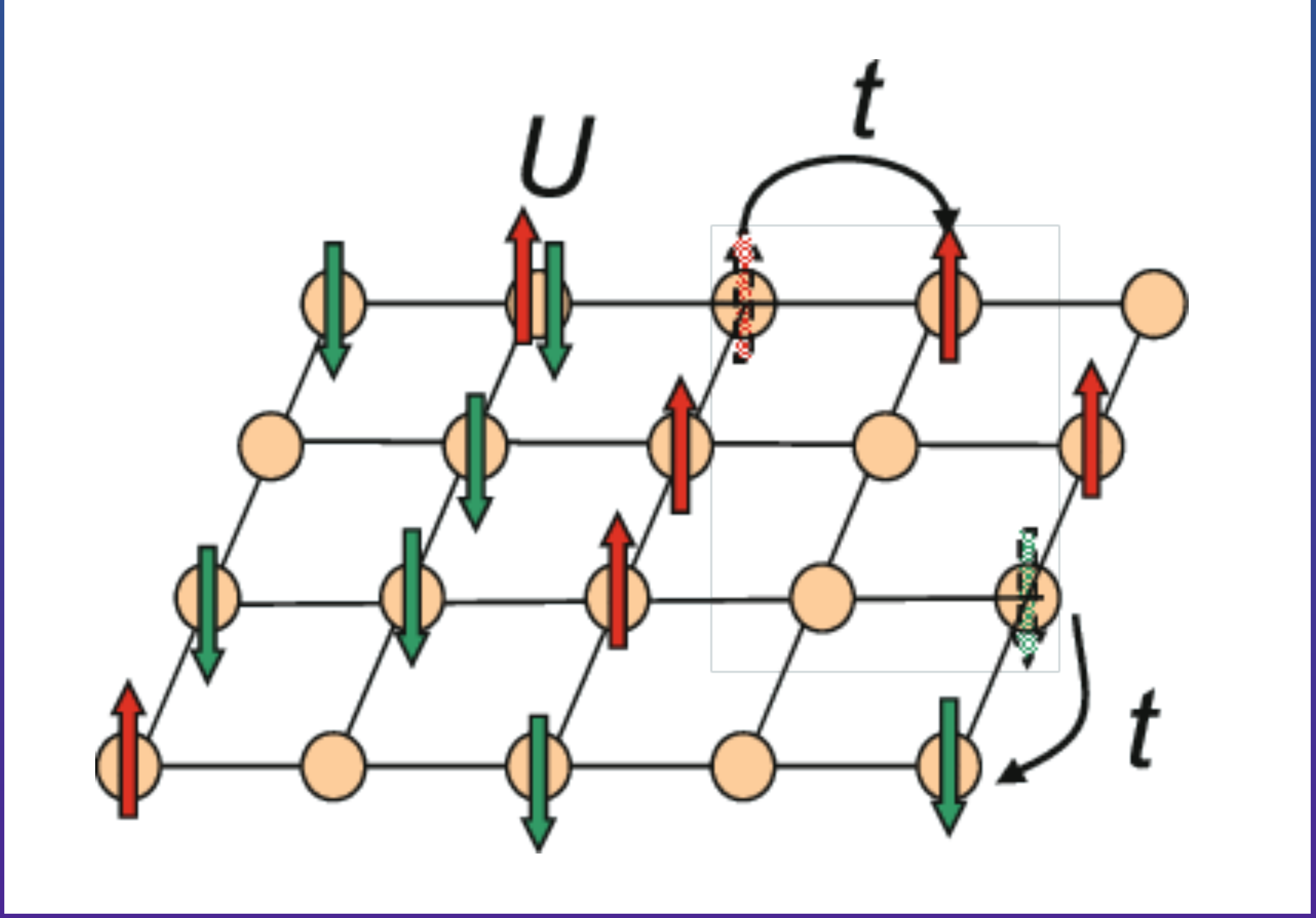
$\langle Z_i Z_j \rangle$

$\langle X_i X_j \rangle$



B-Fermionic Systems

Electron Gas, Hubbard Model, Superconductivity,….



Fermionic Systems

$|\Psi\rangle$

$-|\Psi\rangle$

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

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?

How to create a fermion?

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

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

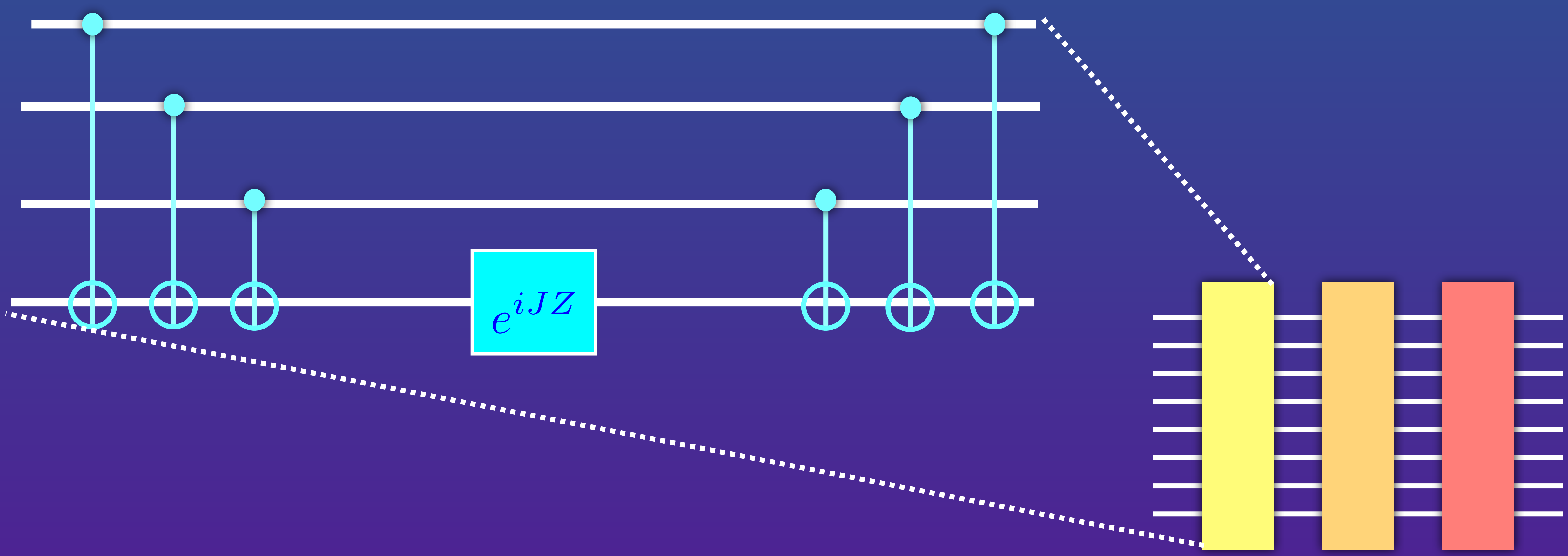
$$= \cos\frac{\pi}{2}I + i\sin\frac{\pi}{2}(c+c^\dagger) \;\; = i(c+c^\dagger)$$

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

$$|\Psi\rangle = c_{j_1}^\dagger c_{j_2}^\dagger \cdots c_{j_n}^\dagger |0\rangle$$

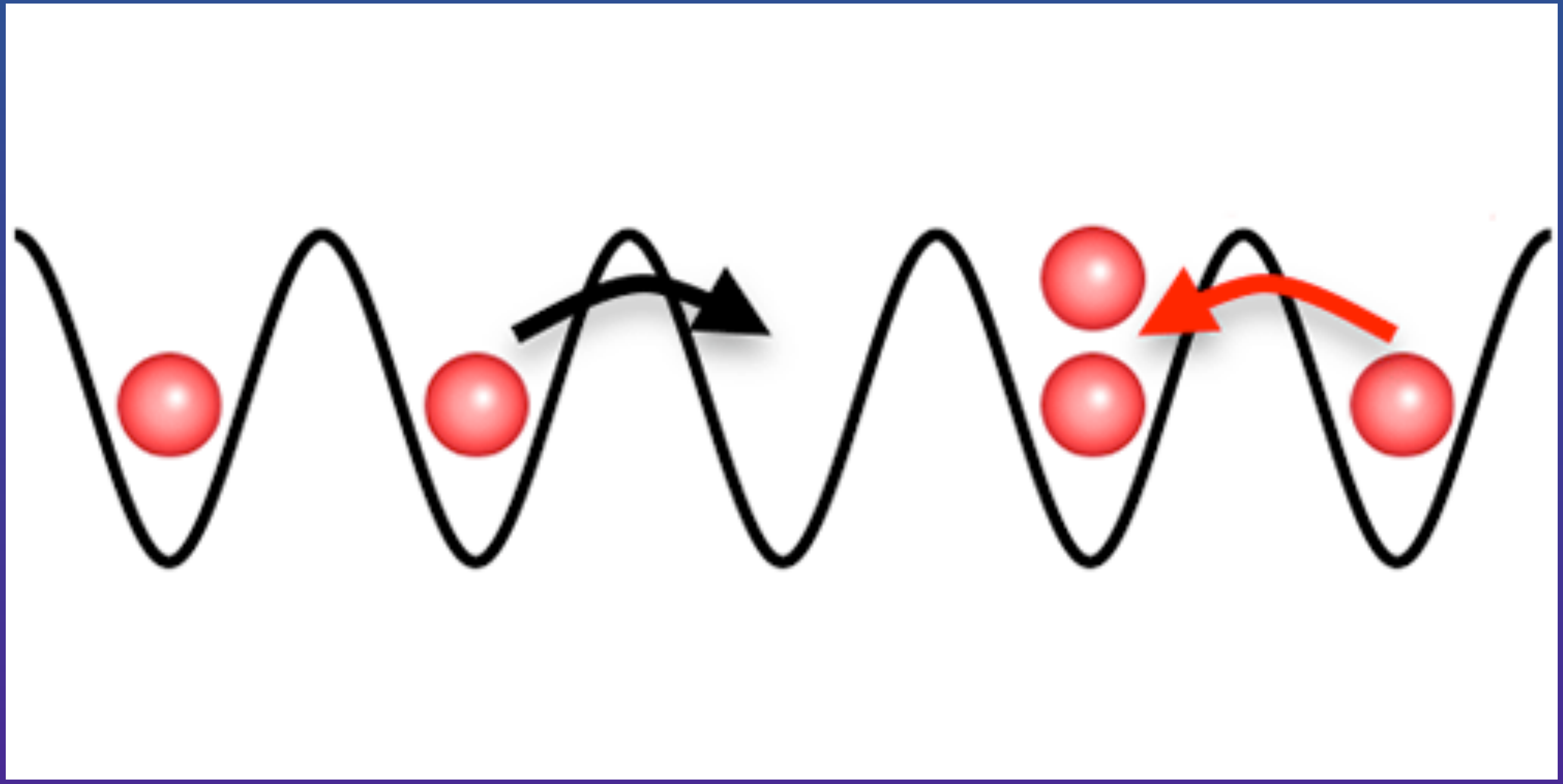
$$= e^{i\frac{\pi}{2}(c_{j_1}+c_{j_1}^\dagger)} \ldots e^{i\frac{\pi}{2}(c_{j_n}+c_{j_n}^\dagger)}|0\rangle$$

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



C-Bosonic Systems

Bose-Hubbard Model,…



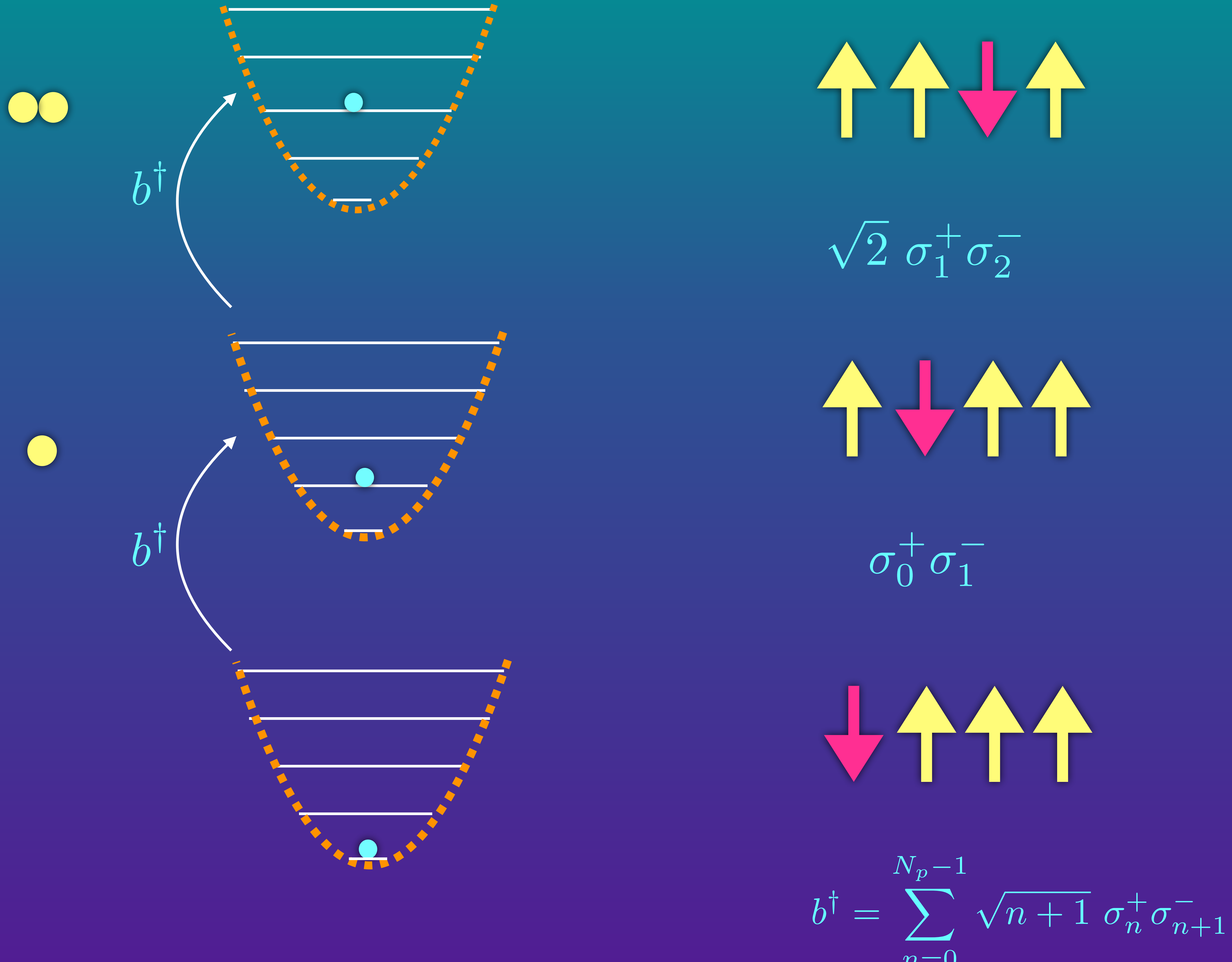
$$|0\rangle_b = |1, 0, 0, \cdots 0\rangle$$

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

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

$$\cdots\cdots\cdots\cdots$$

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



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

$$\hat{n} = \frac{(1 - Z)}{2} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

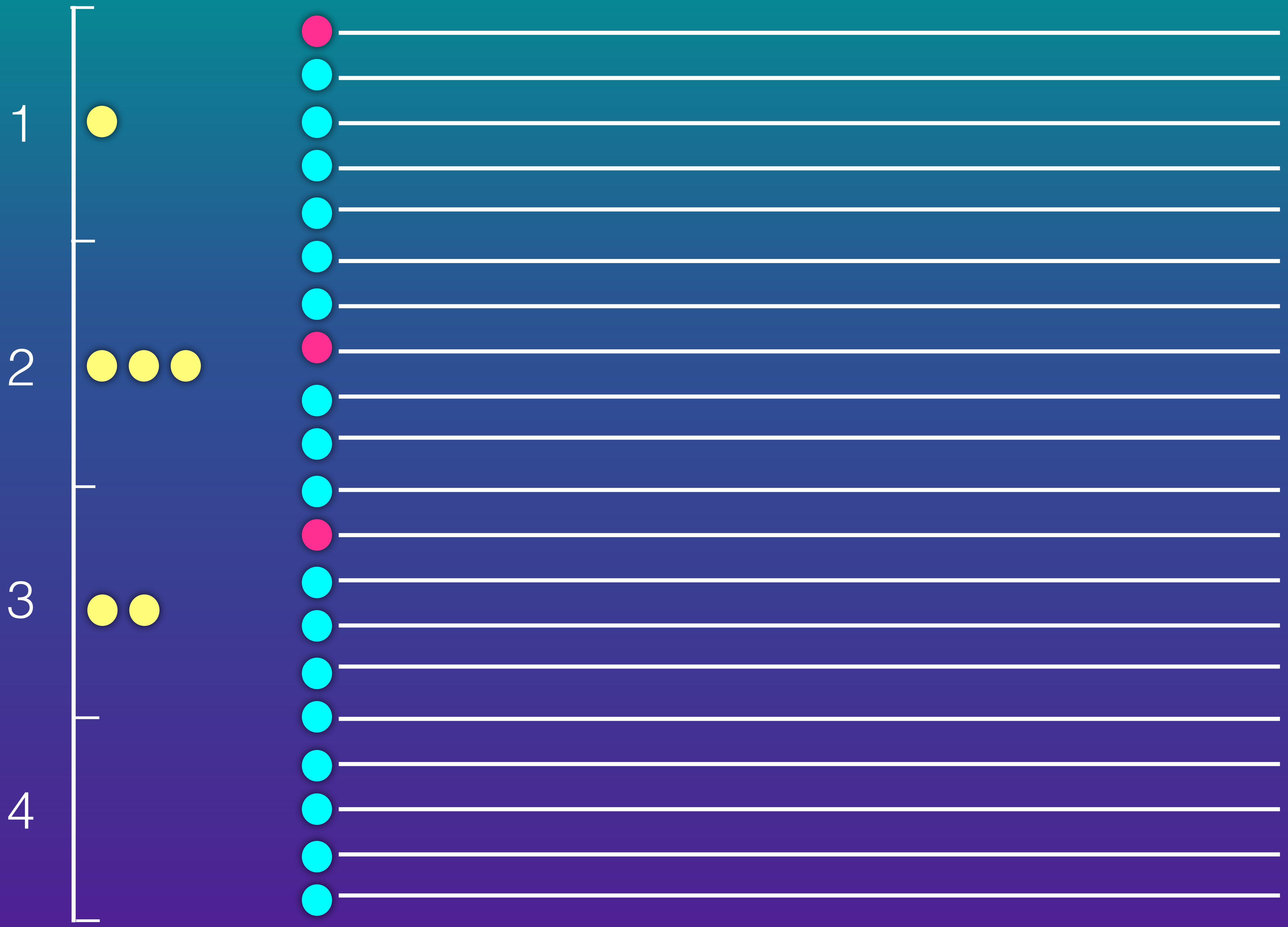
0 0 1 0 0

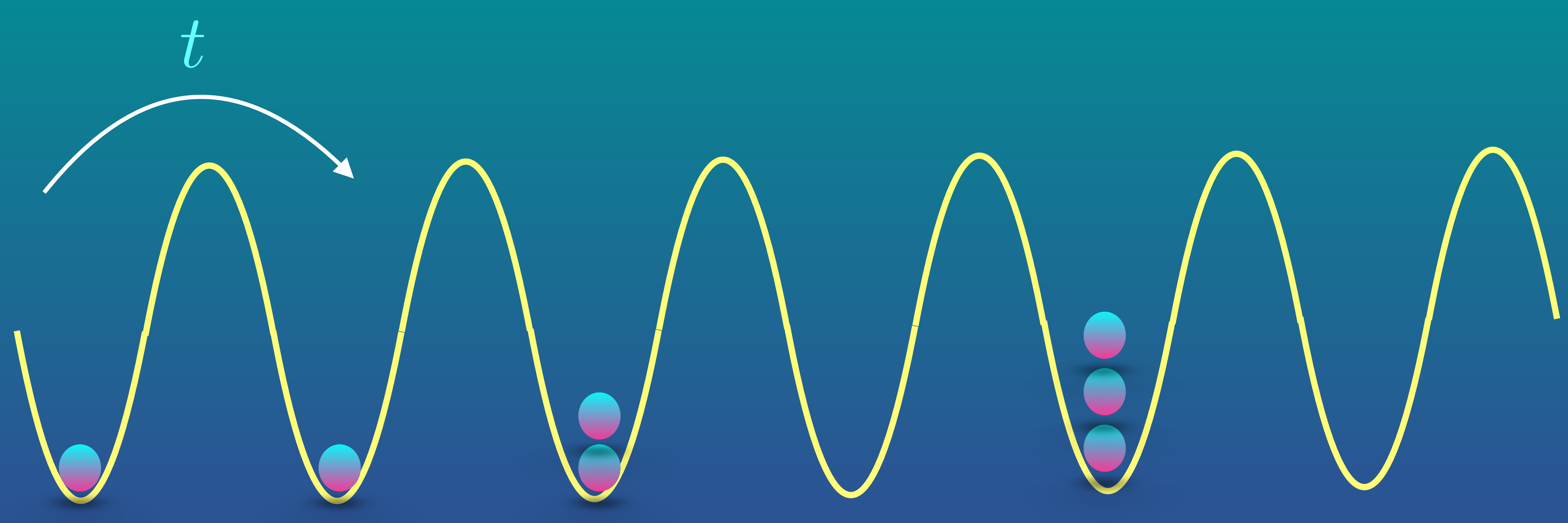
$$\hat{n}_k = \frac{1 - Z_k}{2}$$

0 1 0 0 0

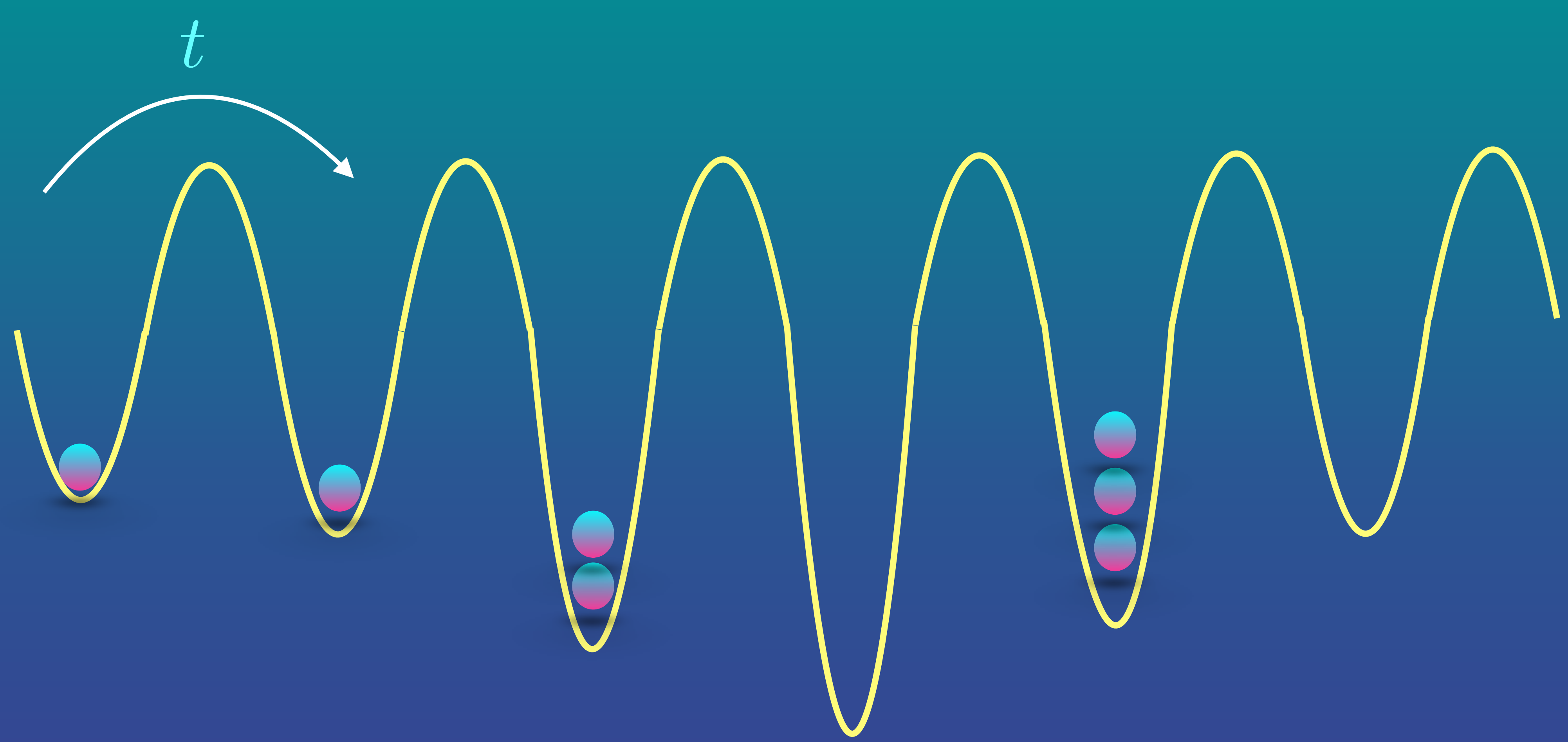
$$\hat{Q} = \sum_{k=0}^{N} \hat{n}_k$$

1 0 0 0 0

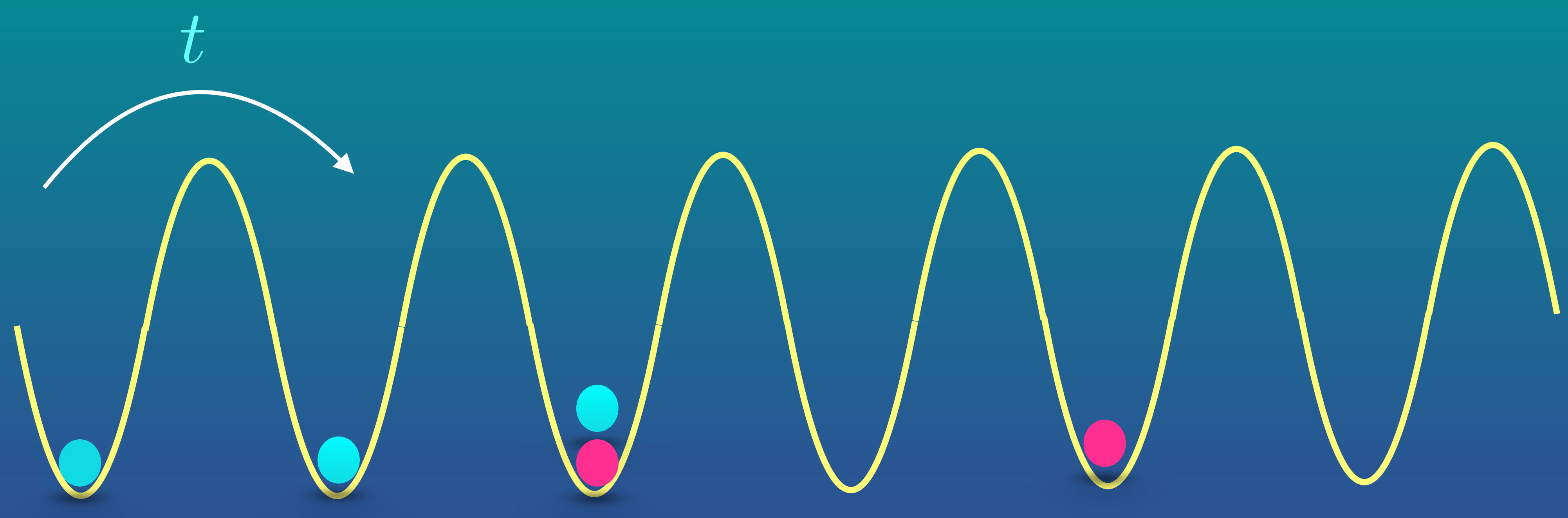

1
2
3
4



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

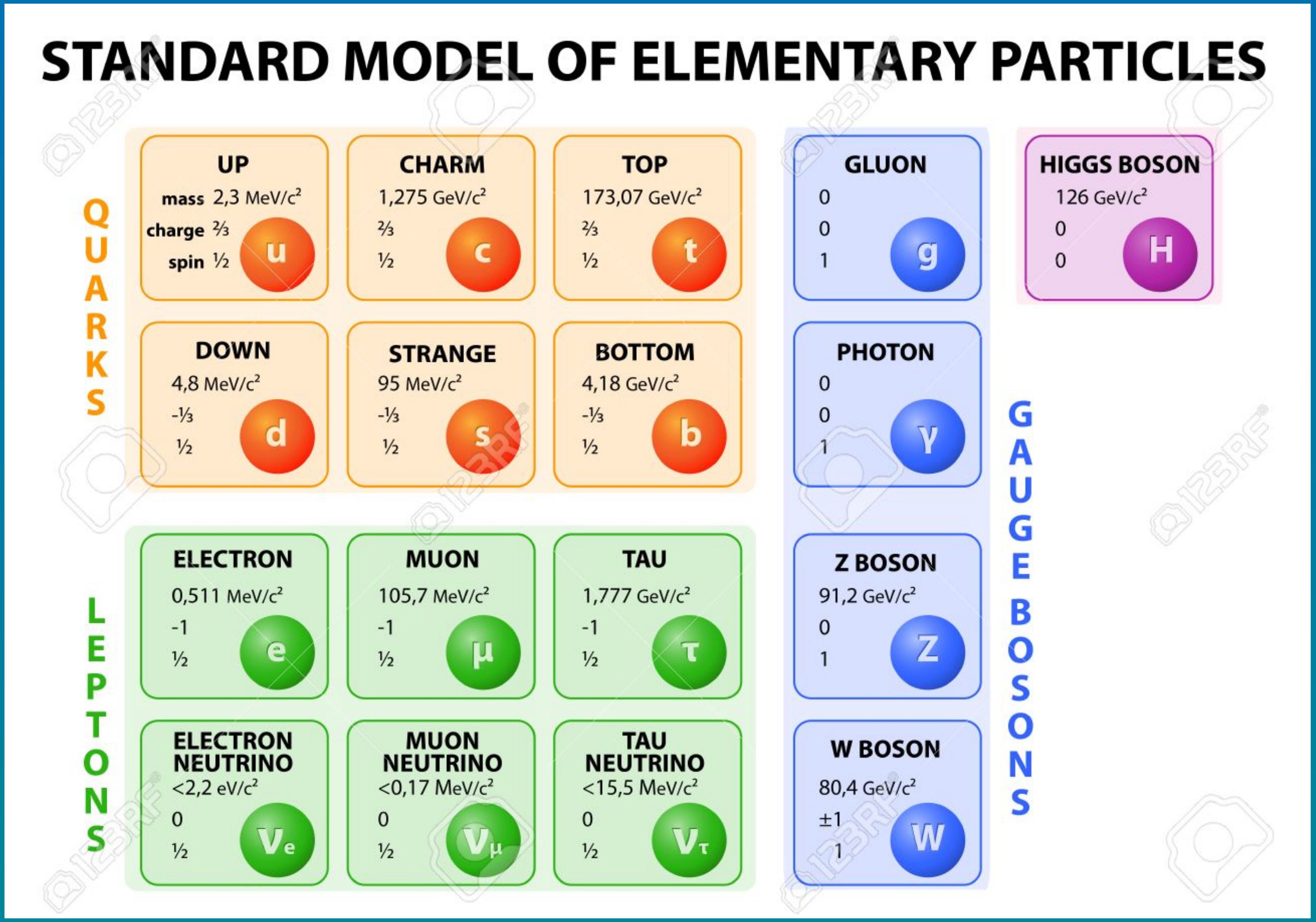


$$H = \sum_{\langle i,j \rangle} b_i^\dagger b_j + \sum_i \epsilon_i n_i + \sum_i n_i(n_i - 1)$$



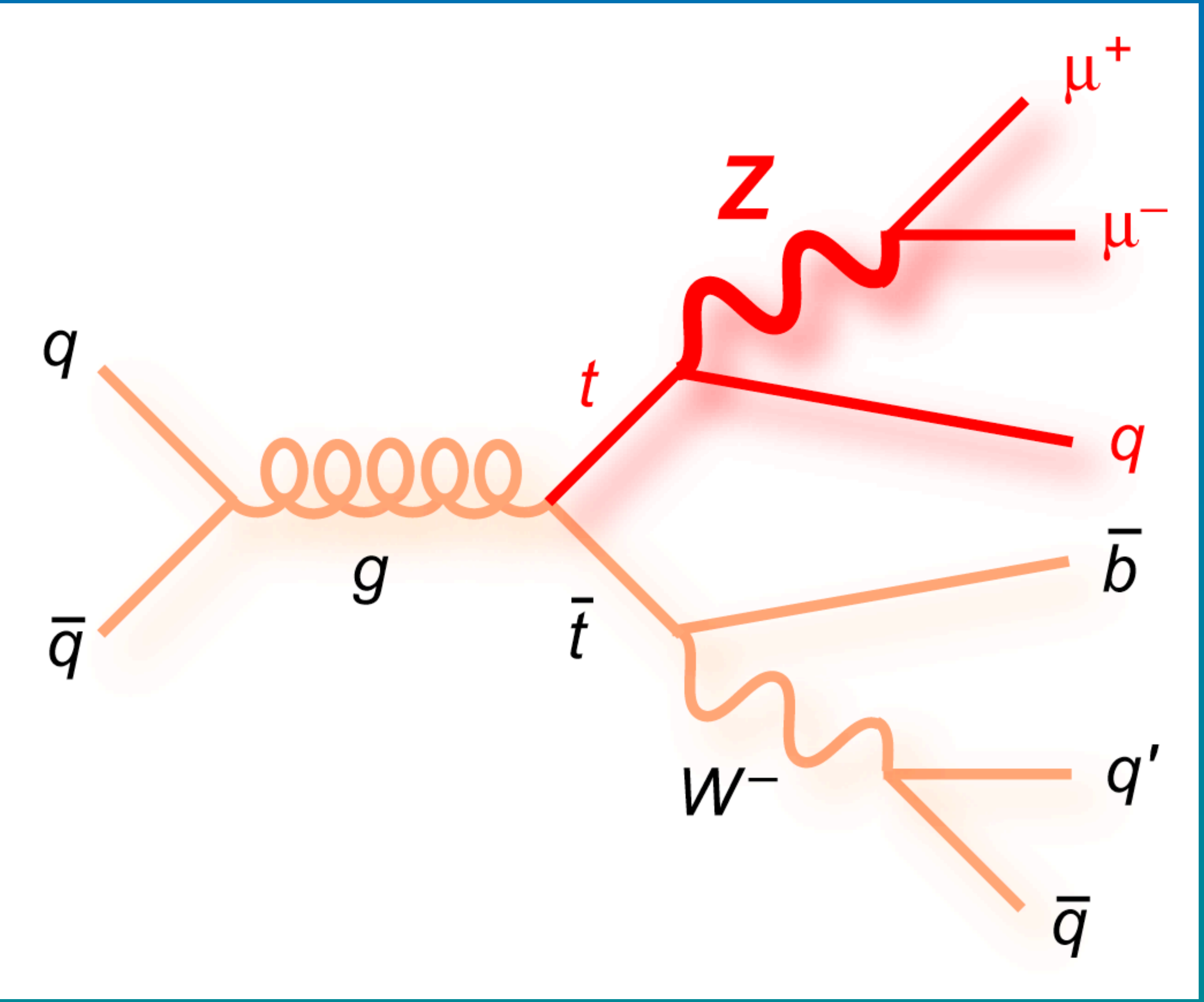
$$H = t \sum_{\langle i,j,\sigma \rangle} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \sum_{i} \epsilon_{i,\sigma} n_{i,\sigma} + U \sum_{i,\sigma} n_{i,\sigma} n_{i,\overline{\sigma}}$$

D-Particle Physics and Field Theory

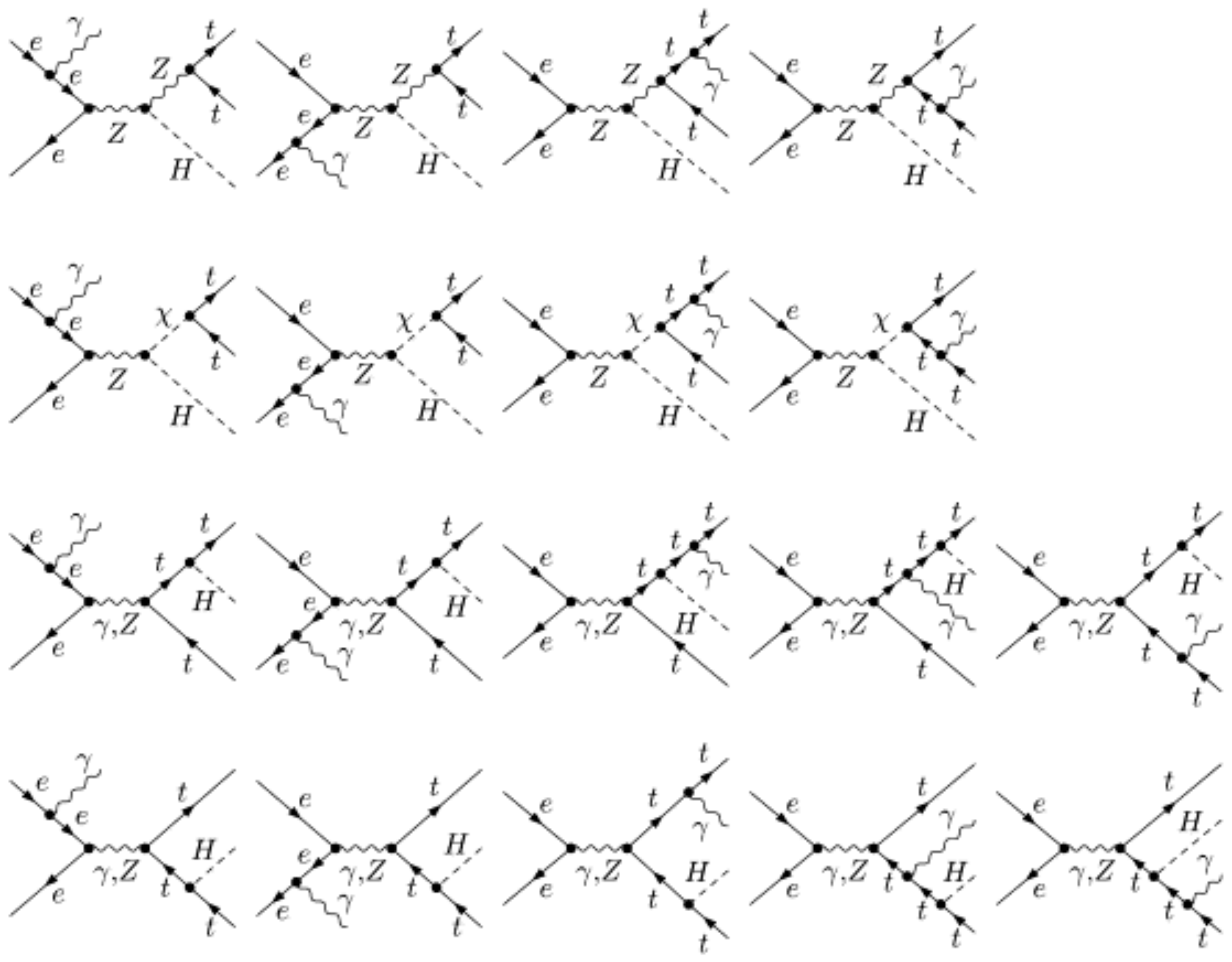


Feynman diagrams

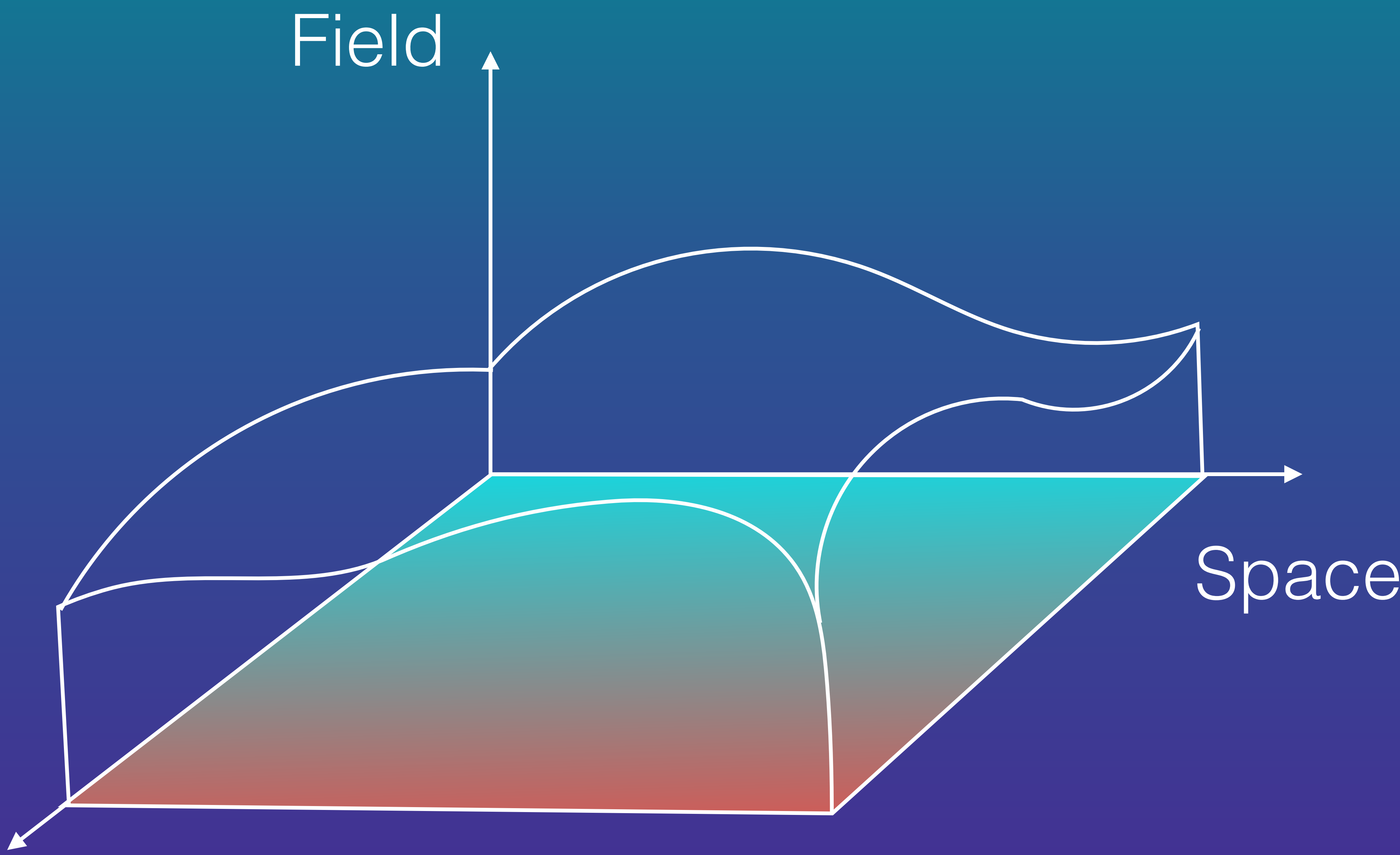
Perturbative Calculations



Thousands of Feynman diagrams

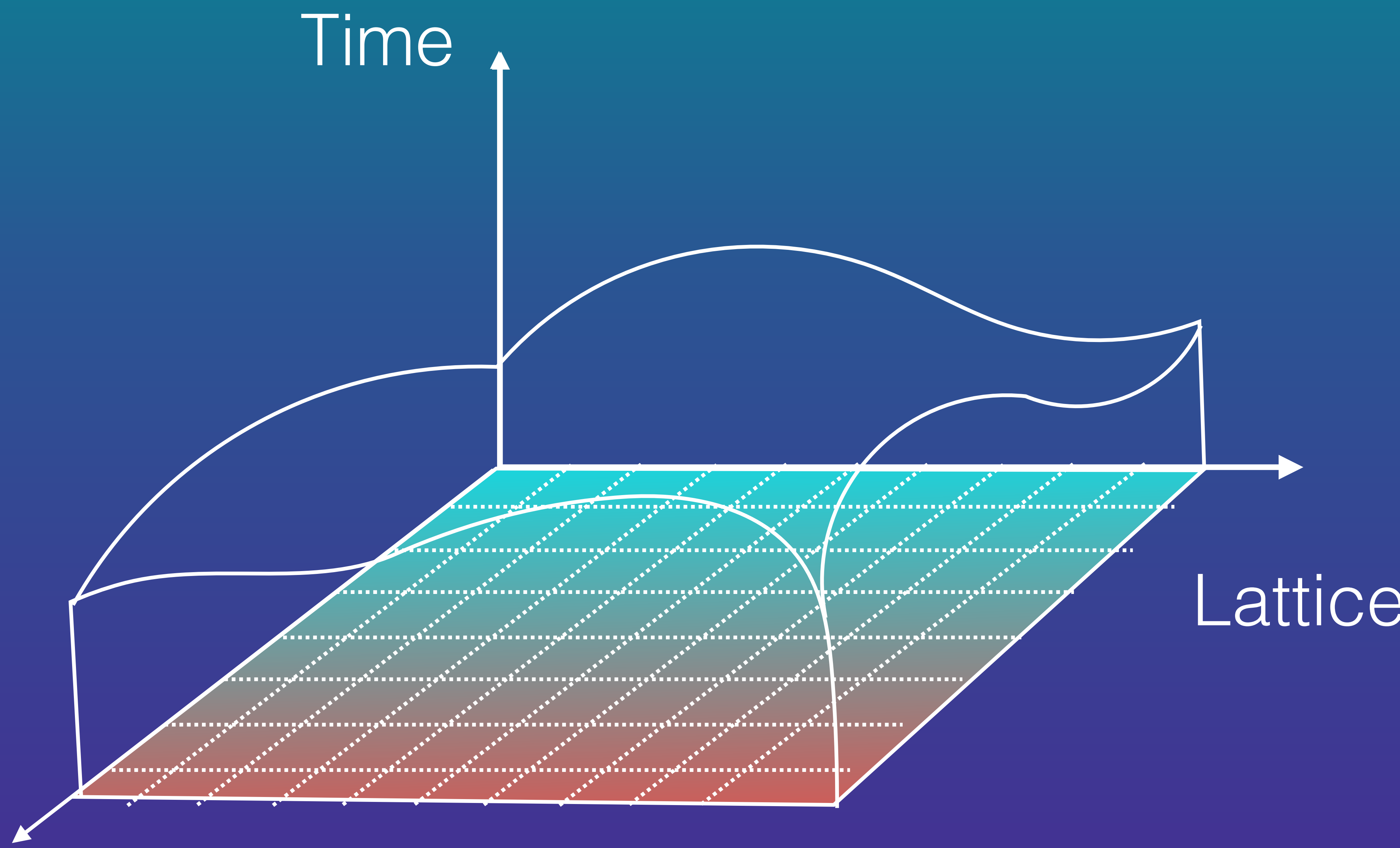


Quantum Field Theory



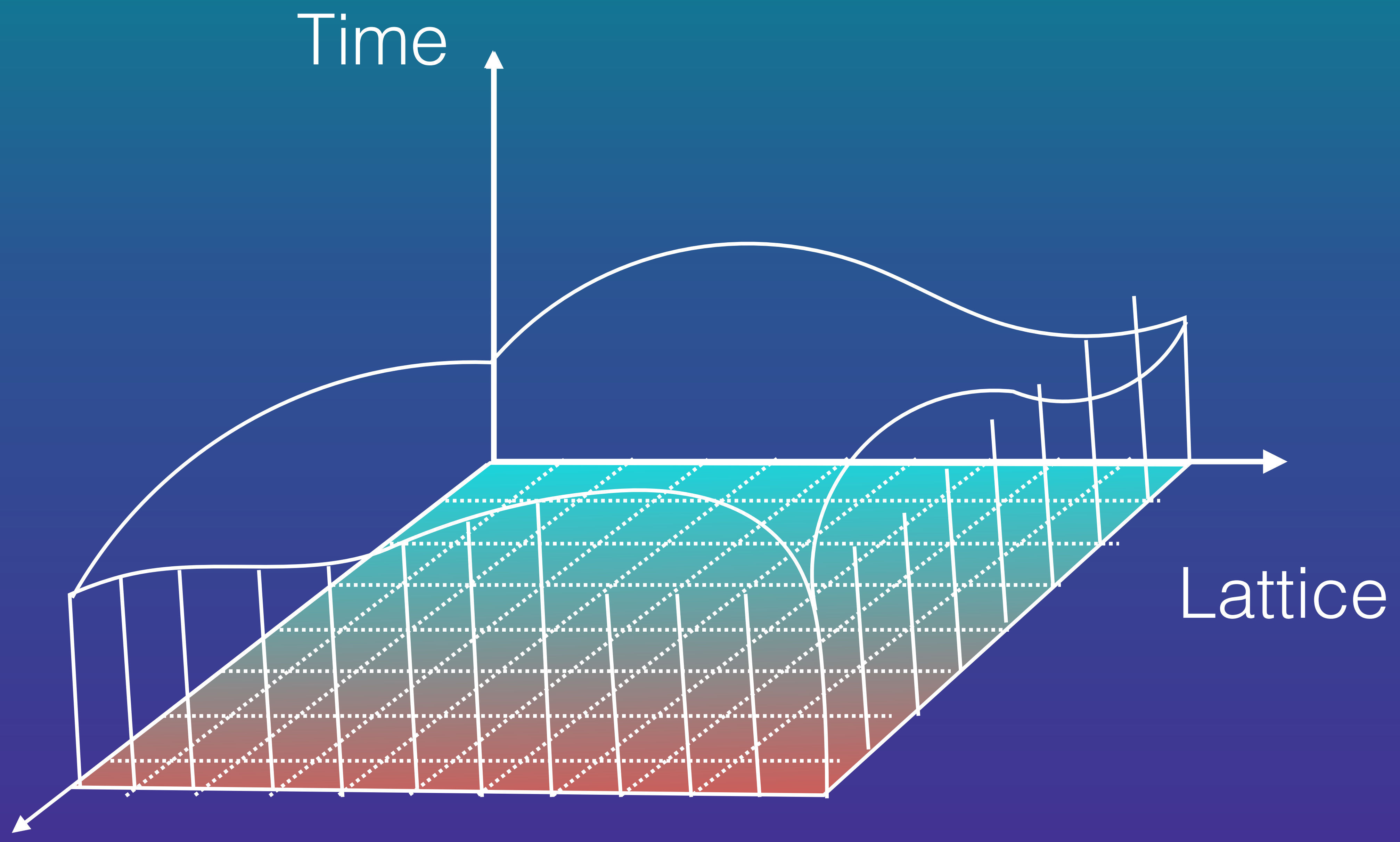
$$H = \int d^D x [\frac{1}{2}\pi(x)^2 + \frac{1}{2}(\nabla\phi)^2(x) + \frac{1}{2}m^2\phi(x)^2 + \frac{\lambda}{4}\phi(x)^4]$$

Quantum Field Theory



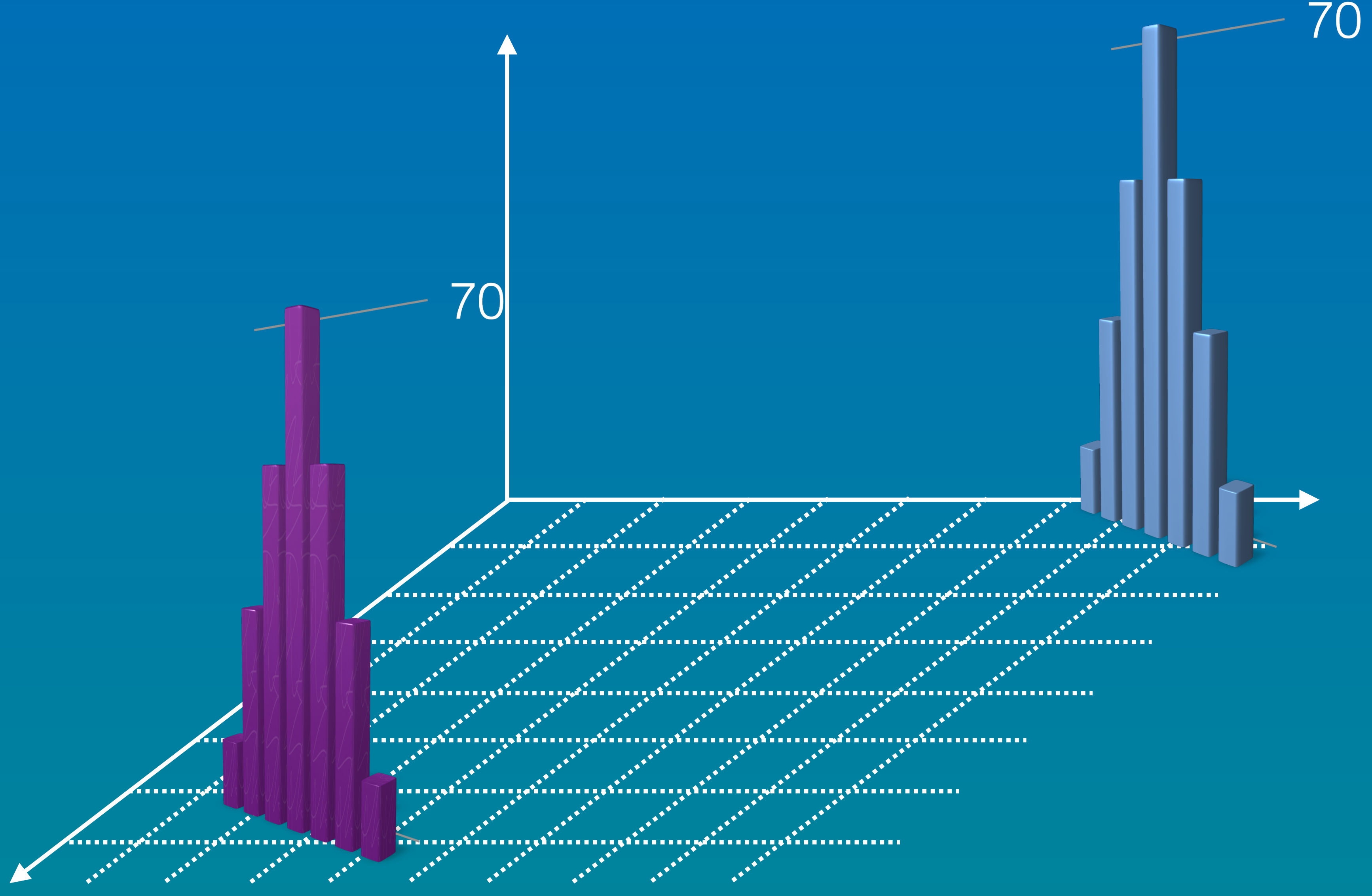
$$H = a^D \sum_{\mathbf{n}} [\frac{1}{2}\pi(\mathbf{n})^{\mathbf{2}} + \frac{\mathbf{1}}{\mathbf{2}}(\nabla\phi)^{\mathbf{2}}(\mathbf{n}) + \frac{\mathbf{1}}{\mathbf{2}}\mathbf{m}^{\mathbf{2}}\phi(\mathbf{n})^{\mathbf{2}} + \frac{\lambda}{\mathbf{4}}\phi(\mathbf{n})^{\mathbf{4}}]$$

Many body boson or fermion

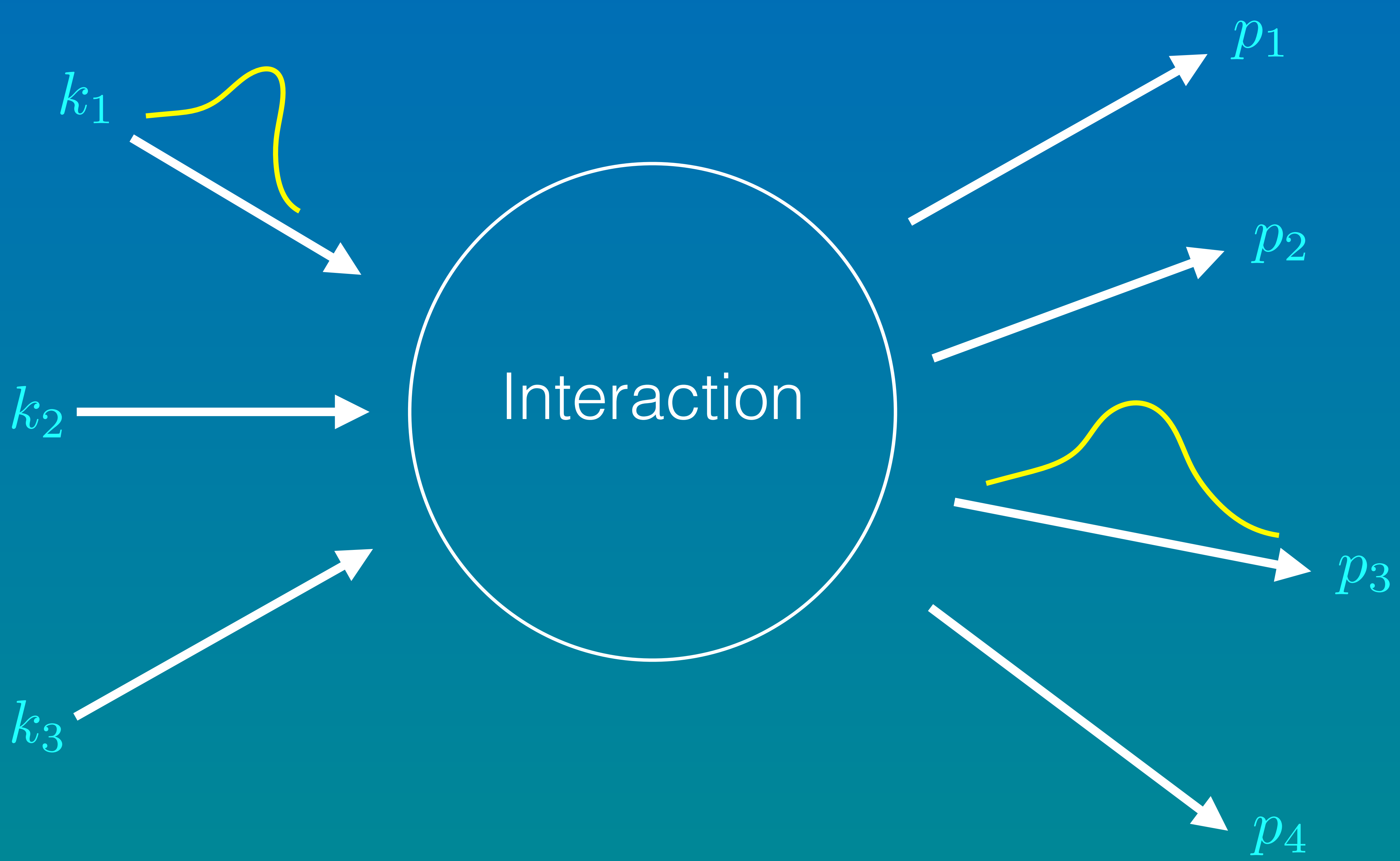


$$H = a^D \sum_{\mathbf{n}} [\frac{1}{2}\pi(\mathbf{n})^{\mathbf{2}} + \frac{\mathbf{1}}{\mathbf{2}}(\nabla\phi)^{\mathbf{2}}(\mathbf{n}) + \frac{\mathbf{1}}{\mathbf{2}}\mathbf{m}^{\mathbf{2}}\phi(\mathbf{n})^{\mathbf{2}} + \frac{\lambda}{\mathbf{4}}\phi(\mathbf{n})^{\mathbf{4}}]$$

Scattering



Quantum Field Theory



Thank you for your attention