

# Algorithms for quantum dynamics

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Quantum Computing and Nuclear Few- and Many-Body Problems

June 20, 2022



MICHIGAN STATE  
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NUCLEI  
Nuclear Computational Low-Energy Initiative  
A SciDAC-4 Project



## Outline

Nuclear dynamics

Time-dependent Schrödinger equation

Spin model Hamiltonians

CNOT gates

Unitary operators on two qubits

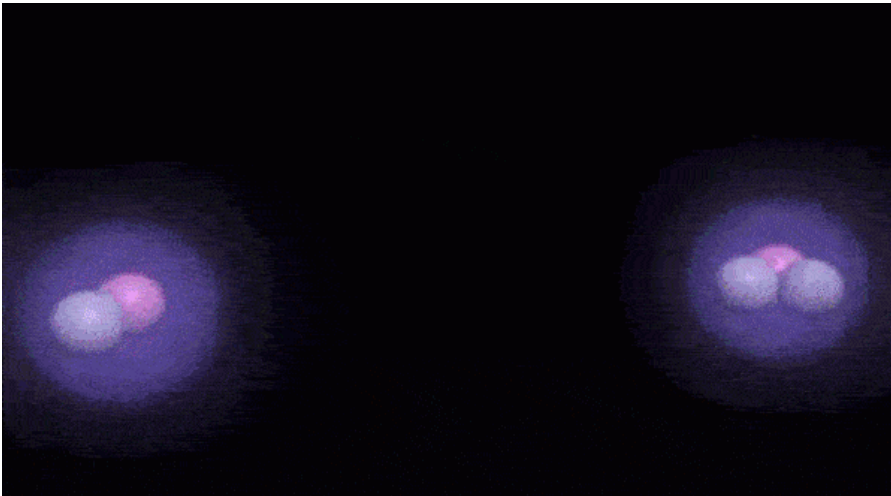
Trotter decomposition

Time evolution of Heisenberg spin chains

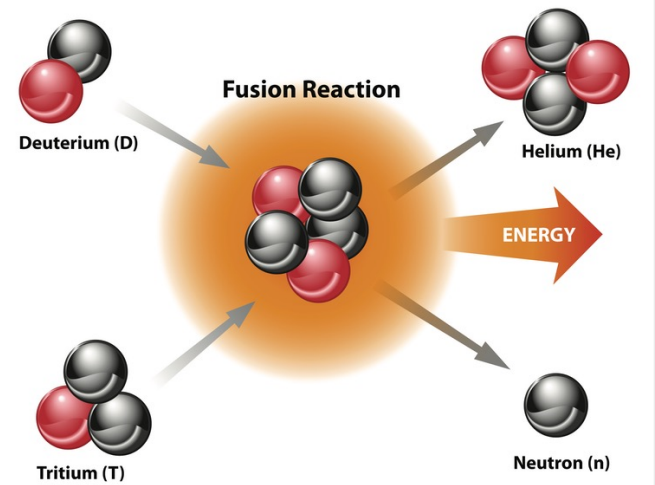
Projected cooling algorithm

# Nuclear dynamics

## Fusion

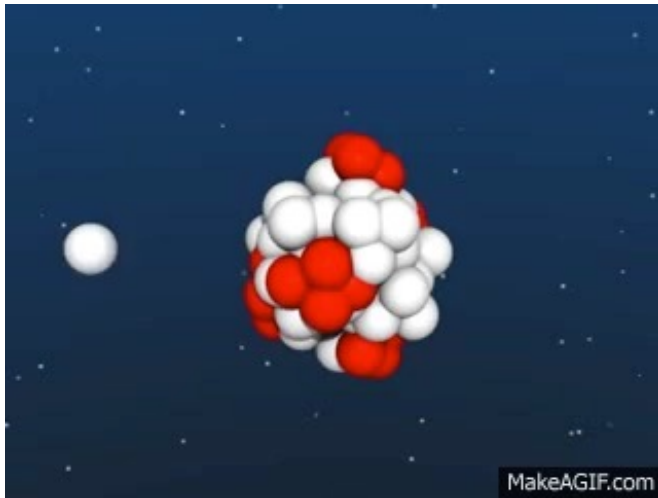


thehustle.co

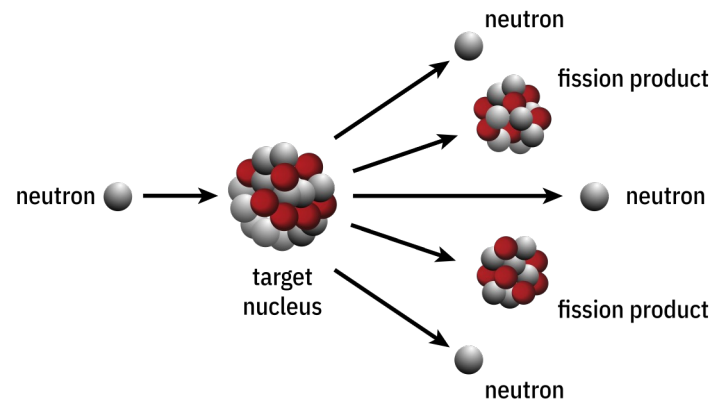


Shutterstock/OSweetNature

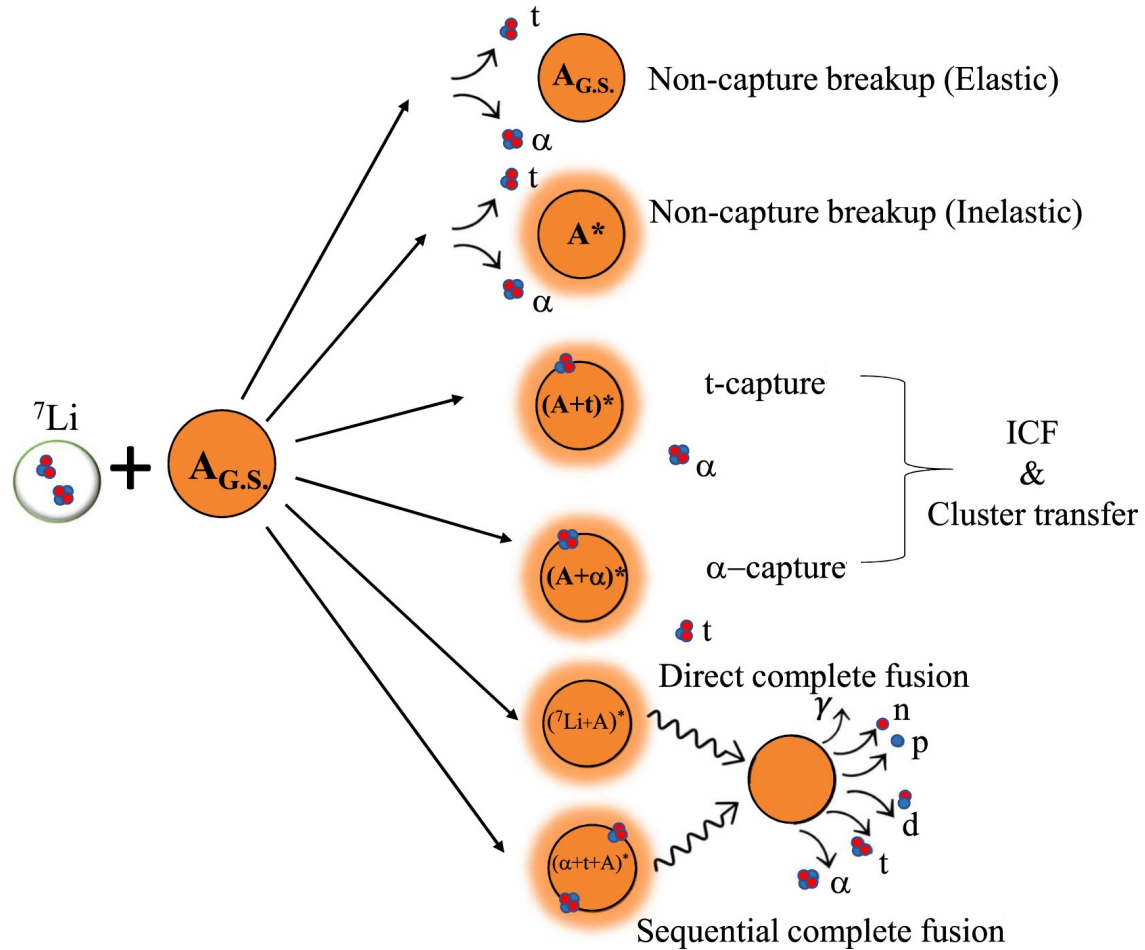
## Neutron-induced fission



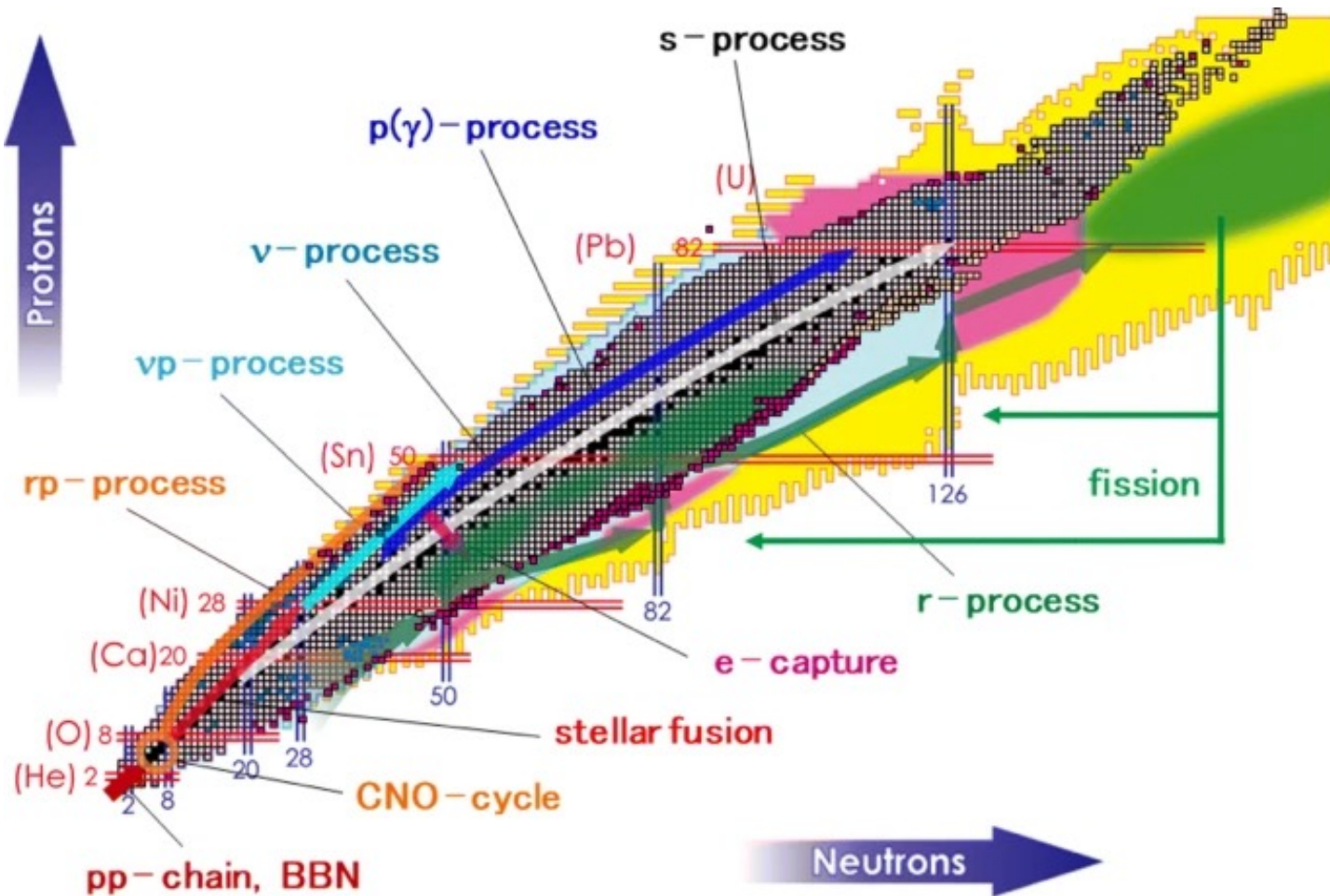
[www.youtube.com/user/jordi3736](http://www.youtube.com/user/jordi3736)



# Breakup, capture, and fusion



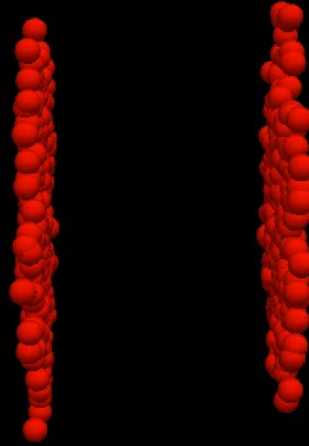
# Astrophysical reactions



# Relativistic heavy ion collisions

Time: 0.10

red: Baryons  
blue: Mesons  
light: Antiparticles



*MADAI.us*

yellow: strange mesons  
green: strange baryons

## Time-dependent Schrödinger equation

Let us consider a Hamiltonian  $H$  that does not vary with time. The time-dependent Schrödinger equation tells us that the wave function evolves as

$$\frac{d}{dt} |\psi(t)\rangle = -iH |\psi(t)\rangle$$

We can solve by exponentiating

$$|\psi(t)\rangle = \exp(-iHt) |\psi(0)\rangle$$

In classical computing we can compute as

$$|\psi(t + \Delta t)\rangle = [1 - iH\Delta t + \dots] |\psi(t)\rangle$$



Let us consider the normalized energy eigenstates of  $H$ ,

$$H |\psi_n\rangle = E_n |\psi_n\rangle \quad n = 0, 1, \dots$$

We can decompose the initial wave function in terms of the energy

$$|\psi(0)\rangle = \sum_n c_n |E_n\rangle$$

Since energy eigenstate evolves with a complex phase determined by its energy, we have

$$|\psi(t)\rangle = \sum_n c_n e^{-iE_n t} |E_n\rangle$$

We see that the dynamics is complicated. We get different oscillations for each energy eigenvalue. For general dynamics, we need to be able to store vectors with the full dimension of the linear space.

This is quite different from Euclidean time evolution

$$\frac{d}{d\tau} |\psi(\tau)\rangle = -H |\psi(\tau)\rangle$$

In Euclidean time evolution we instead get

$$|\psi(\tau)\rangle = \exp(-Ht) |\psi(0)\rangle$$

The exponential of the kinetic energy term gives a diffusion operator, and we can calculate the Euclidean time evolution using quantum Monte Carlo simulations.

For Euclidean time evolution, the energy eigenstate decomposition gives

$$|\psi(\tau)\rangle = \sum_n c_n e^{-E_n \tau} |E_n\rangle$$

The Euclidean time evolution is dominated by low-energy energy states.

None of these simplifying features occur for real time evolution.

## Spin model Hamiltonians

We consider the Hamiltonians that we can construct based on sums of single-qubit Pauli operators and products of Pauli operators on two different qubits

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

We start with single qubit Hamiltonians of the form

$$c_X X + c_Y Y + c_Z Z$$

Because the square of each Pauli matrix equals the identity, we can exponentiate the Pauli matrices as

$$\begin{aligned}\exp(i\alpha X) &= 1 + \frac{i\alpha}{1!}X + \frac{(i\alpha)^2}{2!}X^2 + \frac{(i\alpha)^3}{3!}X^3 + \frac{(i\alpha)^4}{4!}X^4 + \dots \\ &= \cos(\alpha) + i\sin(\alpha)X\end{aligned}$$

$$\exp(i\alpha Y) = \cos(\alpha) + i\sin(\alpha)Y$$

$$\exp(i\alpha Z) = \cos(\alpha) + i\sin(\alpha)Z$$

In general, we have

$$\exp(i\alpha_X X + i\alpha_Y Y + i\alpha_Z Z) = \cos(|\alpha|) + i\sin(|\alpha|)\left[\frac{\alpha_X}{|\alpha|}X + \frac{\alpha_Y}{|\alpha|}Y + \frac{\alpha_Z}{|\alpha|}Z\right]$$

On the IBM devices, the  $X$ ,  $Y$ ,  $Z$  rotation gates are defined as

$$R_x(\theta) = \exp(-i\frac{\theta}{2}X) = \cos(\frac{\theta}{2}) - i \sin(\frac{\theta}{2})X$$

$$R_y(\theta) = \exp(-i\frac{\theta}{2}Y) = \cos(\frac{\theta}{2}) - i \sin(\frac{\theta}{2})Y$$

$$R_z(\theta) = \exp(-i\frac{\theta}{2}Z) = \cos(\frac{\theta}{2}) - i \sin(\frac{\theta}{2})Z$$

Also on the IBM devices, the general  $U_3$  gate is defined in terms of Euler angles

$$U_3(\theta, \phi, \lambda) = R_z(\phi)R_y(\theta)R_z(\lambda)e^{i\frac{\phi+\lambda}{2}} = \begin{bmatrix} \cos(\frac{\theta}{2}) & -e^{i\lambda} \sin(\frac{\theta}{2}) \\ e^{i\phi} \sin(\frac{\theta}{2}) & e^{i(\phi+\lambda)} \cos(\frac{\theta}{2}) \end{bmatrix}$$

The overall phase factor is irrelevant since it is not observable. If we use the phase to set the determinant to 1, this corresponds to a general element of the Lie group  $SU(2)$ . This is a manifold with 3 dimensions.

We now consider two-qubit systems. We use the basis ordering

$$|00\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad |01\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad |10\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad |11\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Let us first consider the product of  $Z$  gates on two qubits

$$Z_1 Z_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Similarly, the product of  $X$  gates on two qubits is

$$X_1 X_0 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

The product of  $Y$  gates on two qubits is

$$Y_1 Y_0 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \otimes \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}$$



It turns out that  $X_1X_0$ ,  $Y_1Y_0$ ,  $Z_1Z_0$  all commute with each other

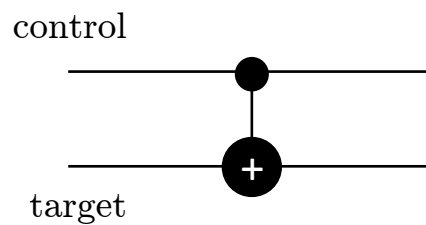
$$\begin{aligned}X_1X_0Y_1Y_0 &= X_1Y_1X_0Y_0 = -Y_1X_1X_0Y_0 \\ &= Y_1X_1Y_0X_0 = Y_1Y_0X_1X_0\end{aligned}$$

Similarly

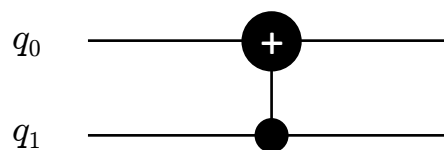
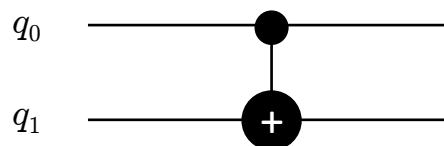
$$Y_1Y_0Z_1Z_0 = Z_1Z_0Y_1Y_0$$

$$Z_1Z_0X_1X_0 = X_1X_0Z_1Z_0$$

## CNOT gates



input ( $t, c$ )	output ( $t, c$ )
00	00
01	11
10	10
11	01



$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

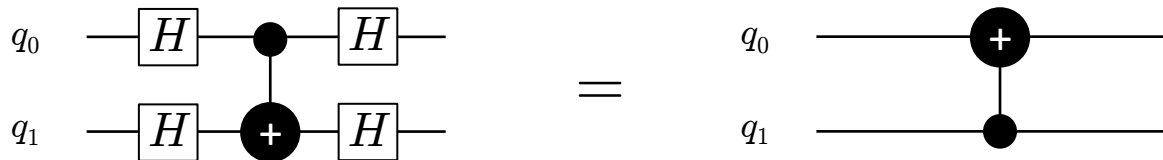
If we apply Hadamard gates on both qubits, we get

$$H_1 H_0 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \otimes \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}$$

We note that

$$\frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \cdot \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

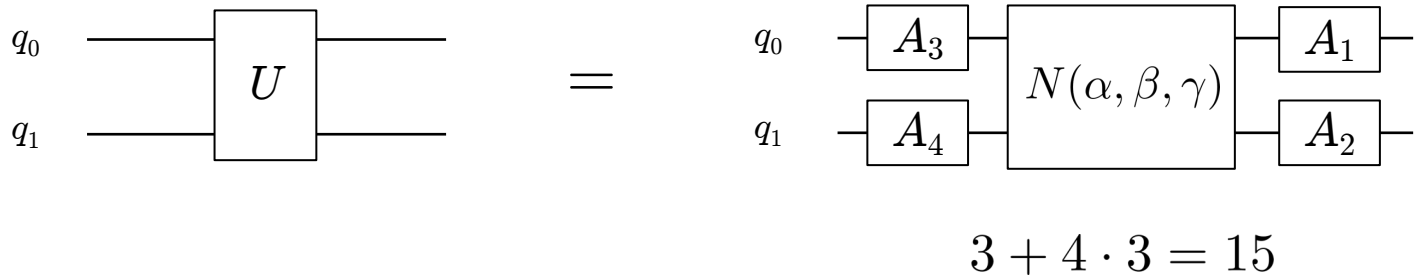
We can therefore switch the roles of the control and target qubits for the CNOT gate using the product of Hadamards on the qubits before and after



## Unitary operators on two qubits

The set of  $4 \times 4$  unitary matrices corresponds with the Lie group  $U(4)$ . If we use the overall phase, which is unobservable, to set the determinant to 1, then the Lie group  $SU(4)$ . This is a manifold with 15 dimensions.

Up to an overall phase, we can represent any  $4 \times 4$  unitary matrix as

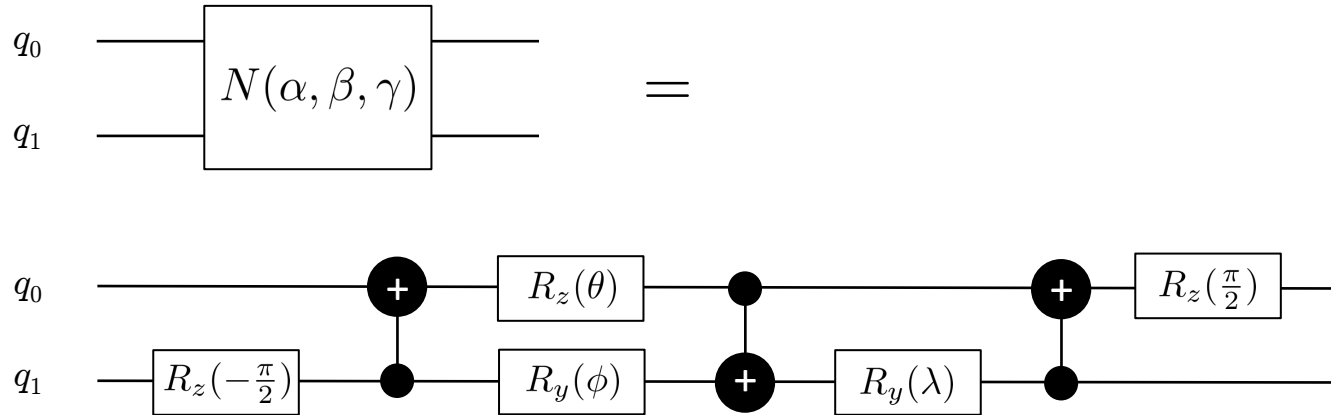


Kraus, Cirac, PRA 63, 8 (2001)

Where we define

$$N(\alpha, \beta, \gamma) = \exp[i(\alpha X_1 X_0 + \beta Y_1 Y_0 + \gamma Z_1 Z_0)]$$

We can write the circuit as



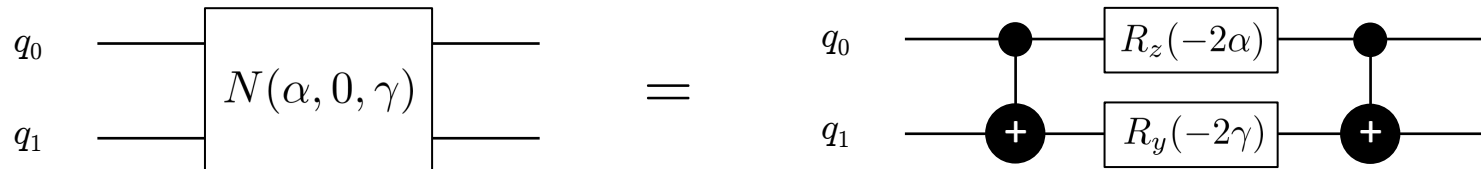
$$\theta = \frac{\pi}{2} - 2\gamma, \quad \phi = 2\alpha - \frac{\pi}{2}, \quad \lambda = \frac{\pi}{2} - 2\beta$$

Smith *et al.*, npj Quant. Info. 5 106 (2019)

When one of the parameters is zero, the corresponding expressions can be simplified. For example,

$$N(\alpha, 0, \gamma) = \exp[i(\alpha X_1 X_0 + \gamma Z_1 Z_0)]$$

In this case, the circuit has the form



## Trotter-Suzuki approximations

The Baker-Campbell-Hausdorff formula says that if

$$\exp(A) \exp(B) = \exp(C)$$

then we can perform an expansion in commutators

$$C = A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] - \frac{1}{12}[B, [A, B]] \cdots$$

We can use this to exponentiate a Hamiltonian with pieces that do not commute.



If our Hamiltonian has two non-commuting pieces

$$H = H_A + H_B$$

then we can use either of the first-order Trotter-Suzuki approximations

$$\exp(-iH\Delta t) = \exp(-iH_A\Delta t) \exp(-iH_B\Delta t) + O(\Delta t^2)$$

$$\exp(-iH\Delta t) = \exp(-iH_B\Delta t) \exp(-iH_A\Delta t) + O(\Delta t^2)$$

If our Hamiltonian has three non-commuting pieces

$$H = H_A + H_B + H_C$$

Then we have the first-order Trotter-Suzuki expressions

$$\exp(-iH\Delta t) = \exp(-iH_A\Delta t) \exp(-iH_B\Delta t) \exp(-iH_C\Delta t) + O(\Delta t^2)$$

$$\exp(-iH\Delta t) = \exp(-iH_B\Delta t) \exp(-iH_A\Delta t) \exp(-iH_C\Delta t) + O(\Delta t^2)$$

(also other orderings)

The second-order Trotter-Suzuki approximation has the form

$$\exp(-iH\Delta t) =$$

$$\exp(-iH_C \frac{\Delta t}{2}) \exp(-iH_B \frac{\Delta t}{2}) \exp(-iH_A\Delta t) \exp(-iH_B \frac{\Delta t}{2}) \exp(-iH_C \frac{\Delta t}{2}) \\ + O(\Delta t^3)$$

(also other orderings)

## Time evolution of Heisenberg spin chains

Let us consider a one-dimension spin chain with an external magnetic field and couplings between nearest neighbor sites

$$H = -J \sum_j X_{j+1} X_j - J \sum_j Y_{j+1} Y_j + U \sum_j Z_{j+1} Z_j + h_j \sum_j Z_j$$

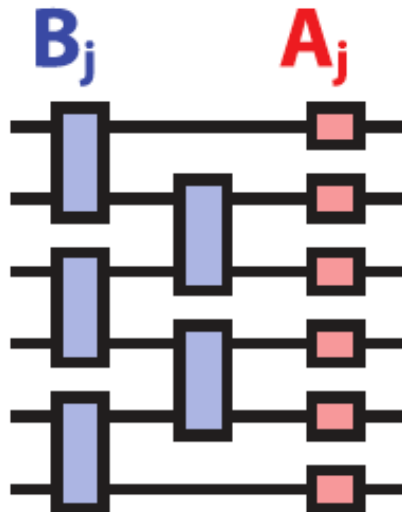
Let us define

$$A_j = \exp(-ih_j Z_j \Delta t)$$

$$B_j = \exp[-i(-JX_j X_{j+1} - JY_j Y_{j+1} + UZ_j Z_{j+1})\Delta t]$$

We can use the first-order Trotter-Suzuki approximation

$$\exp(-H\Delta t) = \left(\prod_j A_j\right) \left(\prod_{j \text{ even}} B_j\right) \left(\prod_{j \text{ odd}} B_j\right)$$



Smith *et al.*, npj Quant. Info. 5 106 (2019)

If we think of the state

$$|0\rangle \otimes |0\rangle \otimes |0\rangle \otimes \dots$$

as the vacuum state and each  $|1\rangle$  as a particle excitation, then we can view the Heisenberg model as a model of bosons with hard core repulsion. The term

$$-J \sum_j X_{j+1} X_j - J \sum_j Y_{j+1} Y_j$$

is a nearest-neighbor hopping term for the bosons. The term

$$h_j \sum_j Z_j$$

is an external potential plus an overall constant.

To remove the extra overall constant we simply write

$$h_j \sum_j (Z_j - 1)$$

The term

$$U \sum_j Z_{j+1} Z_j$$

is a nearest neighbor interaction between bosons, plus a chemical potential and an overall constant.

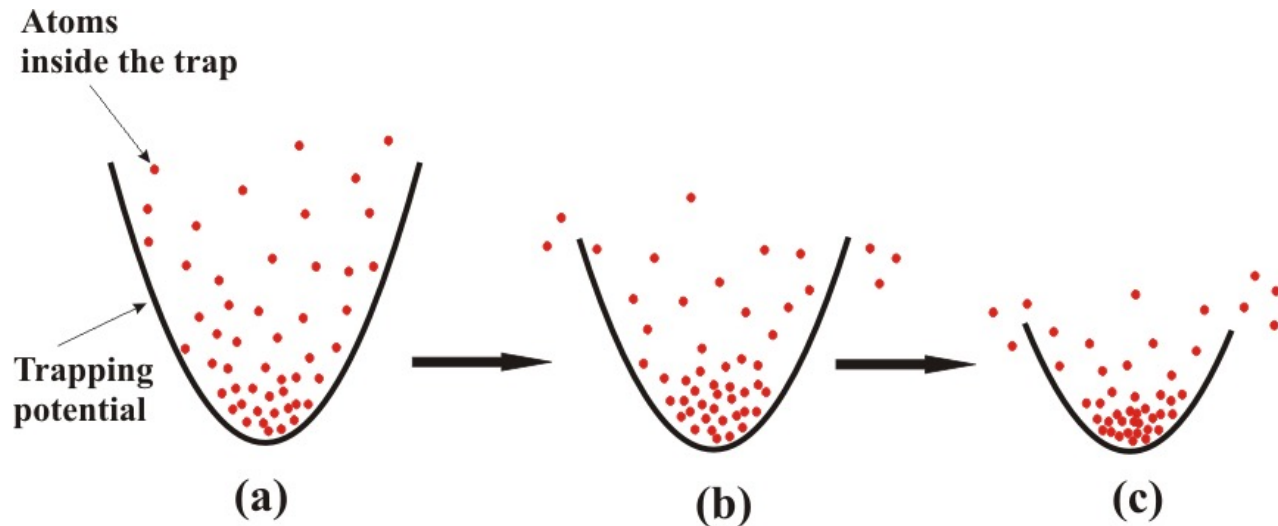
To remove these extra terms, we simply write

$$U \sum_j (Z_{j+1} - 1)(Z_j - 1)$$

# Projected cooling algorithm

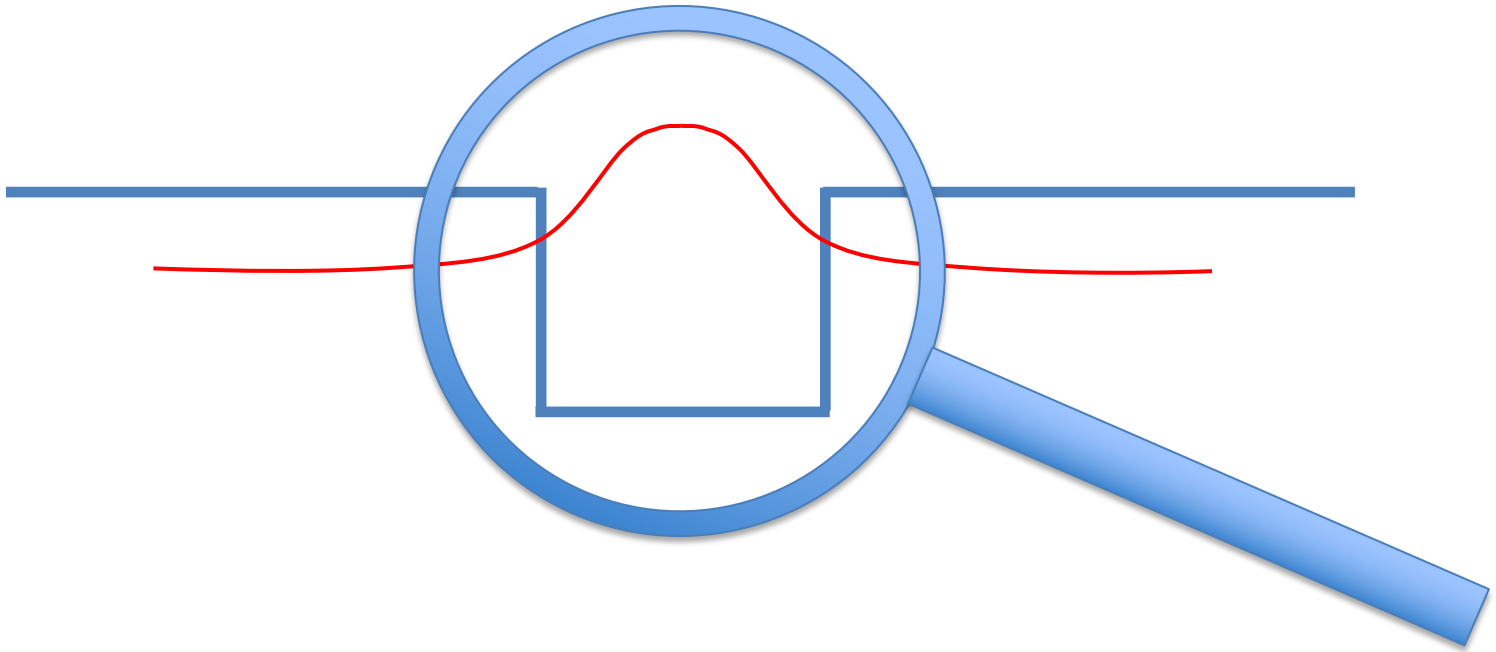
D.L, Bonitati, Given, Hicks, Li, Lu, Rai, Sarkar, Watkins, Phys. Lett. B 807, 135536 (2020)

Analogy: Evaporative cooling



credit: George Raithel

## Projected cooling





Consider a Hamiltonian  $H$  with translational invariance and exactly one localized state (i.e., the ground state)

$$H |\psi_0\rangle = E_0 |\psi_0\rangle$$

We take the system volume to be large enough to avoid rebounding reflections from the boundary. Let  $P$  be a projection operator onto a localized region. In the limit of large time  $t$ , the projected time evolution has a stable fixed point

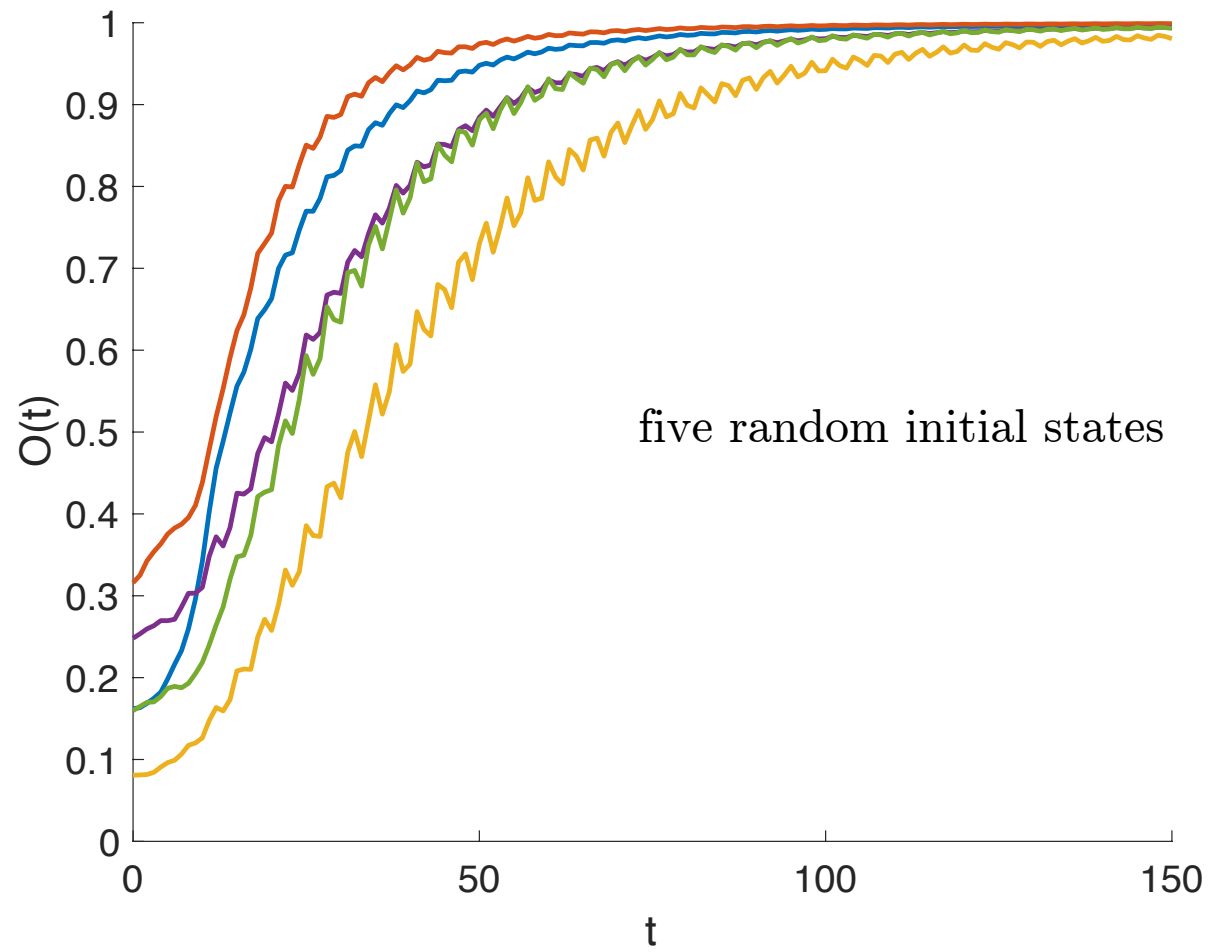
$$Pe^{-iHt}P |\psi_I\rangle \rightarrow e^{-iE_0t}P |\psi_0\rangle \langle\psi_0|P|\psi_I\rangle$$

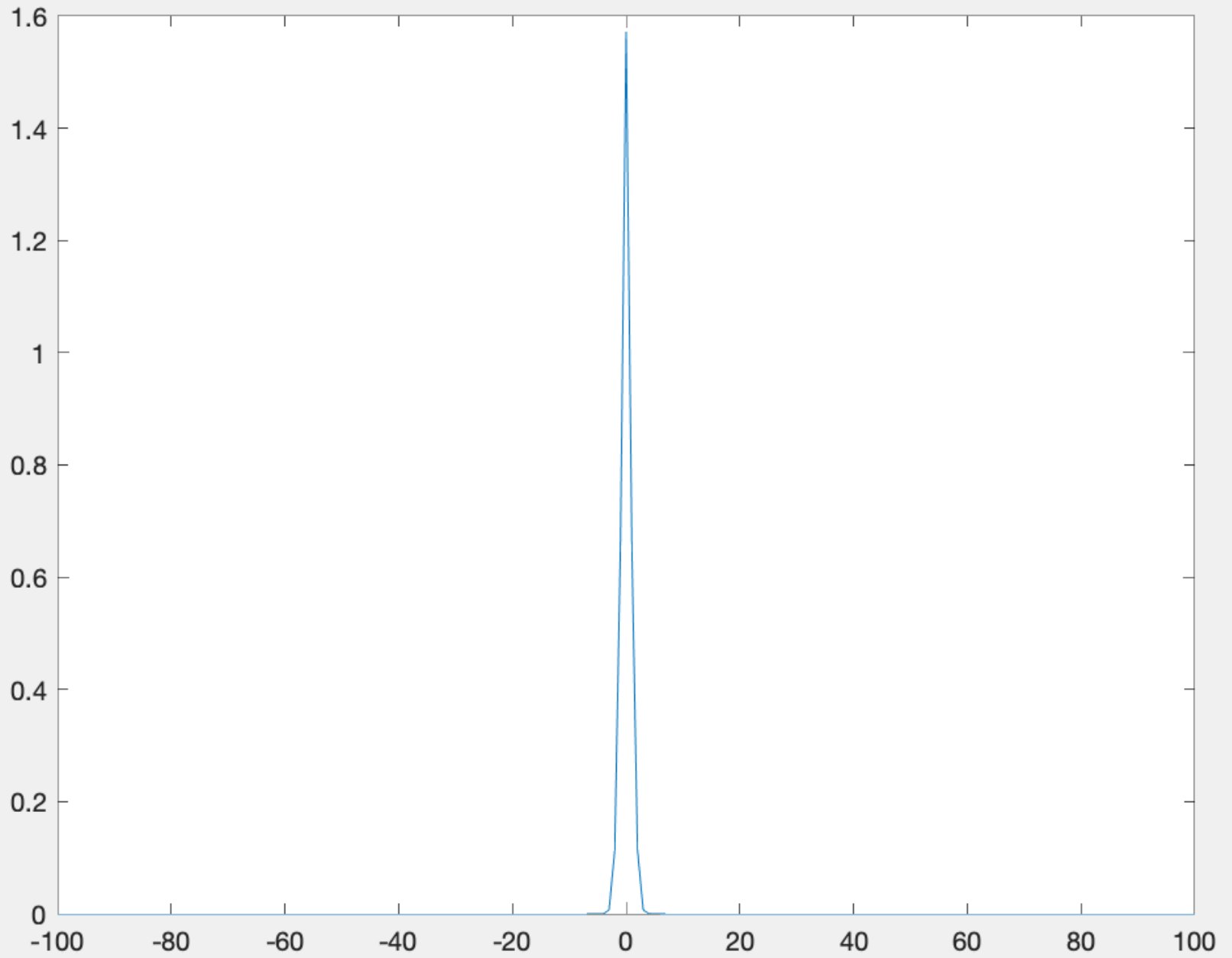
Example:

Consider a single hardcore boson placed in a short-range potential well with only one bound state

$$H = -J \sum_j X_{j+1} X_j - J \sum_j Y_{j+1} Y_j + \sum_j V_j \frac{1-Z_j}{2}$$

Overlap with  $P |\psi_0\rangle$





## Recap of lecture

Nuclear dynamics

Time-dependent Schrödinger equation

Spin model Hamiltonians

CNOT gates

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