# Dimer model implementations of quantum loop gases

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# Outline

- *d*-isotopic quantum loop gases and dimer model implementations
- generalized RK points - Monte Carlo sampling for ground and excited states
- dimer model implementation on triangular lattice
- realization of extended Hubbard Hamiltonian approximate representation on surrounding Kagome lattice with trapped atoms/molecules

# Exotic phases and critical points in lattice models of loops and string-nets:

- certain quantum loop gas models sit on quantum critical points that are related to a class of non-Abelian topological phases

  Freedman, Nayak, Shtengel, Walker, Wang Ann. Phys **310** 428 (2004); Fendley, Fradkin PRB **72** 024412 (2005)

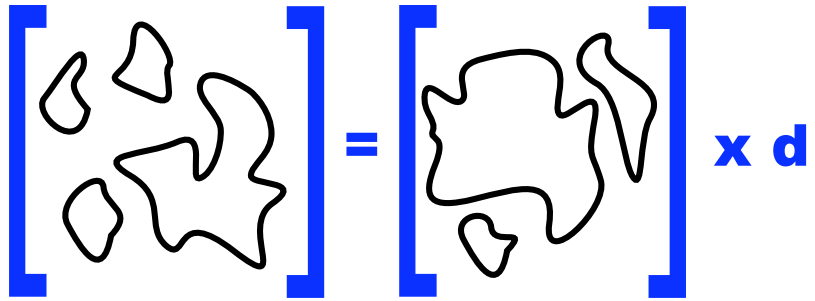
- string-net models can realize a variety of topological phases with Abelian and non-Abelian quasi-particles

  Levin, Wen PRB **71** 045110 (2005)

# *d*-isotopic Quantum Loop Gases (QLG) I:

(Freedman, Nayak, Shtengel, Walker, Zhang)

- Hilbert space of closed, non-intersecting loops
- configurations related by isotopy are given equal weight
- configurations related by the addition of a contractible loop are given a relative weight of the parameter *d*




$$\Psi\left[\{\alpha\} \cup \circ\right] = d\Psi\left[\{\alpha\}\right]$$

# *d*-isotopic Quantum Loop Gases II:

- ground state: $|\Psi_0\rangle = \sum_{\{\alpha\}} d^{n\{\alpha\}} |\alpha\rangle$

- norm of the ground state wavefunction is equivalent to the partition function of the self-dual Potts Model and O(n) model:

$$\langle \Psi_0 | \Psi_0 \rangle = Z_{O(n=d^2)} = Z_{Potts(q=d^4)}$$

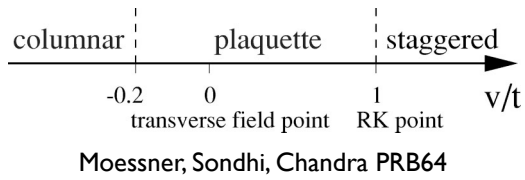
- for $1 \leq d \leq \sqrt{2}$, *d*-isotopic quantum loop gas (QLG) lives on a critical line with gapless $\omega \sim k^2$ excitations

Freedman, Nayak, Shtengel PRL **94** 147205 (2005); cond-mat/0508508

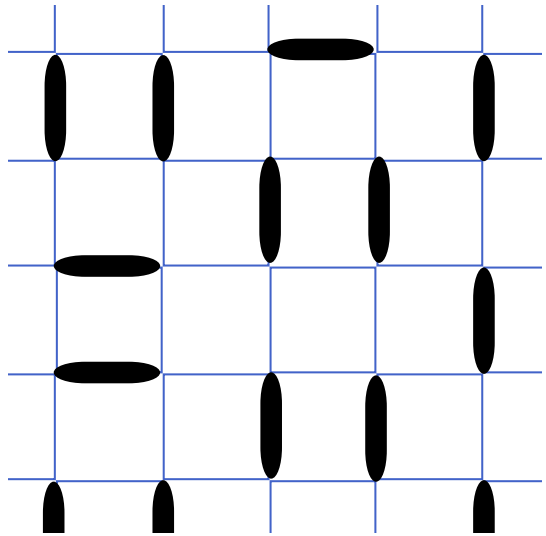
# *d*-isotopic Quantum Loop Gases III:

- the critical line has been conjectured to be described by the *SU(2)* analog of the critical *U(1)* gauge theory that is seen at the RK point on bipartite lattices
  - Rokhsar-Kivelson (RK) : $V = t$

$$H = \sum_{\square} V\left(|\square\rangle\langle\square| + |\square\rangle\langle\square|\right)$$
$$-t\left(|\square\rangle\langle\square| + \ h. \ .c\right)$$

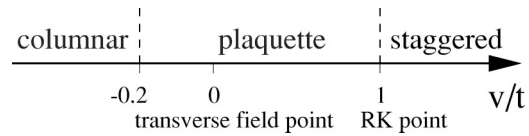



Moessner, Sondhi, Chandra PRB64



# RK point in dimer models:

- bipartite lattices:
  - the Rokhsar-Kivelson (RK) ($V = t$) point is described by a critical $U(1)$ gauge theory

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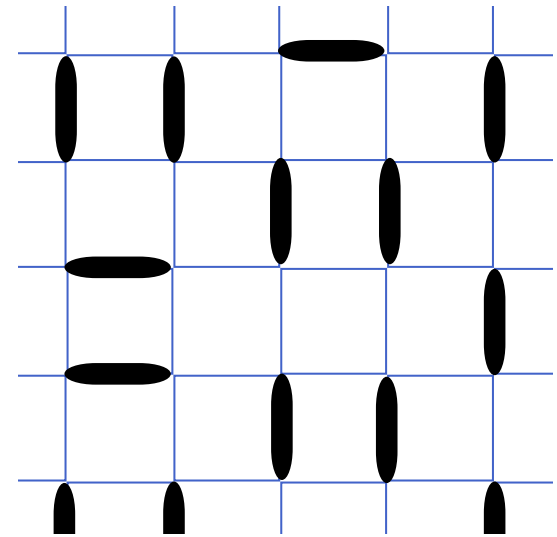
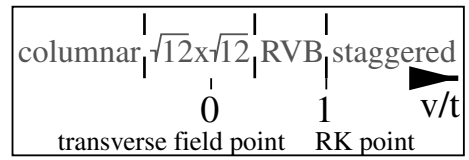


- non-bipartite lattices:
  - RK point is adjacent to a topological phase described by $Z_2$ gauge theory

$$H = \sum_{\square} V\left(|\square\rangle\langle\square| + |\square\rangle\langle\square|\right)$$

$$-t\left(|\square\rangle\langle\square| + \ h. \ .c\right)$$




Moessner, Sondhi PRL86

# *d*-isotopic Quantum Loop Gases III:

- the *d-isotopy* condition is related to the Wilson loop algebra of doubled $SU(2)_k$ Chern-Simons theories for particular values of *d*

$$d = 2\cos\left(\frac{\pi}{k+2}\right)$$

- has been conjectured that there may be proximate phases with related topological order

Freedman, Nayak, Shtengel PRL **94**, 147205 (2005)

# *d*-isotopic QLG's as generalized RK points:

- the square norm of the ground state wave function is equivalent to the partition function of the classical model
- exact zero energy ground state is a superposition of classical configurations (e. g., a dimer or loop covering of the lattice)
- each classical configuration is weighted by the square root of the Boltzmann weight of a corresponding classical model
- this point may be an isolated quantum critical point, or adjacent to a related phase (topological?)

# Strategy for study of topological phases and related critical points in microscopic lattice models

1. characterize ground state and excitations of d-isotopic QLG at generalized RK points

   - classical Monte Carlo

2. look at effects of perturbations (e.g., loop surgeries...), opening of gap, nature of excitations ...

   - quantum Monte Carlo

3. use dimer Hamiltonian on triangular lattice that has an extended Hubbard Hamiltonian approximation on surrounding Kagome lattice (Freedman, Nayak, Shtengel PRL **94**, 066401 (2005))

# Quantum dynamics from classical Monte Carlo I

C. L. Henley, J Phys Cond Mat **16**, S891 (2004)

Generalized RK Hamiltonians:

$$H = \sum_{\square} V\left(|\square\rangle\langle\square| + |\square\rangle\langle\square|\right) - t\left(|\square\rangle\langle\square| + \ h. \ .c\right)$$

classical partition function: $K$=1/T

$$Z_{cl} = \sum_{\alpha} e^{-KE_{\alpha}^{cl}}$$

RK Hamiltonian:

$$H_{RK} = \sum_{\{(\alpha,\beta\})} V\left(e^{-K\left(E_{\alpha}^{cl}-E_{\beta}^{cl}\right)/2}|\alpha\rangle\langle\alpha| + e^{K\left(E_{\alpha}^{cl}-E_{\beta}^{cl}\right)/2}|\beta\rangle\langle\beta|\right) - t\left(|\alpha\rangle\langle\beta| + h.c.\right)$$

exact zero energy ground state:

$$|\Phi_0\rangle = \frac{1}{\sqrt{Z}} \sum_{\alpha} e^{-KE_{\alpha}^{cl}/2}|\alpha\rangle$$

$$@\ t = V$$

# Quantum dynamics from classical Monte Carlo II

- master eqn: $$\frac{dp_\alpha}{d\tau}(\tau) = W_{\alpha\beta}\ p_\beta(\tau)$$ $$\begin{aligned} W_{\alpha\beta} &= min\left(1, e^{-K\left(E_\alpha^{cl} - E_\beta^{cl}\right)}\right) \\ W_{\alpha\alpha} &\equiv -\sum_{\beta\neq\alpha} W_{\alpha\beta} \end{aligned}$$

- similarity transform: $$\tilde{W}_{\alpha\beta} \equiv e^{KE_\alpha^{cl}/2} W_{\alpha\beta} e^{-KE_\beta^{cl}/2}$$

$$\tilde{W}_{\alpha\beta} \sim H_{RK}$$

- eigenvalues of the classical MC master equation are proportional to the eigenvalues of the quantum Hamiltonian

# Quantum dynamics from classical Monte Carlo III

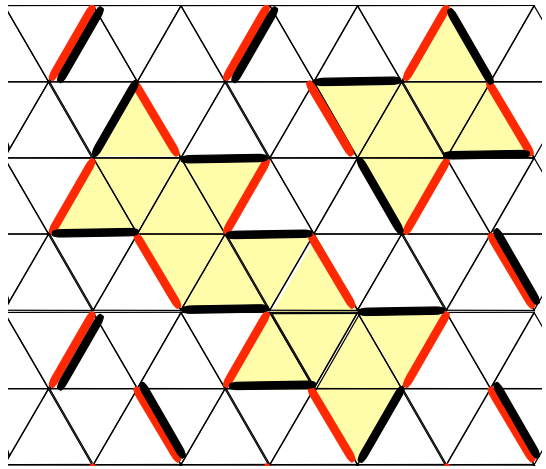
- sampling the classical model related to the quantum ground state => sampling the quantum ground state
- low lying excitations of the quantum Hamiltonian can be extracted from dynamic correlation functions of a classical Metropolis walk that samples the exact GS using the quantum dynamics:

$$C\left(|i-j|,\tau\right) \sim \left\langle O_i^{\dagger}\left(\tau\right) O_j\left(0\right)\right\rangle$$

$$C\left(k,\tau\right) \propto e^{-\Delta(k)\tau}$$

# Dimer model implementation of *d*-isotopic quantum loop gas (QLG)

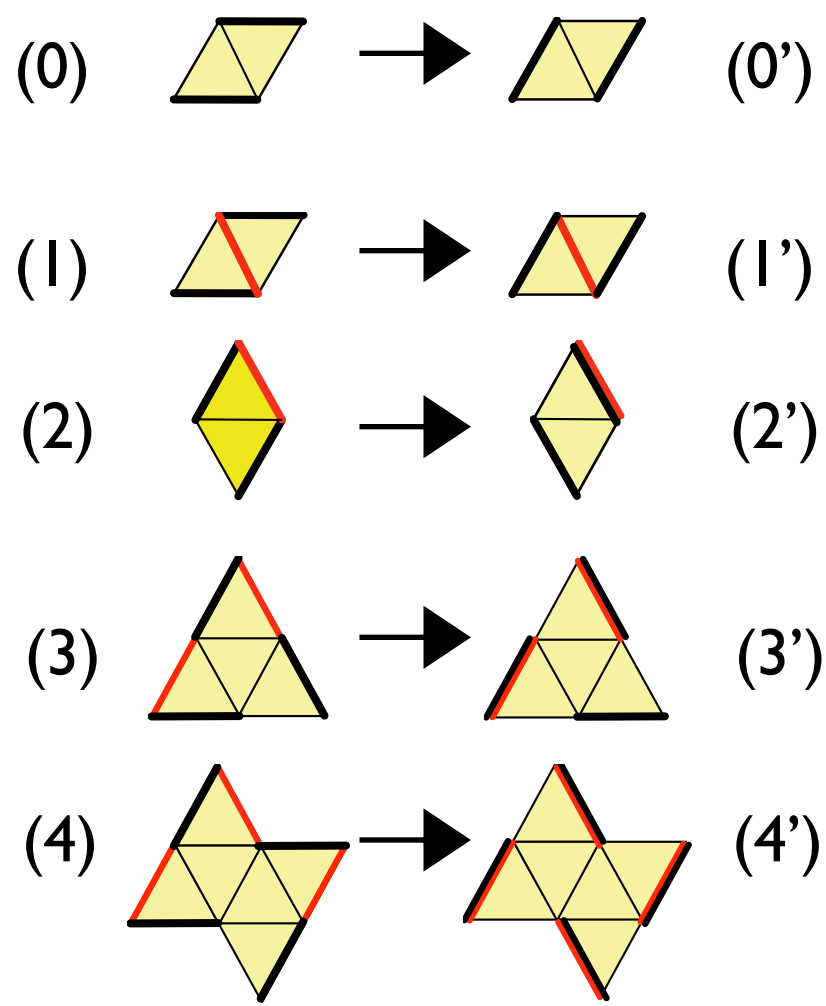
- Hilbert space: fully packed dimer coverings of the triangular lattice
- red bonds are a fixed background dimerization -- transition graph with dimer covering forms fully packed loop covering
- dimers living on red bonds are considered minimal loops with length 2



Freedman, Nayak, Shtengel PRL **94**, 066401 (2005)

# Dimer model QLG dynamics

- Plaquette flips correspond to isotopy (1), *d*-isotopy (2,3,4), and surgery (0) moves
- Surgeries (0) are forbidden; for ergodicity in a single winding sector three and four dimer moves (3,4) are needed



# Dimer model Hamiltonian

$$H = \sum V \left( |1\rangle\langle 1| + |1'\rangle\langle 1'| + d|2\rangle\langle 2| + \frac{1}{d}|2'\rangle\langle 2'| + \epsilon_1 \left( d^2|3\rangle\langle 3| + \frac{1}{d^2}|3'\rangle\langle 3'| \right) + \epsilon_2 \left( d^3|4\rangle\langle 4| + \frac{1}{d^3}|4'\rangle\langle 4'| \right) \right)$$
$$-t \left( |1\rangle\langle 1'| + |2\rangle\langle 2'| + \epsilon_1|3\rangle\langle 3'| + \epsilon_2|4\rangle\langle 4'| + \ h.\ c. \right)$$

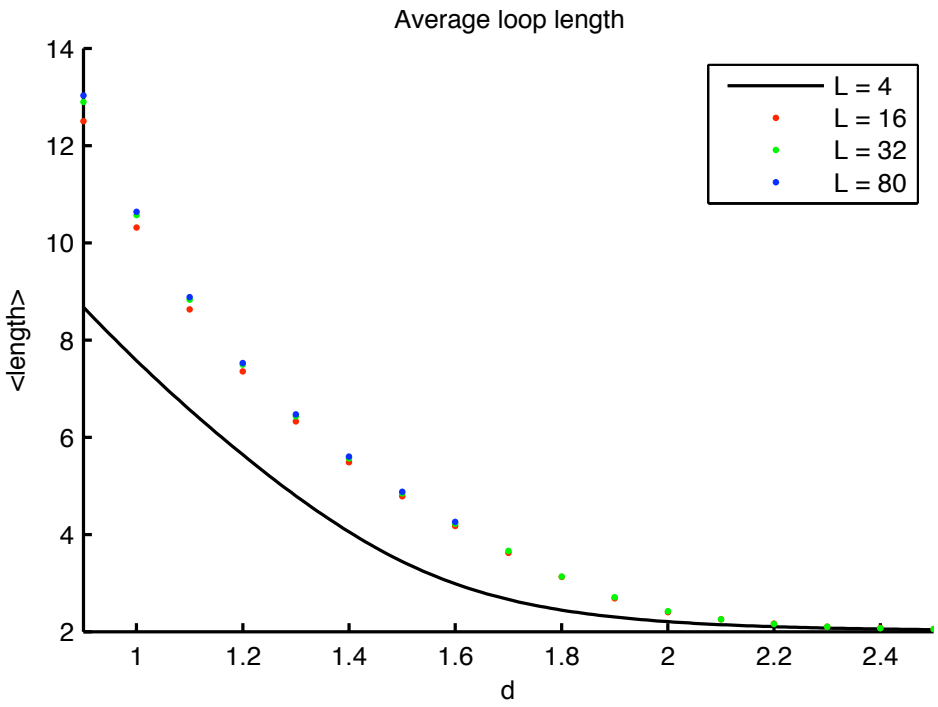
- fine tuned to the *RK* line ( $t = V$) of loop gas Hamiltonian, such that the zero energy ground state is a *d*-isotopic QLG
- one parameter (*d*) class of Hamiltonians
- *d*=1 w/surgeries corresponds to RK point of the pure triangular lattice dimer model
- $(\epsilon_1, \epsilon_2)$ are smallness parameters that do not affect the GS

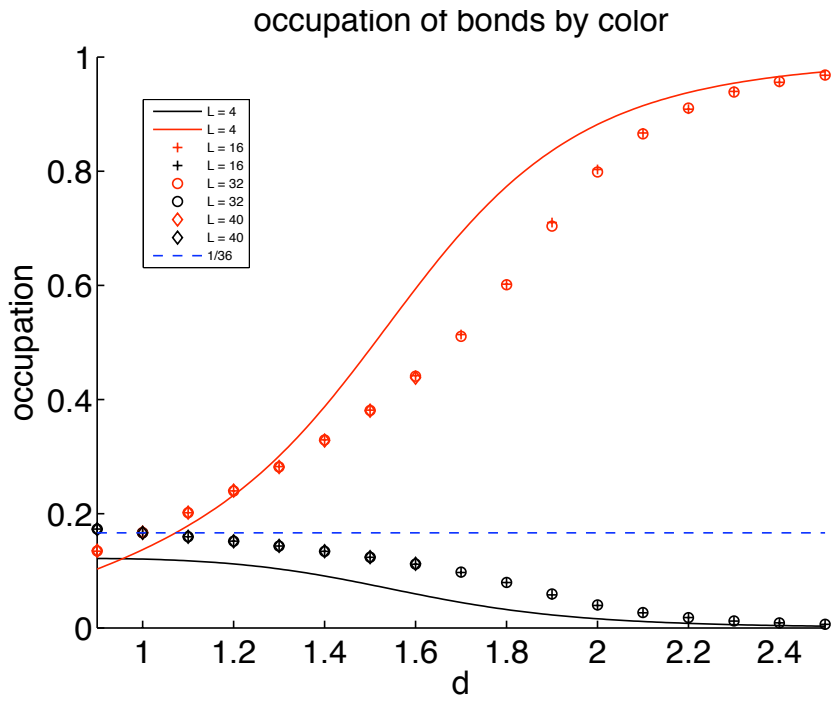
Freedman, Nayak, Shtengel PRL **94**, 066401 (2005); cond-mat/0309120

# Numerical methods

- Metropolis sampling of the ground state wavefunction
  - loop dynamics are critical => inefficient sampling
  - pure dimer dynamics (i.e., with surgeries) on triangular lattice are not critical, can be used for more efficient sampling of ground state
  - non-local moves can also be used
- low-lying excitations can be extracted from the dynamic correlation function (classical sampling corresponding to quantum Hamiltonian) evaluated at generalized RK points with loop dynamics (surgeries switched off during averaging)

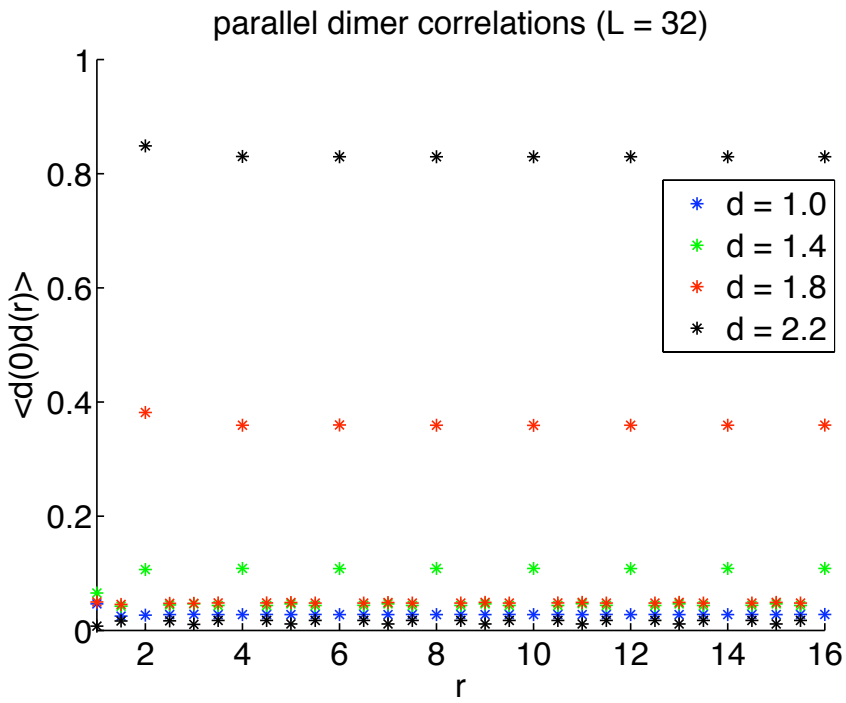
# *d*-isotopic ground state calculations: Global Properties




- transition from longer to shorter loops on average as *d* increases
- dimers on red bonds are minimal loops, dominate at large *d*

# *d*-isotopic ground state calculations: Correlation Functions

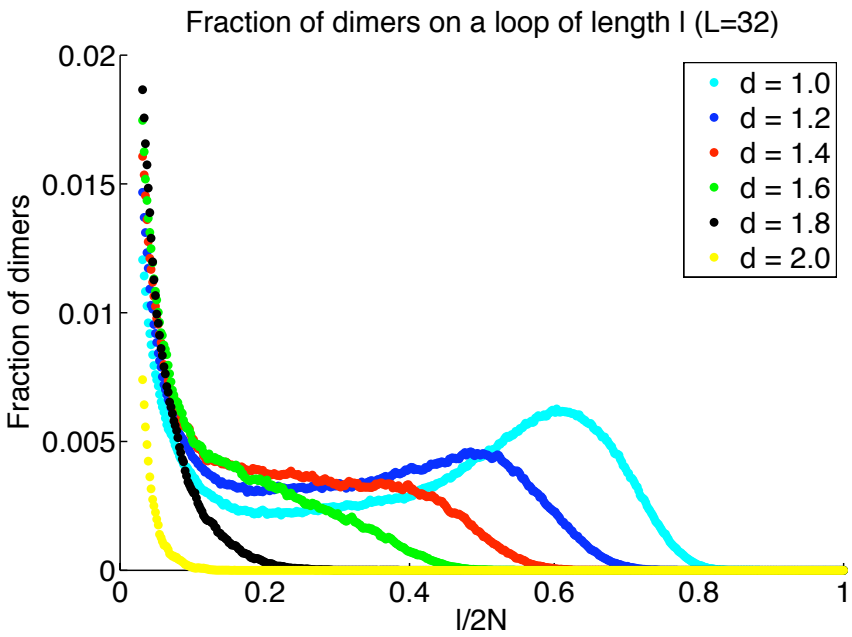


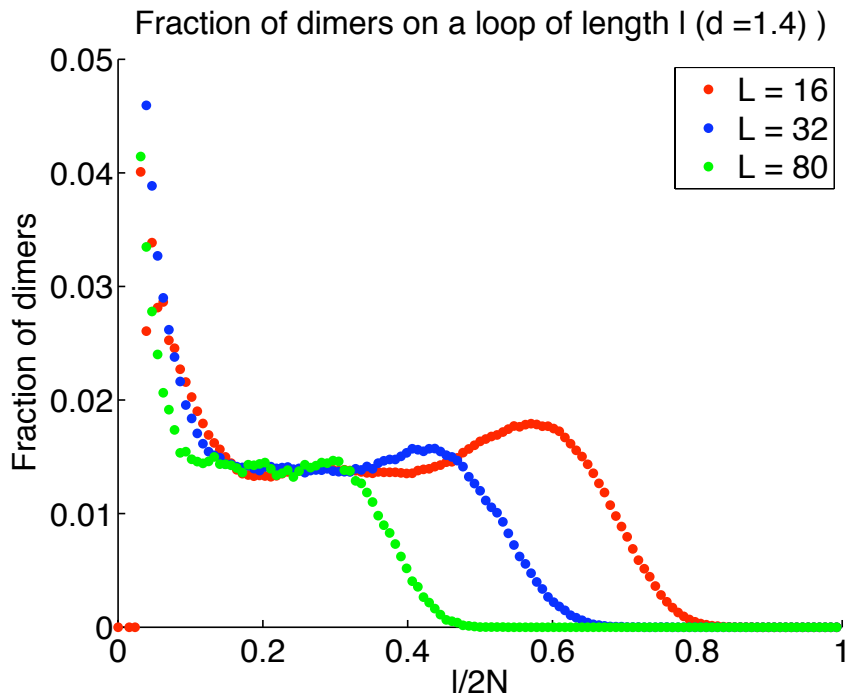

- parallel dimer-dimer correlations from a red site:

$$\langle d_R d\,(r)\rangle$$

- red bonds occur at $r = 2, 4, 6 \ldots$
- residual ordering on red bonds persists for $d > 1$
- no correlations to black bonds, even where finite black occupation persists

# *d*-isotopic ground state calculations: Loop Statistics

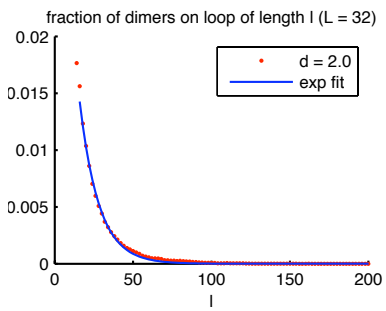


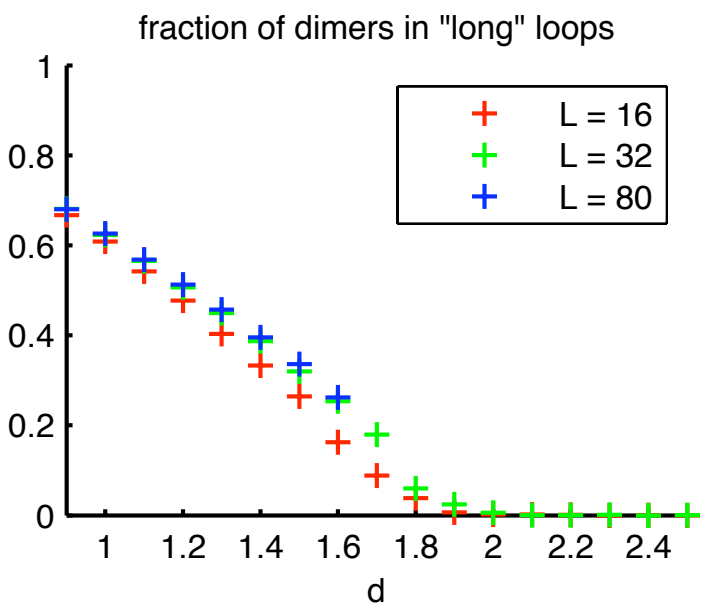




total length of all loops = 2N (N dimers)
for smaller d, broad plateau over large range of length scales emerges

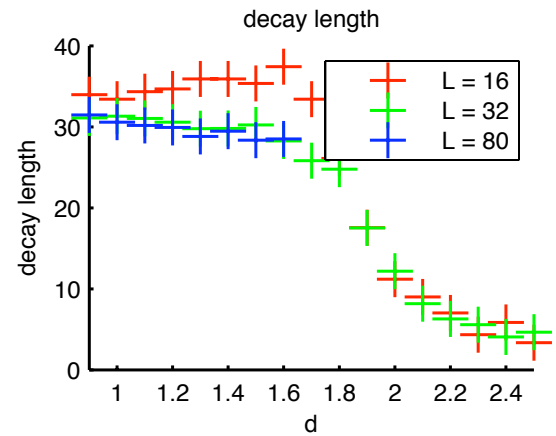
L=16; N=128
L=32; N=512
L=80; N=3200

# *d*-isotopic ground state calculations: "Long" vs. "Short" loops




- at all *d*, exponentially decaying peak at short lengths persists
  - can fit and subtract "short" loops under exponential
- finite fraction of lattice is covered in "long" loops for smaller *d*
- width of short loop exponential decay depends on *d* (width decreases, peak increases for large *d*)

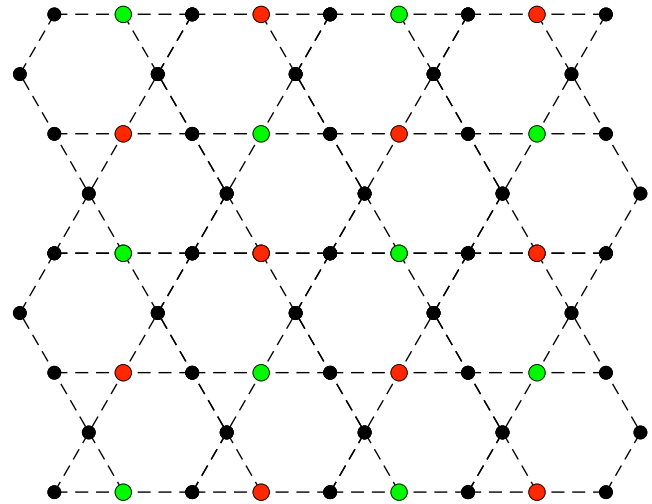


# Future work:

- static intra-loop correlation functions (critical exponents); fractal dimension ...
- imaginary time dynamics of loop gas at generalized RK points −> excitations (dispersion, gap ...)
  - test consistency with conjectured SU(2) gauge theory
- add perturbations to Hamiltonian, use Quantum Monte Carlo instead of Metropolis walks
  - look at neighboring phases, ground and excited states - topological?
- effects of disorder
  - restore criticality for large *d* values?
- other loop models

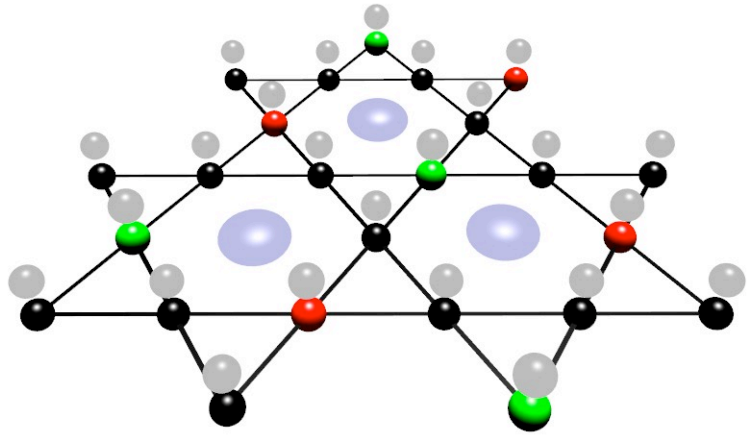
# Extended Hubbard model representation of QLG

- The QLG dimer model can be effectively implemented by a Hubbard-like Hamiltonian on a Kagome lattice (cond-mat/0309120)
- Complicated Hamiltonian, interactions not easy to implement
- Need anisotropic interactions, with very specific ranges
- We are investigating optical lattice implementations



$$H = \sum_i \mu_i n_i + U_0 \sum_i n_i^2 + U \sum_{\langle i,j \rangle \in \hexagon} n_i n_j + \sum_{\langle i,j \rangle \in \bowtie} V_{ij} n_i n_j - \sum_{\langle i,j \rangle} t_{ij} \left( c_i^\dagger c_j + c_j^\dagger c_i \right)$$

# Neutral atom implementation

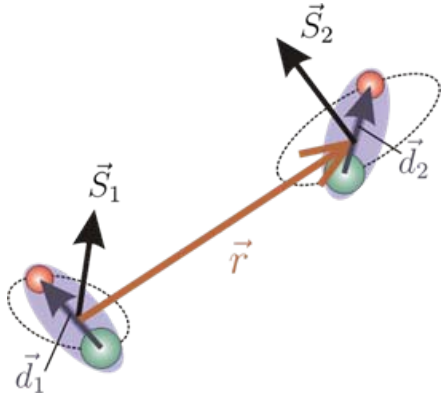


- particle = atom in state $|B\rangle$, vacancy = atom in state $|A\rangle$
- effective tunneling: atoms switching places, $\sim a_1^\dagger b_2^\dagger a_2 b_1$
- Hexagon interaction: State-selective tunneling by state-$|B\rangle$ atoms to auxiliary site in center of hexagon, virtual interaction $\Rightarrow$ energy penalty
- Bowtie interaction: Similar to hexagon interaction, virtual interaction at auxiliary site above every regular site
- Problems: leakage, virtual interactions via auxiliary sites very weak

# Spin-spin coupling with dipolar molecules

- Localized dipolar molecules


$$V_{\mathrm{dd}} = \frac{\vec{d}_1 \cdot \vec{d}_2 - 3\left(\vec{d}_1 \cdot \vec{e}_b\right)\left(\vec{e}_b \cdot \vec{d}_2\right)}{r^3}$$




- Can implement arbitrary (almost, maybe) spin models using dipolar molecules in optical lattices (Micheli et al., Nature Physics **2**, 341 (2006))
- Use diatomic molecules with permanent dipole moment and one net electron spin (e.g. alkali-earth monohalides)
- Create effective spin-spin coupling through *intra*molecular spin-rotation and *inter*molecular dipole-dipole coupling

# Hamiltonians for dipolar molecules and electron spin

- Single molecule: rotational energy and spin-orbit coupling

$$H_i = B\mathbf{N}_i^2 + \gamma \mathbf{N}_i \cdot \mathbf{S}_i$$

- Two molecules: dipole-dipole coupling

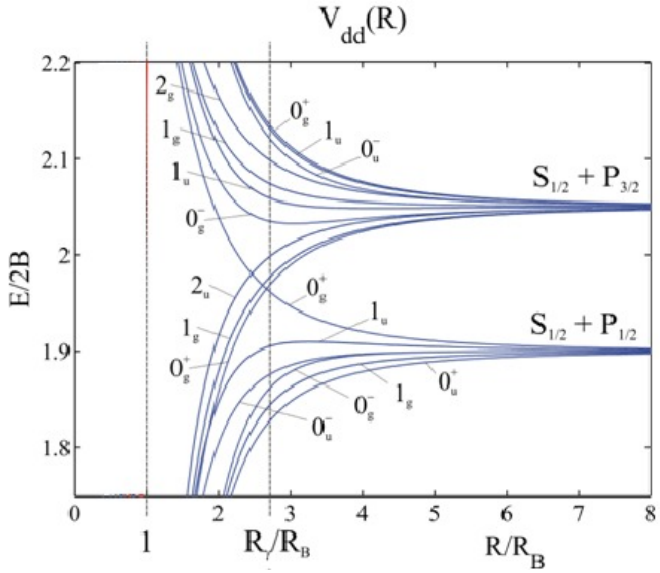
$$H_{dd} = -\frac{d^2}{3r^3}\left(D_1^+ D_2^- + D_1^- D_2^+ + 2D_1^z D_2^z\right)$$

  Couples rotational states of the two molecules

- Ground state, $(\mathbf{N}_1 + \mathbf{N}_2)^2 = 0$: No net dipole moment, only weak interaction to second order, $\sim 1/r^6$

# Dipole coupling in $N_{\text{tot}} = 1$ subspace

- Hamiltonian can be diagonalized *analytically*
- Interaction between two molecules $\sim 1/r^3$ obtained with laser tuned close to an $N_{\text{tot}} = 1$ level
- Spin-orbit coupling results in effective laser-induced spin-spin coupling between electron spins (*selectively* distance dependent)

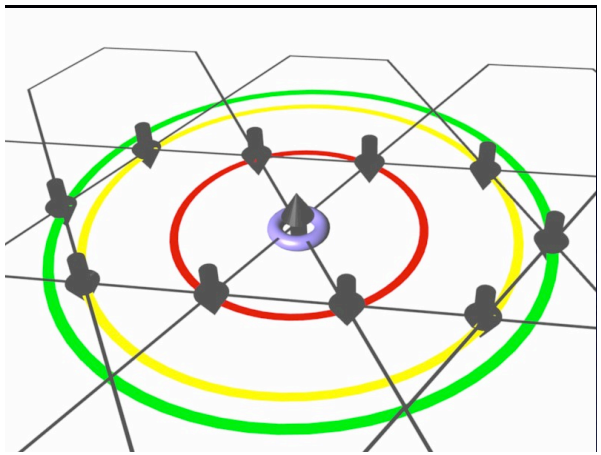


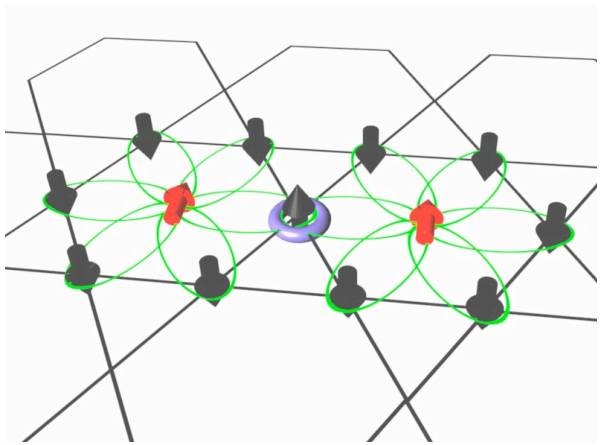

$$H_{\text{eff}} = \sum_{i,f,\lambda(r)} \frac{\langle g_f | V_{\text{las}} | \lambda(r) \rangle \langle \lambda(r) | V_{\text{las}} | g_i \rangle}{\hbar\omega - E(\lambda(r))} |g_f\rangle \langle g_i|$$

$$\longrightarrow \frac{\hbar|\Omega|}{8} \sum_{\alpha,\beta=0}^{3} \sigma_1^\alpha A_{\alpha\beta} \sigma_2^\beta \quad \text{for each intermediate level } |\lambda(r)\rangle$$

# Extended Hubbard model with spins

- Represent particle present by $|\uparrow\rangle$, absence by $|\downarrow\rangle$
- Tunneling through $S_1^y S_2^y + S_1^z S_2^z$ spin-swap
- Repulsive interactions between particles through $(S_1^x + 1/2)(S_2^x + 1/2)$ (Works well for bowties and most hexagon sites, but *not* for furthest hexagon site)
- Add spins at auxiliary sites; but interactions must be non-symmetric (must use different molecules or magnetic fields)





# Summary

- QLG simulation via classical Monte Carlo at generalized RK points
- ground state loop properties easily accessible
- excitations in progress ...
- extension to perturbed QLG's with QMC
- implementation of extended Hubbard approximation to lattice QLG with trapped dipolar molecules