A toolbox for lattice spin-models with polar molecules in optical lattices

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Lattice Spin Models

- Used in CMP as simplified models to
  - describe behavior of more complicated system
  - long range order, phase transitions, broken symmetries, ...

- Can we encode quantum information robustly in many body spin states?
  - Desired features
    - Degenerate ground states encoding logical states with energy gap to excited states
    - Logical states coupled only by highly non local operator
    - Leakage errors that couple to excited states correctable by quasi local operators (local stabilizers)

- Topologically ordered ground-states
  - Robust to arbitrary perturbations in the underlying Hamiltonian
  - no long-range pair-wise correlations, rather
    long-range correlations in strings of operators

- These types of spin models are highly anisotropic in spin and space, often involve N>2 body interactions

- Challenge: find physical systems where
  - these models can be build and
  - their properties can be probed
Outline

- Brief! introduction to topological order
- Description of polar molecules --how to control them
- Building spin models with polar molecules
  - This is not a simulation, i.e. does not involve short time pulse sequencing
- Protocol for building two spin models that encode noise protected quantum memory
  - One on a square lattice with two fold degenerate states
  - One on a honeycomb lattice with topologically protected ground states
- Conclusions
Topologically ordered states

- **Definition:**
  - Hilbert space of $n$, $d$-level spins
    \[ \mathcal{H} = (\mathbb{C}^d)^\otimes n \]
  - Isomorphic to
    \[ \mathcal{H} = \mathbb{C}^{C_1(\Gamma, \mathbb{F}_d)} \]
  - Topologically ordered if ground state degeneracy reflects the homology
    \[ H_1(\Gamma, \mathbb{F}_d) = \ker(\partial_1)/\text{image}(\partial_2) \]
    - i.e. ground states described by equivalence classes of cycles on the lattice that are not themselves boundaries of areas
    \[ \dim(\mathcal{H}_g) = d^{2g} \]

- **Example:** Qubits represented by edges on a planar lattice with two holes
  - Code subspace is two qubits:
    \[ H_1(C; \mathbb{Z}_2)/\bigoplus_{f} H_1(f, \partial f; \mathbb{Z}_2) \]
  - Ground states invariant under loops of Pauli
  - operators that are contractible
  - Hamiltonian
    \[ H = J \left( \sum_{+} (\sigma^z)^\otimes 4 + \sum_{\Box} (\sigma^x)^\otimes 4 \right) \]
    \[ n = |E| \]
Realization with molecular quantum gases:
Physical Ingredients

- lattices:
  - prepare exactly one molecule per site in optical lattice, e.g. starting from a BEC.
  - cf. AMO-Hubbard models

- spin by internal structure of:
  - rotating hetero-nuclear molecules
  - dipole-moment in electronic ground state

- spin-spin interactions
  - via dipole-dipole interactions
  - strong anisotropic off-site interactions
Polar molecules*

- System: $^2\Sigma_{1/2}$ hetero-nuclear molecules in electronic-vibrational ground-states
  - Alkaline-earth monohalogenides (CaF, CaCl, ...)
  - single electron in outer shell
- Look like alkali-atoms ...
  - can be cooled and trapped in optical lattices
  - ground states as spin-1/2-system (neglect hyperfine)
- But: rotation and electric dipole moment in el. gs

here e.g. CaF

\[ \text{el.spin} \rightarrow S \rightarrow e^- \]

\[ \text{optical excitation} \]

\[ \text{Alkali-like} \]

\[ \text{dipole moment} \]

\[ \text{talks to optical radiation, like an alkali atom} \]

\[ \text{talks to microwave radiation \ldots as rotations on } \sim 20 \text{ GHz} \]

* exp: Demille, Doyle, Mejer, Rempe, ...
Rotational spectra of a single molecule

- single hetero-nuclear molecule (without spin)

\[ H = B N^2 \]

\[ | N, M_N \rangle \]

\[ E_N = B N(N+1) \]

- dipole-moment \( d \sim 10 \) Debye 😊
- rotation \( B \sim 10 \) GHz ... anharmonic 😊
- essentially no spontaneous emission 😊
  black-body scatt. rate \( \Gamma N(kT) \sim 10^{-3} \)Hz 😊
  i.e. excited states useable 😊
Rotational spectra of a single molecule

- rigid rotor
  \[ H = B \, N^2 \]
  \[ |N, M_N\rangle \]
  \[ E_N = B \, N(N+1) \]

- add spin-rotation coupling
  \[ H = B \, N^2 + \gamma \, N \cdot S \]
  \[ |N, J, M_J\rangle \quad (J=|N\pm 1/2|) \]
  \[ E_{N,J=N\pm 1/2} = B \, N(N+1) + \begin{cases} +\gamma N/2 \\ -\gamma(N+1)/2 \end{cases} \]

N=2: "D"

N=1: "P"

N=0: "S"

2B \sim 20GHz

rotational ground state...

N=0: "S_1/2" J=1/2

N=1: "P_1/2" J=1/2

N=2: "D_{3/2}" "D_{5/2}" J=3/2 J=5/2

3\gamma/2 \sim 60MHz

... as spin-1/2-system
Two polar molecules: dipole-dipole interactions

- interactions of two polar molecules
  \[ V_{dd} = \frac{\vec{d}_1 \cdot \vec{d}_2 - 3(\vec{d}_1 \cdot \vec{e}_b)(\vec{e}_b \cdot \vec{d}_2)}{r^3} \]

- features of dipole-dipole interaction:
  - long range \( \sim 1/r^3 \)
  - angular dependence (anisotropic)

- include spin-rotation coupling in adiabatic potentials for molecular dimers

- At typical optical lattice spacing: \( \lambda/2 \sim r_\gamma = (2d^2/\gamma)^{1/3} \)
  - rotation of dimers strongly coupled to spins
  - Hund's case (c) excited states, \( \{\alpha(r)\} \quad (Y = \Sigma_{i=1,2} M_{N,i} + M_{S,i}) \)
  - solvable in closed form due to symmetries
Two molecules: Adiabatic Potentials $E_\lambda(r)$

- Adiabatic potential curves for two dimers (rotor + spin-rotation + dipole-dipole)

\[
\begin{align*}
E/2B &= \frac{\gamma}{4B}^{1/3} r / r_\gamma \\
&= \frac{\gamma}{4B}^{1/3} \left( \frac{d^2}{3B} \right)^{1/3} \\
&\approx 300 \text{ nm}
\end{align*}
\]

- In joint rotational ground-state (S+S) only van der Waals interaction
  - weak and (essentially) spin-independent
  \[
  V_{\text{eff}}(r) = -\frac{C_6}{r_\gamma^6} \left[ 1 + \left( \frac{\gamma}{2B} \right)^2 (S_1 \cdot S_2 - S_1^b S_2^b) + O \left( \frac{\gamma}{2B} \right)^4 \right] \\
  C_6 = \frac{d^4}{6B}
  \]
  - while ground + excited (S+P) have strong resonant dipole-dipole interactions
    - competition with spin-rotation coupling at lattice spacings $r \sim \lambda/2$
    \[
    \{|Y\rangle_{g,u}^{\pm}(r)\} \quad (Y=\sum_{i=1,2} M_{N_i}^{\pm} + M_{S_i}^{\pm})
    \]
Microwave coupling with tunable spin patterns

- Adiabatic mixing with dipole-dipole coupled states by microwave fields $E(t)$

Mathematical expressions:

\[
H_{\text{eff}}(r) = \sum_{i,f} \sum_{\lambda(r)} \frac{\langle g_f | H_{\text{mf}} | \lambda(r) \rangle \langle \lambda(r) | H_{\text{mf}} | g_i \rangle}{\hbar \omega_F - E(\lambda(r))} |g_f \rangle \langle g_i|
\]

\[
H_{\text{mf}} = -\sum_{j=1}^{2} \vec{d}_j \cdot \vec{E}(\vec{x}_j, t) = -\hbar \Omega \sum_{j} \vec{d}_j \cdot \vec{e}_F e^{-i(\vec{k}_F \cdot \vec{x}_j - \omega_F t)}/d + h.c.
\]
Microwave coupling with tunable spin patterns

- Adiabatic mixing with dipole-dipole coupled states by microwave fields

\[ H_{\text{eff}}(r) = \sum \sum_{i, f} \frac{\langle g_f | H_{\text{mf}} | \lambda(r) \rangle \langle \lambda(r) | H_{\text{mf}} | g_i \rangle}{\hbar \omega_F - E(\lambda(r))} | g_f \rangle | g_i \rangle \]

\[ H_{\text{spin}} = \langle H_{\text{eff}}(r) \rangle_{\text{rel}} = \sum_{\alpha, \beta} A_{\alpha, \beta} \sigma^\alpha \sigma^\beta \]

- Feature 1: Tuning close to a resonance one select a specific spin pattern, e.g.

<table>
<thead>
<tr>
<th>Polarization</th>
<th>Resonance</th>
<th>Spin pattern</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \hat{x} )</td>
<td>2_g</td>
<td>( \sigma^z \sigma^z )</td>
</tr>
<tr>
<td>( \hat{z} )</td>
<td>0^+_u</td>
<td>( \tilde{\sigma} \cdot \tilde{\sigma} )</td>
</tr>
<tr>
<td>( \hat{z} )</td>
<td>0^-_g</td>
<td>( \sigma^x \sigma^x + \sigma^y \sigma^y - \sigma^z \sigma^z )</td>
</tr>
<tr>
<td>( \hat{y} )</td>
<td>0^-_g</td>
<td>( \sigma^x \sigma^x - \sigma^y \sigma^y + \sigma^z \sigma^z )</td>
</tr>
<tr>
<td>( \hat{y} )</td>
<td>0^+_g</td>
<td>( -\sigma^x \sigma^x + \sigma^y \sigma^y + \sigma^z \sigma^z )</td>
</tr>
<tr>
<td>((\hat{y} - \hat{x})/\sqrt{2})</td>
<td>0^+_g</td>
<td>( -\sigma^x \sigma^x - \sigma^y \sigma^y + \sigma^z \sigma^z )</td>
</tr>
</tbody>
</table>

polarization rel. to body axis, here set \( \vec{e}_b = \hat{z} \)
Lattice Spin Models using multiple fields

- **Feature 2:** for a *multifrequency* field spin textures are *additive* => toolbox

1D XYZ model

\[ H = \sum_{\langle i,j \rangle} J_x \sigma_i^x \sigma_j^x + J_y \sigma_i^y \sigma_j^y + J_z \sigma_i^z \sigma_j^z \]

2D Ising model

\[ H = \sum_{\langle i,j \rangle} J \sigma_i^z \sigma_j^z \]

3D Heisenberg model

\[ H = \sum_{\langle i,j \rangle} J \vec{\sigma}_i \cdot \vec{\sigma}_j \]

**Typical coupling strengths:** \(|J| \sim 10 - 100\text{kHz}\)

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<td>(\hat{z})</td>
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</tr>
<tr>
<td>(\hat{y})</td>
<td>0(_g^-)</td>
</tr>
<tr>
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</tr>
<tr>
<td>(\hat{x})</td>
<td>2(_g)</td>
</tr>
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</tr>
<tr>
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</tr>
<tr>
<td>(\hat{z})</td>
<td>0(_u^+)</td>
</tr>
<tr>
<td>(\hat{x})</td>
<td>1(_u)</td>
</tr>
</tbody>
</table>

*sign adjustable by tuning above or below given resonance*
Model I: Error protected ground states

- Model on 2D square lattice

\[ H_{\text{spin}}^{(1)} = \sum_{i=1}^{\ell-1} \sum_{j=1}^{\ell-1} J(\sigma_{i,j}^z \sigma_{i,j+1}^z + \cos \zeta \sigma_{i,j}^x \sigma_{i+1,j}^x) \]

- gapped spectrum with 2-fold degenerate ground-state (for \( \zeta \neq \pm \pi/2 \) → \( |0\rangle_L, |1\rangle_L \)
- ground-states robust to local errors up to \( \ell\)-th order
- logical operations correspond to strings of operators along row or column
- tunable coupling by rotating polarization of the driving microwave field \( E(t) \) by angle \( \zeta \)

\( J_z \sum_{i,j} \sigma_{i,j}^z \sigma_{i,j+1}^z \)

\[ \text{Gap } \Delta/J = (E_n - E_0)/J \]

\( J_x \sum_{i,j} \sigma_{i,j}^x \sigma_{i+1,j}^x \)
Spatial orientation dependent Ising interactions

- Realization by tuning MW far blue from bare $S_{1/2} \leftrightarrow P_{3/2}$ transition

- Interaction given effectively by interplay of 3 resonances
  - Outer two yield single effective interaction
  - Optimal regime near $2_g$ as spin-texture

- Feature 3: Can choose the range of the interaction for a given spin texture,
  (cf. reminiscent of optical shielding)
Results: Design and verification on 3x3 lattice

- Noise resilience as measured by rms magnetisation in ground manifold
  - as function of the detuning
  - give worst case scenario for logical bit flip errors / phase flip errors
  - protected region near $2_g$

- Verification by absorption spectroscopy
  - for $\zeta=0$ (polarization along the plane)
    - probe gap at $J/2$
  - for $\zeta=\pi/2$ (polarization along the plane)
    - gap disappears and excitations as spin-waves $S^x$
Model II: Topological order

- Model on a 2D honeycomb lattice*

\[ H_{\text{spin}}^{(\text{II})} = J_\perp \sum_{x-\text{links}} \sigma_j^x \sigma_k^x + J_\perp \sum_{y-\text{links}} \sigma_j^y \sigma_k^y + J_z \sum_{z-\text{links}} \sigma_j^z \sigma_k^z \]


- exactly solvable model
- two phases:
  - \( |J_z| > 2|J_\perp| \): gapped phase with abelian anyonic excitations
  - \( |J_z| \leq 2|J_\perp| \): gapless phase which becomes gapped in presence of a magnetic field with nonabelian anyonic excitations
- Effective Hamiltonian in gapped phase with \( |J_z| \gg |J_\perp| \) encodes topologically protected memory**

\[ H_{\text{eff,spin}}^{(\text{II})} = J_{\text{eff}} \left( \sum_{i=1}^{4} \prod_{i=1}^{4} \sigma_i^x + \sum_{i=1}^{4} \prod_{i=1}^{4} \sigma_i^z \right) \]

\[ J_{\text{eff}} = \frac{J_\perp J_z}{16J_4^z} \]
Construction in an optical lattice

- Implementation in $Q^{*}bert$ lattice:
  - Two staggered triangular lattices
  - Nearest neighbors give honeycombs
  - Their edges form orthogonal triads

- Realization with 3 fields: (several possible choices)
  shown when all 3 being z polarized, resp. near $0^{-g}$, $1^{-g}$, $2^{-g}$

Spin pattern

| Coupling strengths $|J_{lr}|$ |
|---------------------------|
| $\sigma^z \sigma^z$       | $< 10^{-2} |J_z|$ |
| $\sigma^x \sigma^x$       | $< 10^{-3} |J_z|$ |
| $\sigma^y \sigma^y$       | $|J_{\perp}| = 0.4 |J_z|$ |

Operator fidelity (on a 4 spin configuration)

$\sup[||H_{spin} - H^{(II)}_{spin} |\psi||_2; \langle \psi | \psi \rangle = 1] = 10^{-4} |J_z|$
Measuring quasi-particle statistics

- Statistical phase measured by computing relative phase between a path with a braid that cannot be disentangled and one that can.

- Particle types depend on character of the excitation.

- Physical implementation of quasiparticle creation and transport using a different species atom or molecule trapped in a different lattice.

- Guide for braiding operations can be preprepared using state preparation on the ancillaes.
Summary

- **Lattice Spin Models**
  - Realization with Polar Molecules & optical lattices

- **Engineering spin-spin interactions with polar molecules**
  - Structure of a single polar molecule
    - Electronic, vibrational, rotational and spin degrees of freedom
    - Electronic Dipole-moments in ro-vibrational ground-states
  - Interactions between two (unpolarized) rotating polar molecules
    - Competing Dipole-Dipole Interaction and Spin-rotation
    - VdW & Resonant transition between Hund's Cases for Dimers of dipoles
  - Effective spin-spin interactions via long-range resonances

- **Examples of Lattice Spin Models**
  - The Duocot *et al.* Model
    - Error protected degenerate subspace (macroscopic # spins).
  - The Kitaev Model
    - From gapped system with abelian excitations to
    - To ungapped system with nonabelian excitations