

# $(1 + 1)$ -d $U(1)$ Quantum Link Models from Effective Hamiltonians of Dipolar Molecules

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**I** ILLINOIS Physics

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# Our Team



Bryan Clark



Brian DeMarco



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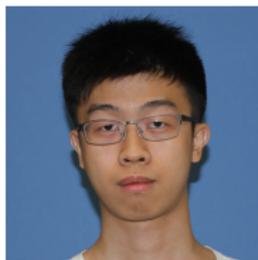
Bryce Gadway



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Jiayu Shen

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# Introduction to Quantum Simulations

- ▶ Quantum mechanics in AMO **experiments** → Quantum theories





# Introduction to Quantum Simulations

- ▶ Real-time evolution with **Hamiltonian** formalism
- ▶ Usually **finite** d.o.f.

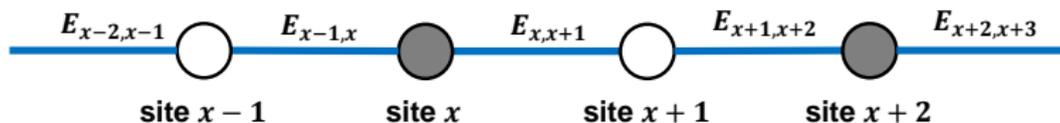
# Introduction to Quantum Simulations

- ▶ Real-time evolution with **Hamiltonian** formalism
- ▶ Usually **finite** d.o.f.
- ▶ States in experiment  $\rightarrow$  States in the theory
- ▶ Match the experimental Hamiltonian with the target Hamiltonian

# Introduction to Quantum Link Models

- ▶  $U(1)$  lattice gauge theory with staggered fermions in  $(1+1)$ -d with the temporal gauge  $A_0 = 0$ :

$$H = -w \sum_x \left[ \psi_x^\dagger U_{x,x+1} \psi_{x+1} + \psi_{x+1}^\dagger U_{x,x+1}^\dagger \psi_x \right] \\ + m \sum_x (-1)^x \psi_x^\dagger \psi_x + \frac{g^2}{2} \sum_x E_{x,x+1}^2,$$

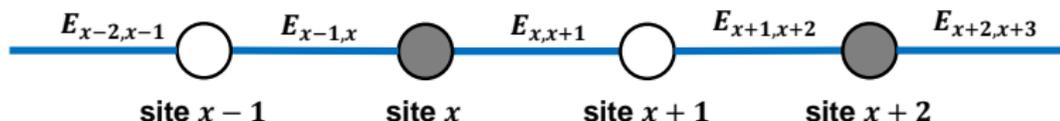


Empty:  Filled: 

# Introduction to Quantum Link Models

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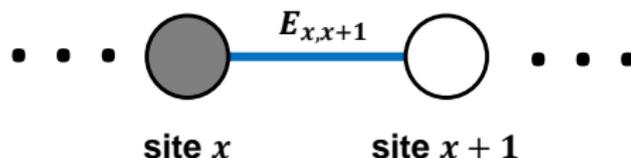
$$U_{x,x+1} = \exp(iagA_{x,x+1}) \in U(1),$$

$$E_{x,x+1} \equiv \frac{1}{g} F_{01,x,x+1} = -i \frac{1}{ag} \frac{\partial}{\partial A_{x,x+1}} \in \mathbb{Z}.$$

Infinite d.o.f.

# Introduction to Quantum Link Models

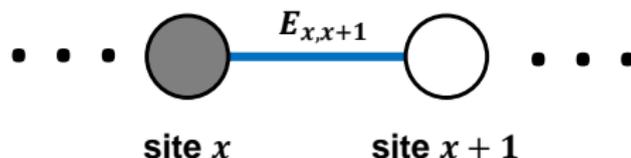
Quantum Link Models (QLMs) (Chandrasekharan, Wiese, Nucl.Phys. B492 (1997) 455-474)



- ▶  $E_{x,x+1} \in \mathbb{Z}$  →  $E_{x,x+1} \in \{-S, -S + 1, \dots, S - 1, S\}$   
Infinite d.o.f. → Finite d.o.f.

# Introduction to Quantum Link Models

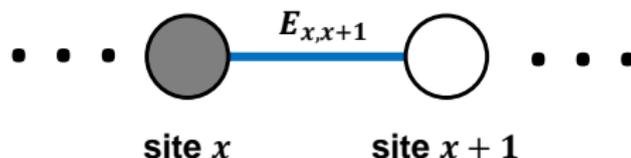
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Infinite d.o.f.  $\rightarrow$  Finite d.o.f.
- ▶  $[E_{x,x+1}, U_{x,x+1}] = U_{x,x+1}, [E_{x,x+1}, U_{x,x+1}^\dagger] = -U_{x,x+1}^\dagger,$   
 $[U_{x,x+1}, U_{x,x+1}^\dagger] = 0$   
are reminiscent of  
 $[S^3, S^+] = S^+, [S^3, S^-] = -S^-, [S^+, S^-] = 2S^3.$

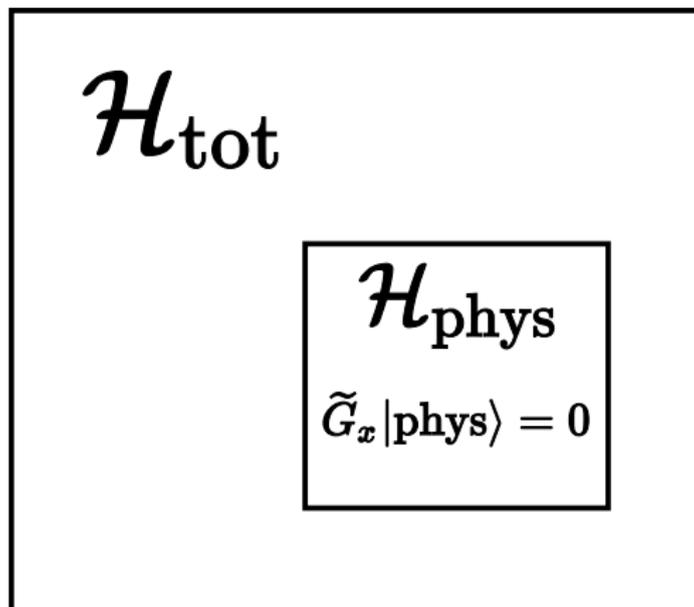
# Introduction to Quantum Link Models

Quantum Link Models (QLMs) (Chandrasekharan, Wiese, Nucl.Phys. B492 (1997) 455-474)



- ▶  $E_{x,x+1} \in \mathbb{Z} \rightarrow E_{x,x+1} \in \{-S, -S+1, \dots, S-1, S\}$   
Infinite d.o.f.  $\rightarrow$  Finite d.o.f.
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- ▶ Impose  $[E_{x,x+1}, U_{x,x+1}] = U_{x,x+1},$   
 $[E_{x,x+1}, U_{x,x+1}^\dagger] = -U_{x,x+1}^\dagger, [U_{x,x+1}, U_{x,x+1}^\dagger] = 2E_{x,x+1}.$

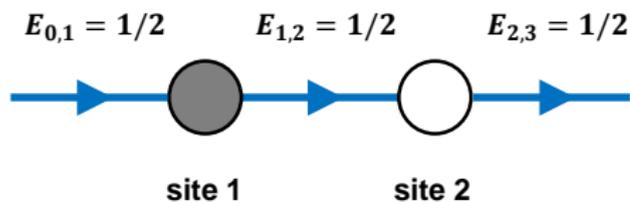
# Introduction to Quantum Link Models



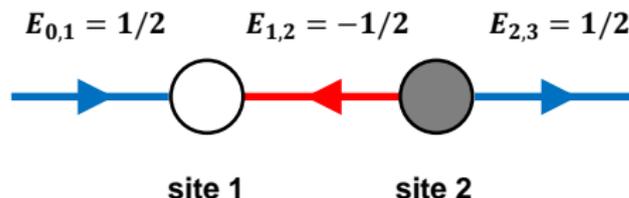
Gauss law operator:  $\tilde{G}_x = \psi_x^\dagger \psi_x - E_{x,x+1} + E_{x-1,x} + \frac{1}{2} [(-1)^x - 1]$   
 $[H, \tilde{G}_x] = 0$

# Introduction to Quantum Link Models

$w$ : Hopping parameter

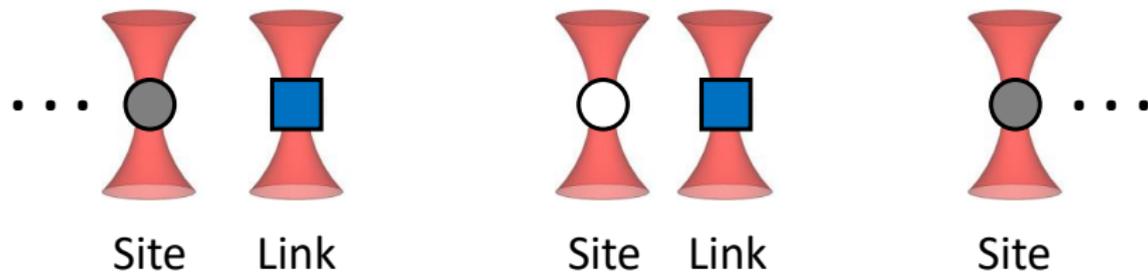


$$-w\psi_x^\dagger U_{x,x+1}\psi_{x+1} + h.c.$$



Gauss law operator:  $\tilde{G}_x = \psi_x^\dagger \psi_x - E_{x,x+1} + E_{x-1,x} + \frac{1}{2} [(-1)^x - 1]$

# Schematic Setup of the Experiment



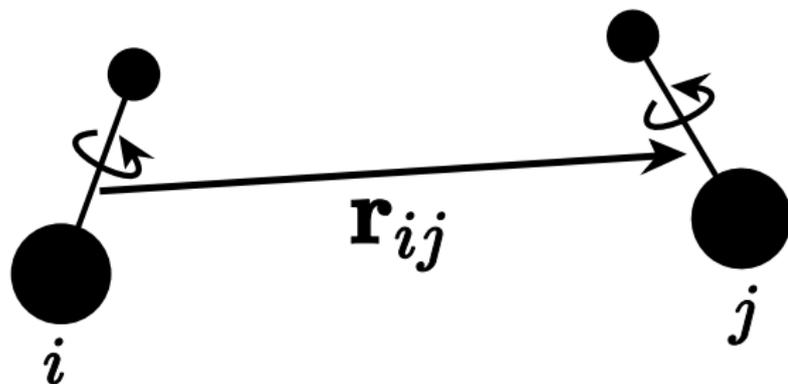
Red cones: Local laser lights



# Physics of Dipolar Molecules

- ▶ Dipole-dipole interaction ( $\mathbf{r}_{ij}$  fixed)

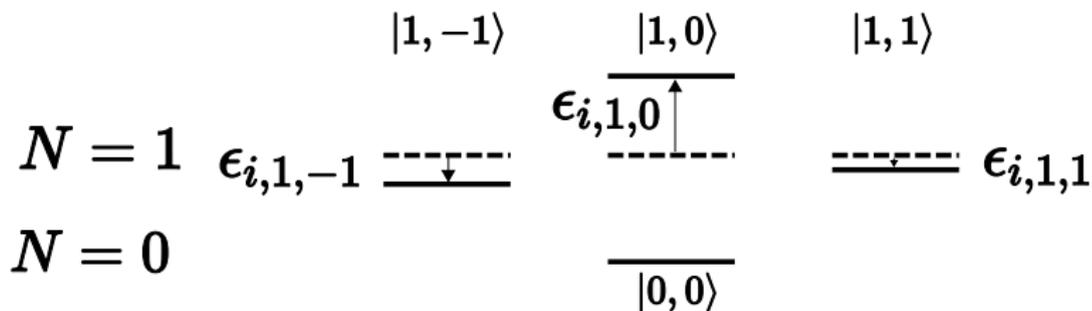
$$V_{ij} = \frac{1}{4\pi\epsilon_0} \frac{\mathbf{d}_i \cdot \mathbf{d}_j - 3(\mathbf{d}_i \cdot \hat{\mathbf{r}}_{ij})(\mathbf{d}_j \cdot \hat{\mathbf{r}}_{ij})}{r_{ij}^3},$$





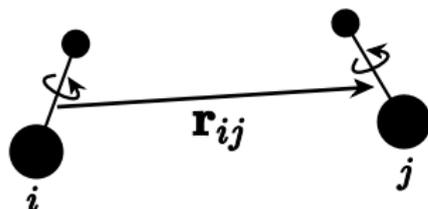
# Physics of Dipolar Molecules

- ▶ Laser lights: **local** energy shifts  $\epsilon_{i,N,m_N}$
- ▶ For molecule  $i$ :



# Physics of Dipolar Molecules

- ▶ Tunable parameters:
- ▶ Inter-molecule separations  $\mathbf{r}_{ij}$   $\rightarrow$  Dipole-dipole  $V_{ij}$

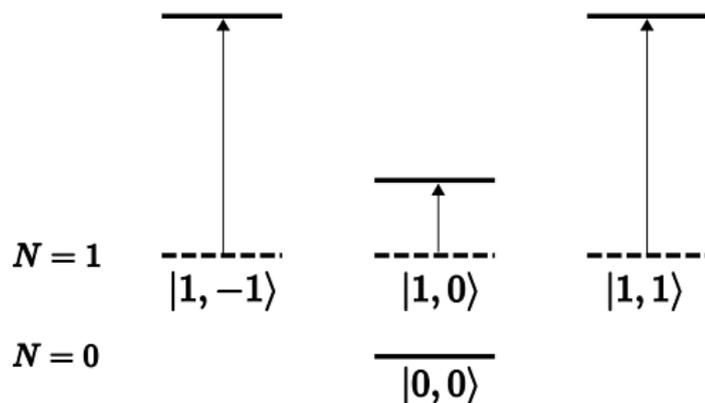


- ▶ Laser lights: Relative local energy shifts  $\epsilon_{i,N,m_N}$

$$\begin{array}{ccccc}
 & & |1, -1\rangle & & |1, 1\rangle \\
 & & \frac{|1, 0\rangle}{\epsilon_{i,1,0}} & & \\
 N = 1 & \epsilon_{i,1,-1} & \frac{\text{---}}{\text{---}} & & \frac{\text{---}}{\text{---}} \epsilon_{i,1,1} \\
 N = 0 & & & & \\
 & & & & \frac{|0, 0\rangle}{\text{---}}
 \end{array}$$

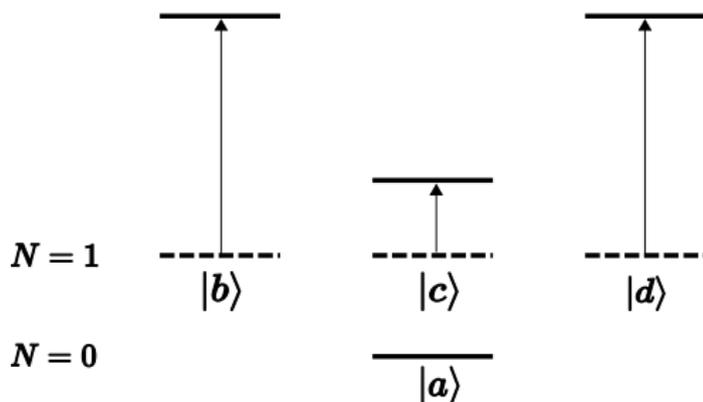
# Mapping from Dipolar Molecules to the QLM States

Fermion Sites:



# Mapping from Dipolar Molecules to the QLM States

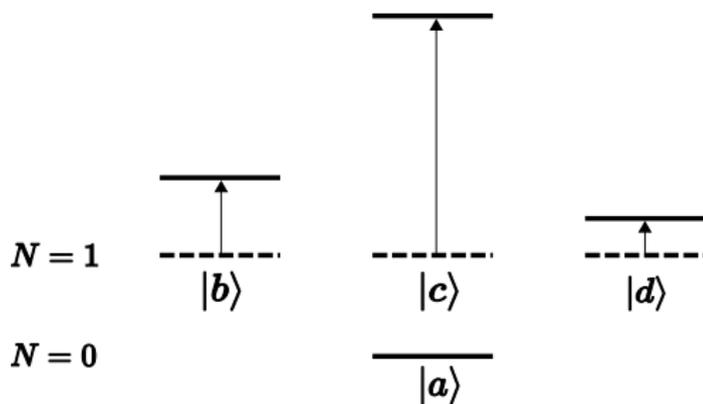
Fermion Sites:



Molecular States	QLM States
$ a\rangle =  0, 0\rangle$	Filled
$ c\rangle =  1, 0\rangle$	Empty
$ b\rangle =  1, -1\rangle$	Off-Resonant
$ d\rangle =  1, 1\rangle$	Off-Resonant

# Mapping from Dipolar Molecules to the QLM States

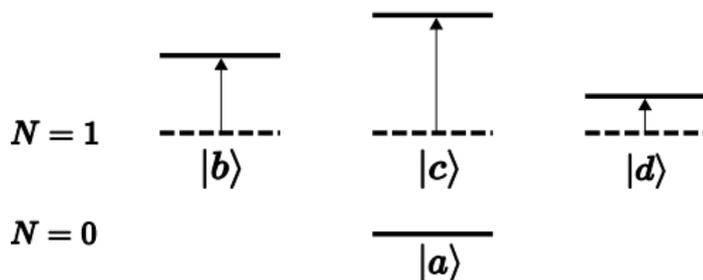
$S = 1/2$  Links:



Molecular States	QLM States
$ b\rangle =  1, -1\rangle$	$S^3 = -1/2$
$ d\rangle =  1, 1\rangle$	$S^3 = 1/2$
$ a\rangle =  0, 0\rangle$	Not Used Directly
$ c\rangle =  1, 0\rangle$	Off-Resonant

# Mapping from Dipolar Molecules to the QLM States

$S = 1$  Links:



Molecular States	QLM States
$ b\rangle =  1, -1\rangle$	$S^3 = -1$
$ d\rangle =  1, 1\rangle$	$S^3 = 0$
$ c\rangle =  1, 0\rangle$	$S^3 = 1$
$ a\rangle =  0, 0\rangle$	Not Used Directly

# Engineering the Effective Hamiltonian

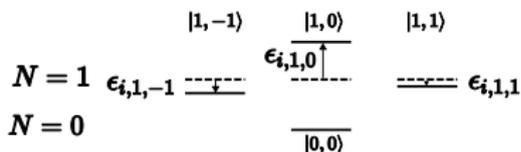
Dipolar Molecules

QLM

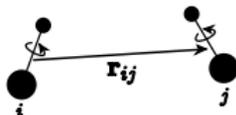
One-body: Rotor  $H_{\text{rot}} = \sum_i hB_{\text{rot}} \mathbf{N}_i^2$



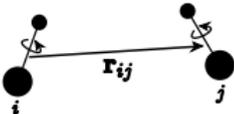
One-body: Laser lights  $\epsilon_{i,N,m_N}$



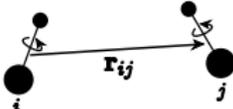
Two-body: Dipole-dipole interactions  $V_{ij}$



# Engineering the Effective Hamiltonian

Dipolar Molecules	QLM
<p data-bbox="141 221 779 270">One-body: Rotor <math>H_{\text{rot}} = \sum_i hB_{\text{rot}} \mathbf{N}_i^2</math></p>  <p data-bbox="141 430 665 479">One-body: Laser lights <math>\epsilon_{i,N,m_N}</math></p> <div style="display: flex; align-items: center; justify-content: center;"> <div style="margin-right: 20px;"> <p data-bbox="234 539 312 570"><math>N = 1</math></p> <p data-bbox="234 588 312 619"><math>N = 0</math></p> </div> <div style="text-align: center;"> <p data-bbox="412 491 467 511"> 1,-1&gt;</p> <p data-bbox="488 491 573 511"> 1,0&gt;</p> <p data-bbox="628 491 683 511"> 1,1&gt;</p> <p data-bbox="488 522 573 542"><math>\epsilon_{i,1,0}</math></p> <p data-bbox="522 605 573 625"> 0,0&gt;</p> </div> <div style="margin-left: 20px;"> <p data-bbox="691 553 746 573"><math>\epsilon_{i,1,1}</math></p> </div> </div> <p data-bbox="141 664 834 712">Two-body: Dipole-dipole interactions <math>V_{ij}</math></p> 	<p data-bbox="879 260 1057 308">One-body:</p> $m \sum_x (-1)^x \psi_x^\dagger \psi_x$ $\frac{g^2}{2} \sum_x E_{x,x+1}^2$ <p data-bbox="879 501 1085 539">Three-body:</p> $-w \psi_x^\dagger U_{x,x+1} \psi_{x+1} + h.c.$

# Engineering the Effective Hamiltonian

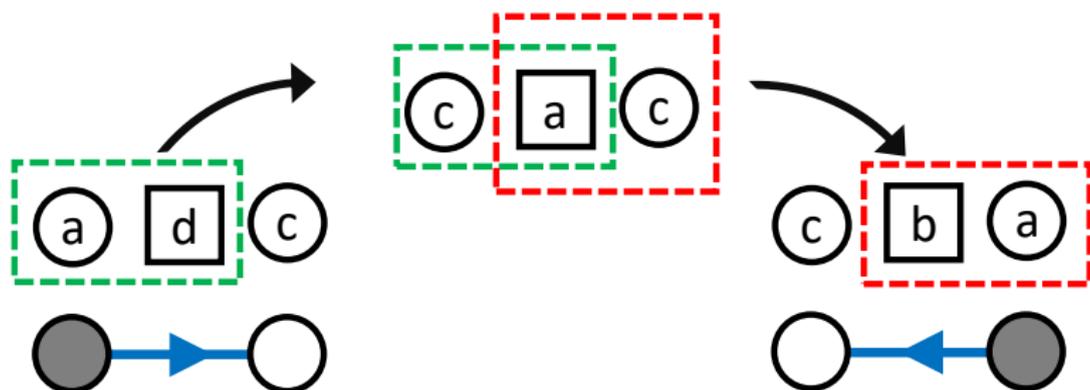
Dipolar Molecules	QLM
<p><b>One-body:</b> Rotor <math>H_{\text{rot}} = \sum_i hB_{\text{rot}} \mathbf{N}_i^2</math></p>  <p><b>One-body:</b> Laser lights <math>\epsilon_{i,N,m_N}</math></p> <p> <math>N = 1</math> <math>\epsilon_{i,1,-1}</math> <math>\xrightarrow{ 1,-1\rangle}</math> <math>\epsilon_{i,1,0}</math> <math>\xrightarrow{ 1,0\rangle}</math> <math>\xrightarrow{ 1,1\rangle}</math> <math>\epsilon_{i,1,1}</math>  <math>N = 0</math> <math>\xrightarrow{ 0,0\rangle}</math> </p> <p><b>Two-body:</b> Dipole-dipole interactions <math>V_{ij}</math></p> 	<p><b>One-body:</b></p> $m \sum_x (-1)^x \psi_x^\dagger \psi_x$ $\frac{g^2}{2} \sum_x E_{x,x+1}^2$ <p><b>Three-body:</b></p> $-w \psi_x^\dagger U_{x,x+1} \psi_{x+1} + h.c.$

2nd-order Effective Hamiltonian

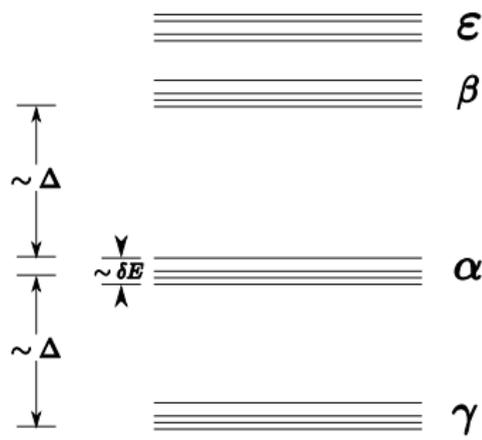
# Engineering the Effective Hamiltonian

An example of second-order processes ( $S = 1/2$ ):

$$-w\psi_x^\dagger U_{x,x+1}\psi_{x+1}$$



# Engineering the Effective Hamiltonian



A generic **many-body** configuration  $m$  in the subspace  $\mathcal{H}_{\text{phys}} = \alpha$

$\dots$   $\circ$   $\square$   $\circ$   $\square$   $\circ$   $\square$   $\circ$   $\dots$

## ▶ Quasi-degenerate effective Hamiltonian (2nd order)

$$\langle m | H_{\text{eff}}^{\alpha} | n \rangle = E_{m\alpha} \delta_{ij} + \langle m, \alpha | V | n, \alpha \rangle + \frac{1}{2} \sum_{l, \gamma \neq \alpha} \langle m, \alpha | V | l, \gamma \rangle \langle l, \gamma | V | n, \alpha \rangle \left[ \frac{1}{E_{m\alpha} - E_{l\gamma}} + \frac{1}{E_{n\alpha} - E_{l\gamma}} \right] + \dots$$

# Engineering the Effective Hamiltonian

- ▶ Quasi-degenerate effective Hamiltonian (2nd order)

$$\begin{aligned} \langle m | H_{\text{eff}}^{\alpha} | n \rangle &= E_{m\alpha} \delta_{mn} + \langle m, \alpha | V | n, \alpha \rangle \\ &+ \frac{1}{2} \sum_{l, \gamma \neq \alpha} \langle m, \alpha | V | l, \gamma \rangle \langle l, \gamma | V | n, \alpha \rangle \left[ \frac{1}{E_{m\alpha} - E_{l\gamma}} + \frac{1}{E_{n\alpha} - E_{l\gamma}} \right] + \dots \end{aligned}$$

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- ▶  $E_{m\alpha} \delta_{mn}$ : Adjust with rotors and laser lights  $\rightarrow$  Gauss' law,  
 $m(-1)^x \psi_x^{\dagger} \psi_x$  and  $\frac{g^2}{2} E_{x, x+1}^2$

# Engineering the Effective Hamiltonian

- ▶ Quasi-degenerate effective Hamiltonian (2nd order)

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- ▶  $E_{m\alpha} - E_{l\gamma} \sim \Delta$ : Adjust with rotors and laser lights

# Engineering the Effective Hamiltonian

- ▶ Quasi-degenerate effective Hamiltonian (2nd order)

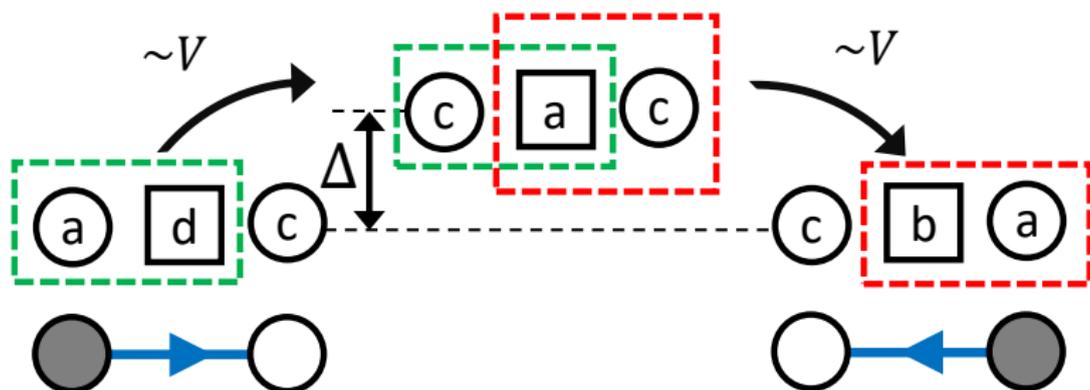
$$\begin{aligned} \langle m | H_{\text{eff}}^{\alpha} | n \rangle &= E_{m\alpha} \delta_{mn} + \langle m, \alpha | V | n, \alpha \rangle \\ &+ \frac{1}{2} \sum_{l, \gamma \neq \alpha} \langle m, \alpha | V | l, \gamma \rangle \langle l, \gamma | V | n, \alpha \rangle \left[ \frac{1}{E_{m\alpha} - E_{l\gamma}} + \frac{1}{E_{n\alpha} - E_{l\gamma}} \right] + \dots \end{aligned}$$

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- ▶  $E_{m\alpha} - E_{l\gamma} \sim \Delta$ : Adjust with rotors and laser lights
- ▶  $\langle m, \alpha | V | l, \gamma \rangle$ : Adjust with dipole-dipole interactions  $V_{ij}$

# Engineering the Effective Hamiltonian

An example of second-order processes ( $S = 1/2$ ):

$$-w\psi_x^\dagger U_{x,x+1}\psi_{x+1}$$



$$w \sim V^2 / \Delta$$

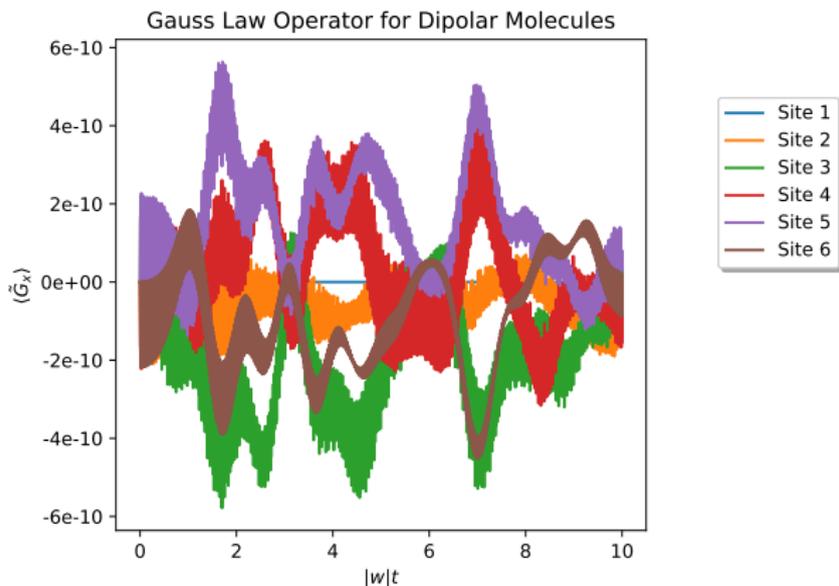
# Numerical Results (Preliminary)

Exact diagonalization (ED), Open boundary conditions

$S = 1/2$ ,  $m = g^2/2 = |w|$  in 6 sites

$w$ : Hopping parameter

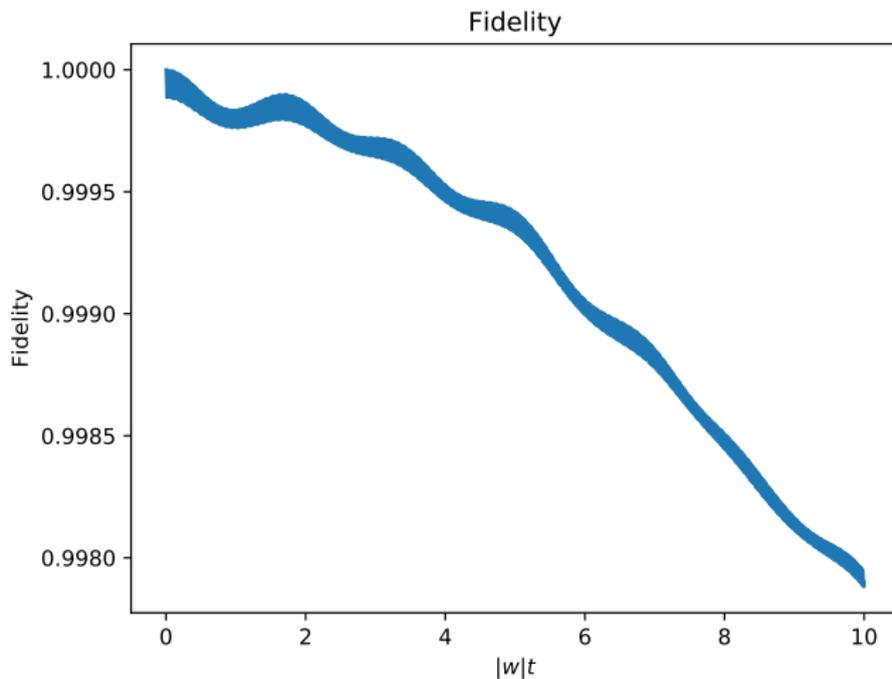
Gauss law operator:  $\tilde{G}_x = \psi_x^\dagger \psi_x - E_{x,x+1} + E_{x-1,x} + \frac{1}{2} [(-1)^x - 1]$



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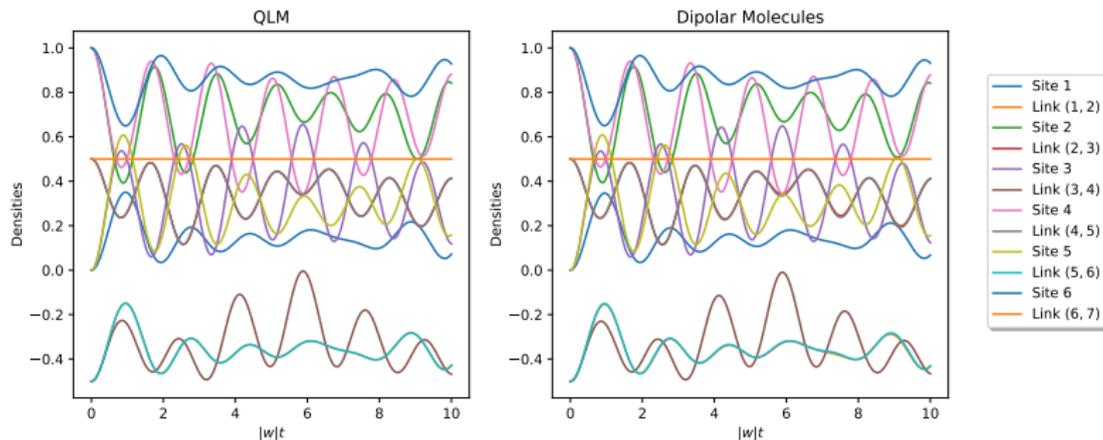
Fidelity:  $|\langle \psi_{\text{QLM}}(t) | \psi_{\text{molecule}}(t) \rangle|^2$



# Numerical Results (Preliminary)

$S = 1/2$ ,  $m = g^2/2 = |w|$  in 6 sites

Site/Link number densities:

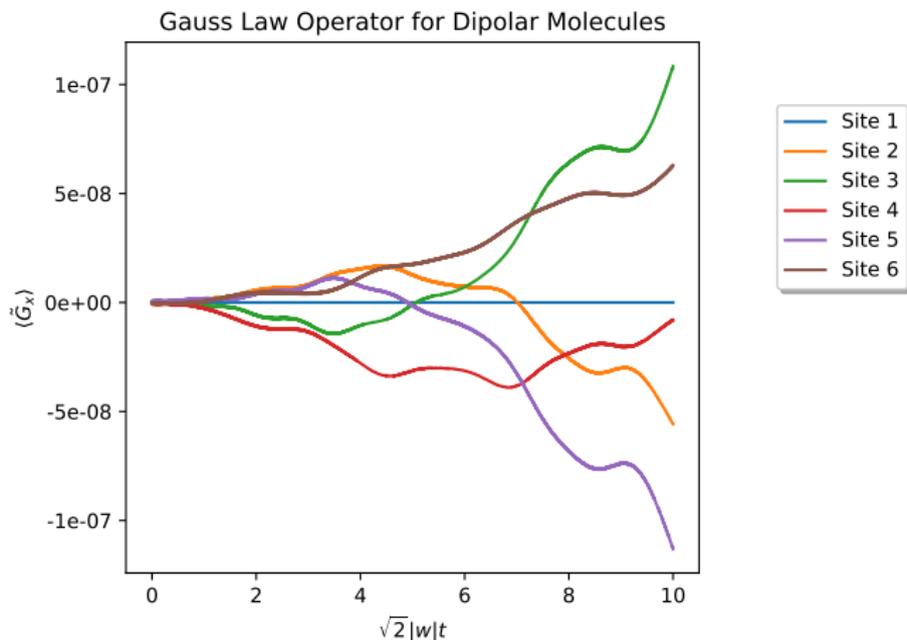


# Numerical Results (Preliminary)

$S = 1$ ,  $m = g^2/2 = \sqrt{2}|w|$  in 6 sites

$w$ : Hopping parameter

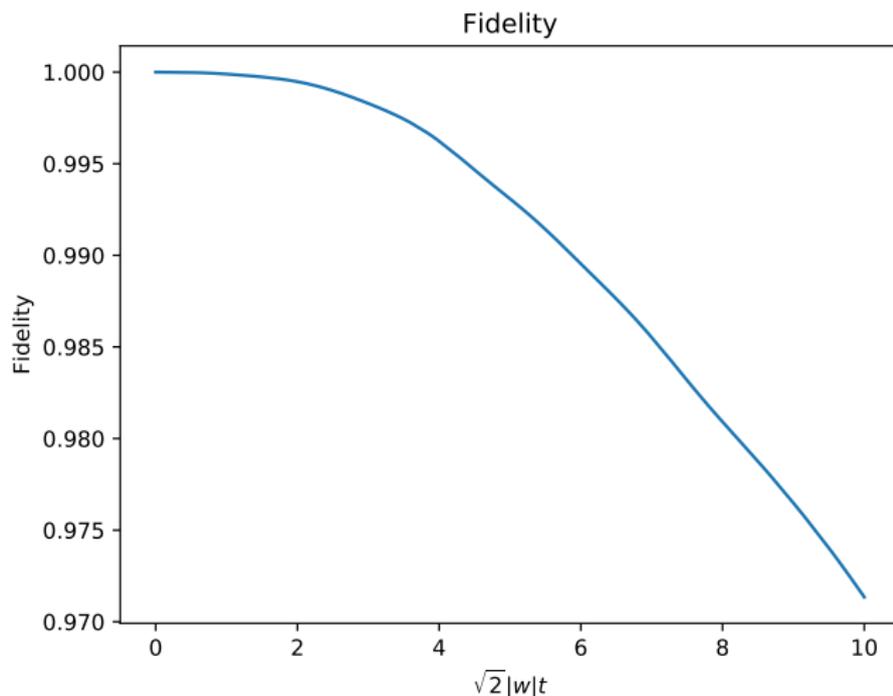
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# Numerical Results (Preliminary)

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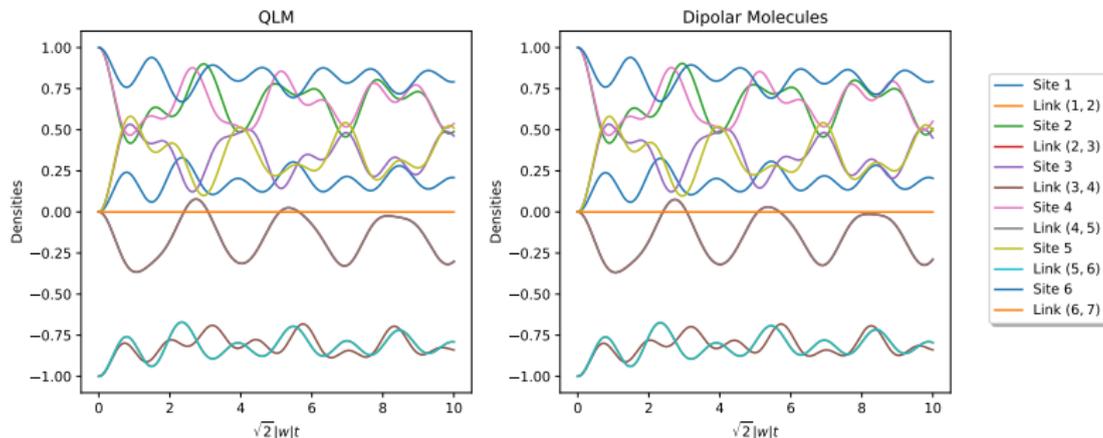
Fidelity:  $|\langle \psi_{\text{QLM}}(t) | \psi_{\text{molecule}}(t) \rangle|^2$



# Numerical Results (Preliminary)

$S = 1$ ,  $m = g^2/2 = \sqrt{2}|w|$  in 6 sites

Site/Link number densities:



# Outlook

- ▶ Parameters of experimental availability
- ▶ Numerical studies on longer chains with the density matrix renormalization group (DMRG)

# Summary

- ▶  $U(1)$  QLMs: Finite d.o.f. on each link
- ▶ Dipolar molecules: Rotors, laser lights, dipole-dipole interactions
- ▶ Mapping of states: from dipolar molecular states to QLM states
- ▶ The effective Hamiltonian of the dipolar molecules simulates the QLM.

**Thank You**

# Backup Info: Introduction to Quantum Simulations

(Zohar, Cirac, Reznik, Rep. Prog. Phys. 79 014401 2016)

- ▶ Quantum simulations are to study quantum mechanics (a theory) using quantum mechanics (a designed experimental setup).
- ▶ AMO systems with tunable parameters can serve as simulators.
- ▶ Analog quantum simulators are non-universal. For a specific model, a specific experimental setup is needed.
- ▶ The simulation is a continuous time evolution  $e^{-iHt}$  for an initial state.
- ▶ Simulating the Hamiltonian for the lattice gauge theory: mapping quantum states and engineering the Hamiltonian.

## Backup Info: (1 + 1)-d U(1) QLMs

- ▶ Even for analog simulations, AMO systems usually only have **finite** degrees of freedom.
- ▶ Discretization of space (already achieved in the lattice theory) and digitization of field degrees of freedom are required.
- ▶ U(1) gauge theory with staggered fermions in (1 + 1)-d with the temporal gauge  $A_0 = 0$ :

$$H = -w \sum_x \left[ \psi_x^\dagger U_{x,x+1} \psi_{x+1} + \psi_{x+1}^\dagger U_{x,x+1}^\dagger \psi_x \right] + m \sum_x (-1)^x \psi_x^\dagger \psi_x + \frac{g^2}{2} \sum_x E_{x,x+1}^2, \quad (1)$$

## Backup Info: Introduction to Quantum Link Models



$$U_{x,x+1} = \exp(iagA_{x,x+1}) \in U(1), \quad (2)$$

$$E_{x,x+1} \equiv \frac{1}{g} F_{01,x,x+1} = -i \frac{1}{ag} \frac{\partial}{\partial A_{x,x+1}}. \quad (3)$$

- ▶  $agA_{x,x+1}$  is defined modulo  $2\pi$ , so the spectrum of the electric flux on each link is  $\mathbb{Z}$ , **infinite** degrees of freedom:  
 $E_{x,x+1} = \dots, -2, -1, 0, 1, 2, \dots$
- ▶ Each Fermion site has two (**finite**) degrees of freedom: occupied and unoccupied.

## Backup Info: Introduction to Quantum Link Models

- ▶  $SU(2)$  representations with any integers or half-integers  $S$  are allowed (only  $S = 1/2$  and  $1$  are considered in this work) so the spectrum of the electric flux is **finite**:

$$E_{x,x+1} = -S, -S + 1, \dots, S - 1, S.$$

## Backup Info: Introduction to Quantum Link Models

- ▶ Each link is associated with an  $SU(2)$  algebra. The gauge field associated with this theory is still  $U(1)$ .
- ▶ The  $U(1)$  Quantum link Hamiltonian in terms of quantum operators look identical to the corresponding lattice gauge theory, but its Hilbert space is finite per link and the commutation relations of quantum operators are modified.
- ▶ The Hamiltonian does not by itself impose the gauge invariance, so the Gauss law needs to be imposed by hand  $\tilde{G}_x |\text{phys}\rangle = 0$  and we only consider states that satisfy the Gauss law. The Gauss law operator is

$$\tilde{G}_x = \psi_x^\dagger \psi_x - E_{x,x+1} + E_{x-1,x} + \frac{1}{2} [(-1)^x - 1]. \quad (4)$$

## Backup Info: Physics of Dipolar Molecules

- ▶ A dipolar molecule is a quantum rotor  $H_{\text{rot}} = hB_{\text{rot}} \mathbf{N}^2$ .  $\mathbf{N}$  is the rotational angular momentum operator. Eigenstates are  $|N, m_N\rangle$  where  $m_N = -N, -N + 1, \dots, N - 1, N$ .
- ▶ A strong uniform magnetic field defines the  $z$  axis of spherical harmonics
- ▶  $N = 0$  and  $1$  states:  $|a\rangle \equiv |0, 0\rangle$ ,  $|b\rangle \equiv |1, -1\rangle$ ,  $|c\rangle \equiv |1, 0\rangle$  and  $|d\rangle \equiv |1, 1\rangle$ .
- ▶ Dipole-dipole interaction is

$$V_{ij} = \frac{1}{4\pi\epsilon_0} \frac{\mathbf{d}_i \cdot \mathbf{d}_j - 3(\mathbf{d}_i \cdot \hat{r}_{ij})(\mathbf{d}_j \cdot \hat{r}_{ij})}{r_{ij}^3}, \quad (5)$$

where  $\mathbf{r}_{ij}$ , the vector connecting positions of two molecules, is fixed and  $\mathbf{d}_i$  is the dipole moment operator, transforming like a vector (rank-1 tensor) under spatial rotation.

## Backup Info: Physics of Dipolar Molecules

- ▶ The dipole selection rules  $\Delta N = \pm 1$  and  $\Delta m_N = 0, \pm 1$  follow from the Wigner 3- $j$  symbols in

$$\begin{aligned} & \langle N', m'_N | \hat{d}_q | N, m_N \rangle \\ &= d(-1)^{m'_N} \sqrt{(2N'+1)(2N+1)} \\ & \quad \begin{pmatrix} N' & 1 & N \\ -m'_N & q & m_N \end{pmatrix} \begin{pmatrix} N' & 1 & N \\ 0 & 0 & 0 \end{pmatrix}. \end{aligned} \quad (6)$$

- ▶ The matrix elements of the dipole-dipole interaction  $\hat{H}_{ij}^{\text{int}}$ , as a two-body interaction, can be directly calculated from multiplying matrix elements of  $\mathbf{d}_i$  and  $\mathbf{d}_j$  and then taking a linear combination.

## Backup Info: Physics of Dipolar Molecules

- ▶ Constrained to  $N = 0$  and 1 states, relative energy shifts depending on molecule positions, angular momenta  $N$  and  $m_N$  are accessible by using laser lights.
- ▶ They are one-body potentials  $\sum_{i,N,m_N} \epsilon_{i,N,m_N} \hat{n}_{i,N,m_N}$ .

## Backup: Mapping of States

- ▶ A molecule is mapped to a site or link. (Positions are mapped to positions.)
- ▶ A molecule state is mapped to a site or link state. (States are mapped to states.)
- ▶ Each fermion site needs two molecule states:  $|a\rangle$  for occupied and  $|c\rangle$  for unoccupied.  $|b\rangle$  and  $|d\rangle$  are made off-resonant.
- ▶ Dipolar molecules used in our case are hardcore bosons and in  $(1+1)$ -d, a Jordan-Wigner transformation converts hardcore bosons to fermions.
- ▶ Each gauge link needs  $2S + 1$  molecule states.
- ▶  $S = 1/2$ :  $|b\rangle$  for  $S^3 = -1/2$  and  $|d\rangle$  for  $S^3 = 1/2$ .  $|c\rangle$  is made off-resonant.
- ▶  $S = 1$ :  $|b\rangle$  for  $S^3 = -1$ ,  $|d\rangle$  for  $S^3 = 0$ ,  $|c\rangle$  for  $S^3 = 1$ .

## Backup Info: Engineering the Effective Hamiltonian

- ▶ In the lab, only one-body potentials (rotors and laser lights) and two-body (dipole-dipole) interactions are accessible.
- ▶ Our target Hamiltonian has one-body terms  $m \sum_x (-1)^x \psi_x^\dagger \psi_x + \frac{g^2}{2} \sum_x E_{x,x+1}^2$  and three-body terms  $\psi_x^\dagger U_{x,x+1} \psi_{x+1} + h.c..$
- ▶ Engineering one-body terms is straight-forward.
- ▶ Engineering three-body terms require the method of quasi-degenerate effective Hamiltonians .

# Backup Info: Engineering the Effective Hamiltonian

- ▶ The quasi-degenerate effective Hamiltonian to the second-order is

$$\begin{aligned} \langle m | H_{\text{eff}}^{\alpha} | n \rangle &= E_{m\alpha} \delta_{mn} + \langle m, \alpha | V | n, \alpha \rangle + \\ &+ \frac{1}{2} \sum_{l, \gamma \neq \alpha} \langle m, \alpha | V | l, \gamma \rangle \langle l, \gamma | V | n, \alpha \rangle \cdot \quad (7) \\ &\times \left[ \frac{1}{E_{m\alpha} - E_{l\gamma}} + \frac{1}{E_{n\alpha} - E_{l\gamma}} \right] + \dots \end{aligned}$$

- ▶ The Gauss law is imposed by laser lights so that only the configurations that satisfy the Gauss law are in the subspace  $\alpha$ .
- ▶ **One-body potentials** are tunable by laser lights while keeping  $m, g^2 \ll \Delta$ .
- ▶ Three-body interactions are **tunable by molecule positioning** and **tunable by laser lights**.