Many-Body Physics with Up and Coming Molecules in Optical Lattices

Michael L. Wall
Colorado School of Mines

In collaboration with
Lincoln D. Carr and
Erman Bekaroglu

Unterstützt von / Supported by
Alexander von Humboldt Stiftung/Foundation

Center for Quantum Dynamics

What sorts of molecules?

$^1\Sigma$

- E.g. KRb, RbCs (talks this week)
- "Assembled" from ultracold alkali gases

$^2\Pi$

- E.g. OH, evaporative cooling

$^2\Sigma$

- E.g. SrF, YO via laser cooling
- Assemble from other ultracold species

Symmetric Tops

- E.g. CH_3F
- Possibility of efficient Stark deceleration, sympathetic cooling

http://coldmoles13.wikispaces.com/

What is new with molecules?

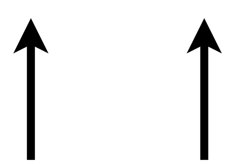
- Large electric dipole moments!
    - Resonant dipole-dipole interactions

$$V_{dd}\left(\mathbf{r}\right) = \frac{d^2}{r^3}\left(1 - 3\cos^2\theta\right)$$

What is new with molecules?

- Large electric dipole moments!
  - Resonant dipole-dipole interactions

$$V_{dd}(\mathbf{r}) = \frac{d^2}{r^3}\left(1 - 3\cos^2\theta\right)$$



repulsive

What is new with molecules?

- Large electric dipole moments!
  - Resonant dipole-dipole interactions

$$V_{dd}\left(\mathbf{r}\right) = \frac{d^2}{r^3}\left(1 - 3\cos^2\theta\right)$$

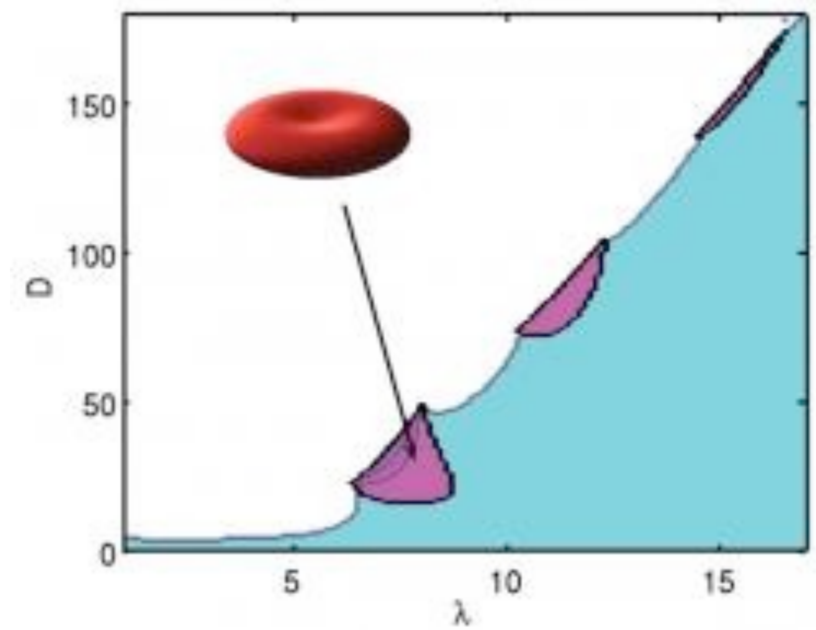
$\longrightarrow \longrightarrow$ Attractive

What is new with molecules?

- Large electric dipole moments!
  - Resonant dipole-dipole interactions

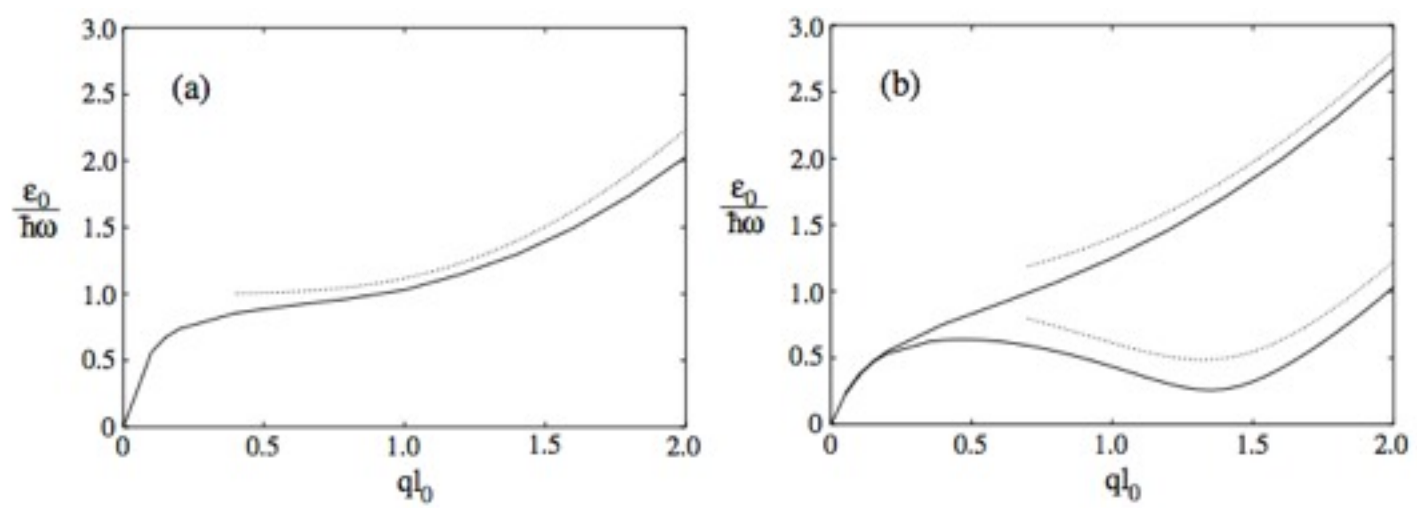
$$V_{dd}(\mathbf{r}) = \frac{d^2}{r^3}\left(1 - 3\cos^2\theta\right)$$

$\longrightarrow \; \longrightarrow$ Attractive



Ronen *et al.* PRL **98** 030406

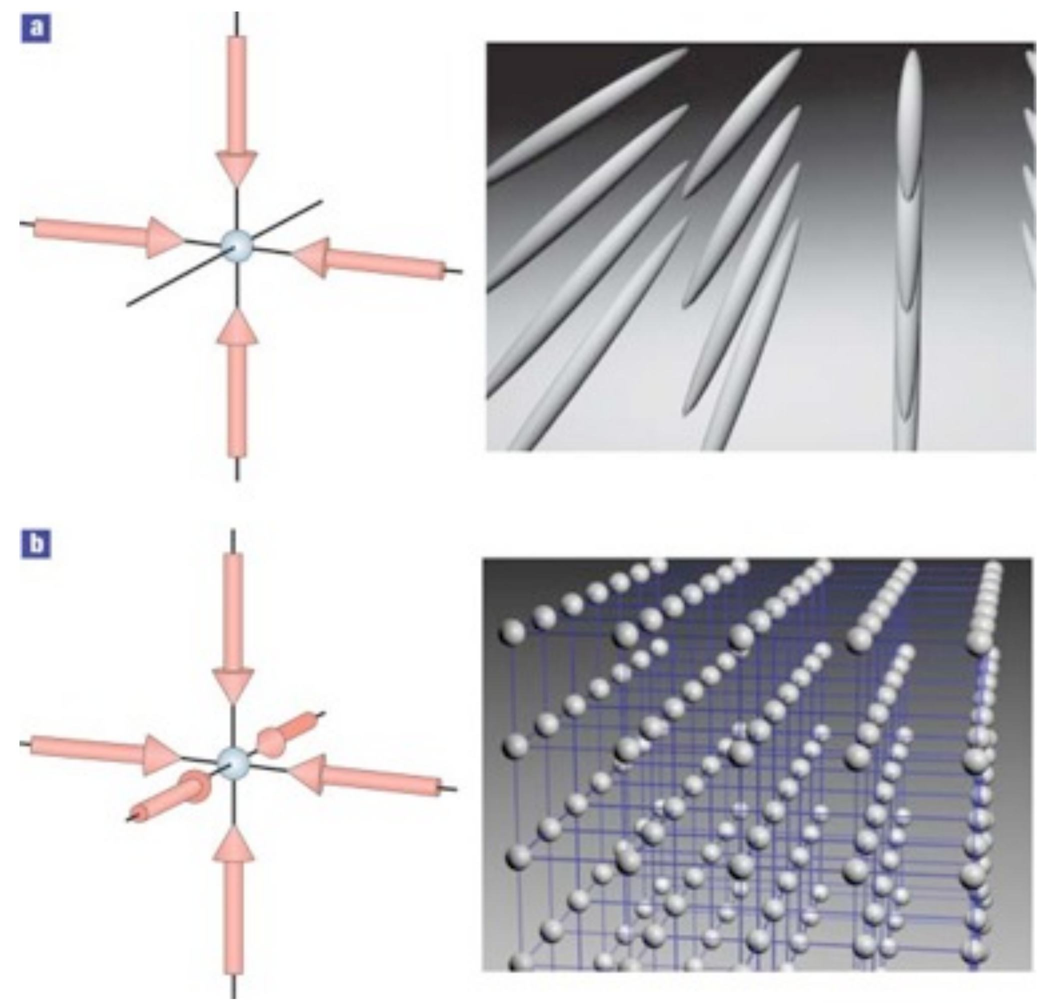
- Several novel predictions for structureless dipoles
- Rotons, "Red blood cell" BEC
- Anisotropic Fermi liquid
- Novel BCS-type pairing

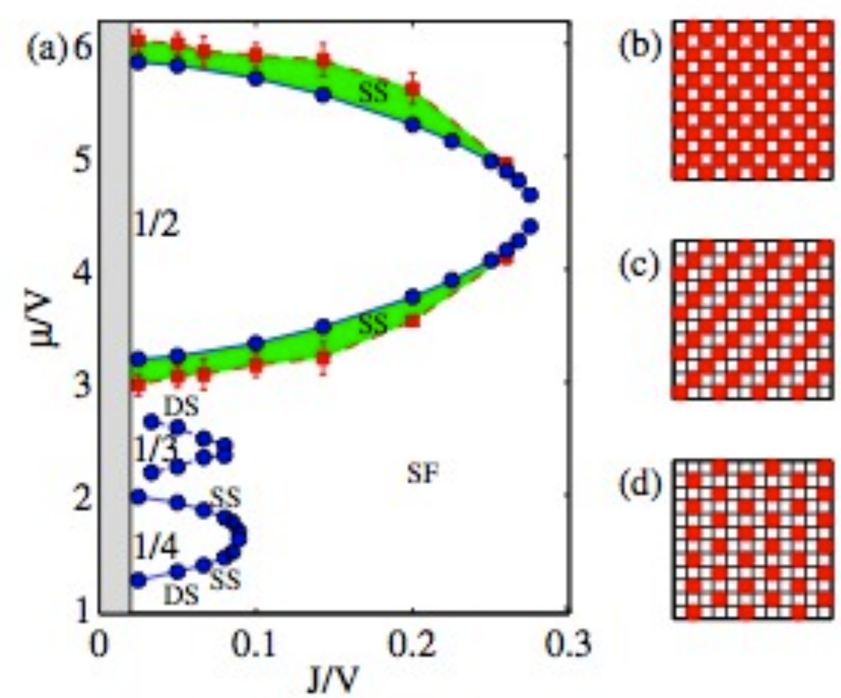


Santos *et al.* PRL **90** 250403

Dipoles in lattices

- Standing wave "Optical lattice"
- "Devil's staircase" of insulating phases
- Supersolidity (Pupillo,...)



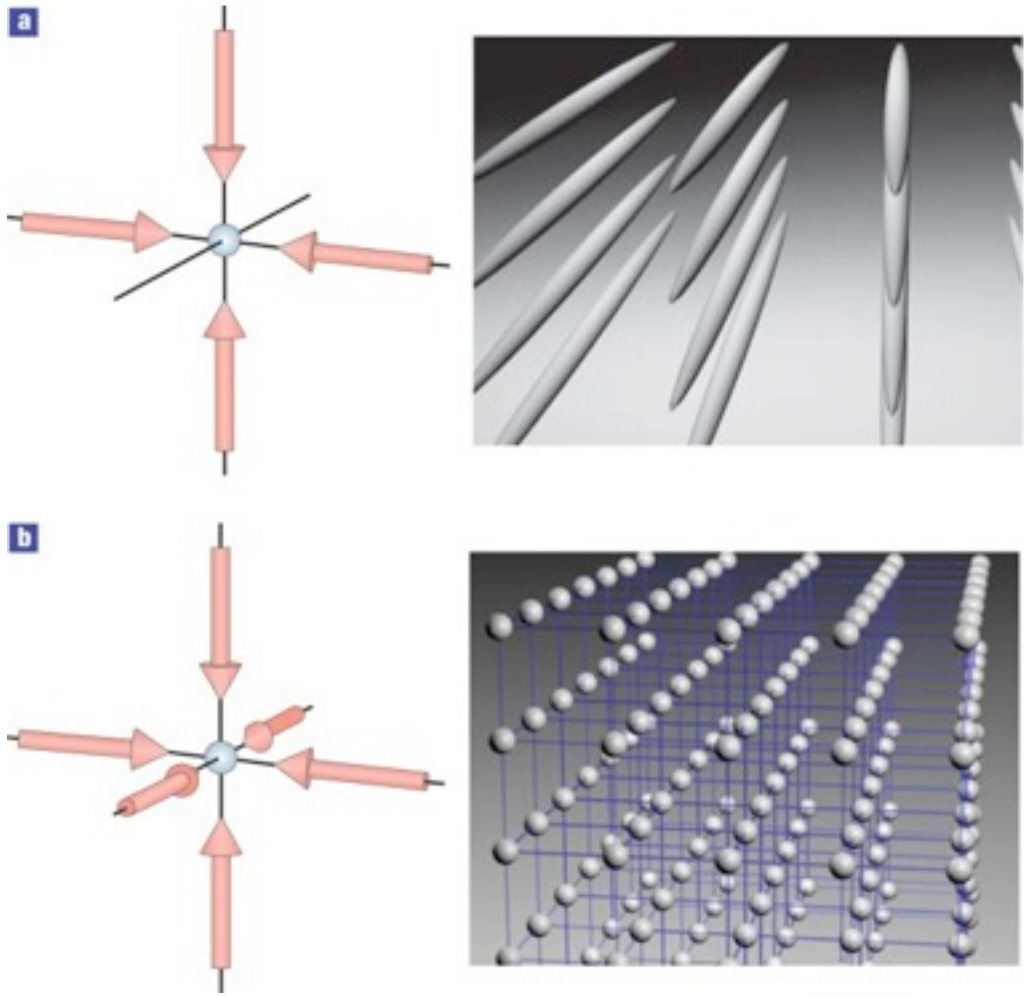


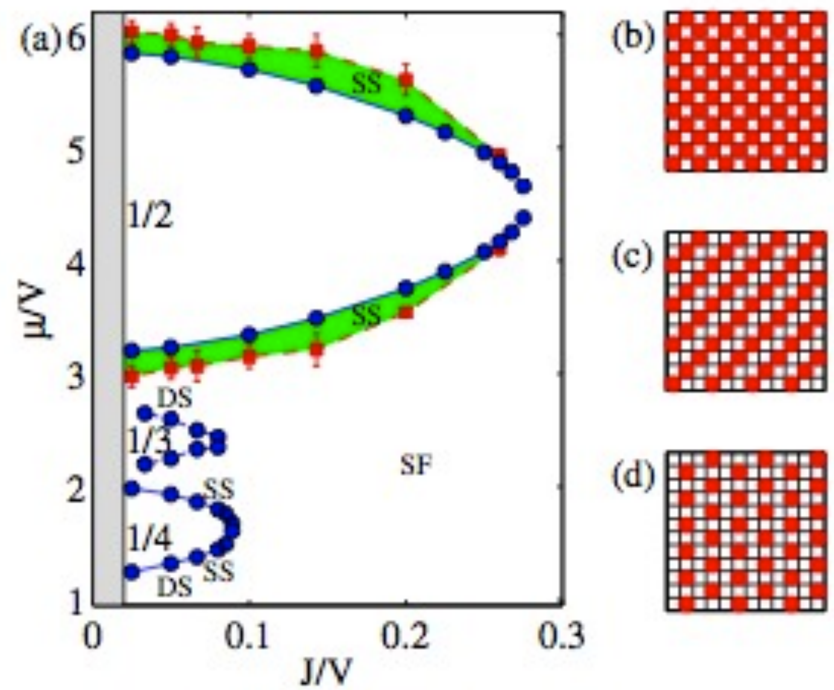
Capogrosso-Sansone *et al.* PRL **104** 125301

Dipoles in lattices

- Standing wave "Optical lattice"
- "Devil's staircase" of insulating phases
- Supersolidity (Pupillo,...)

- Are strong dipoles everything molecules have to offer for many-body physics?





Capogrosso-Sansone *et al.* PRL **104** 125301

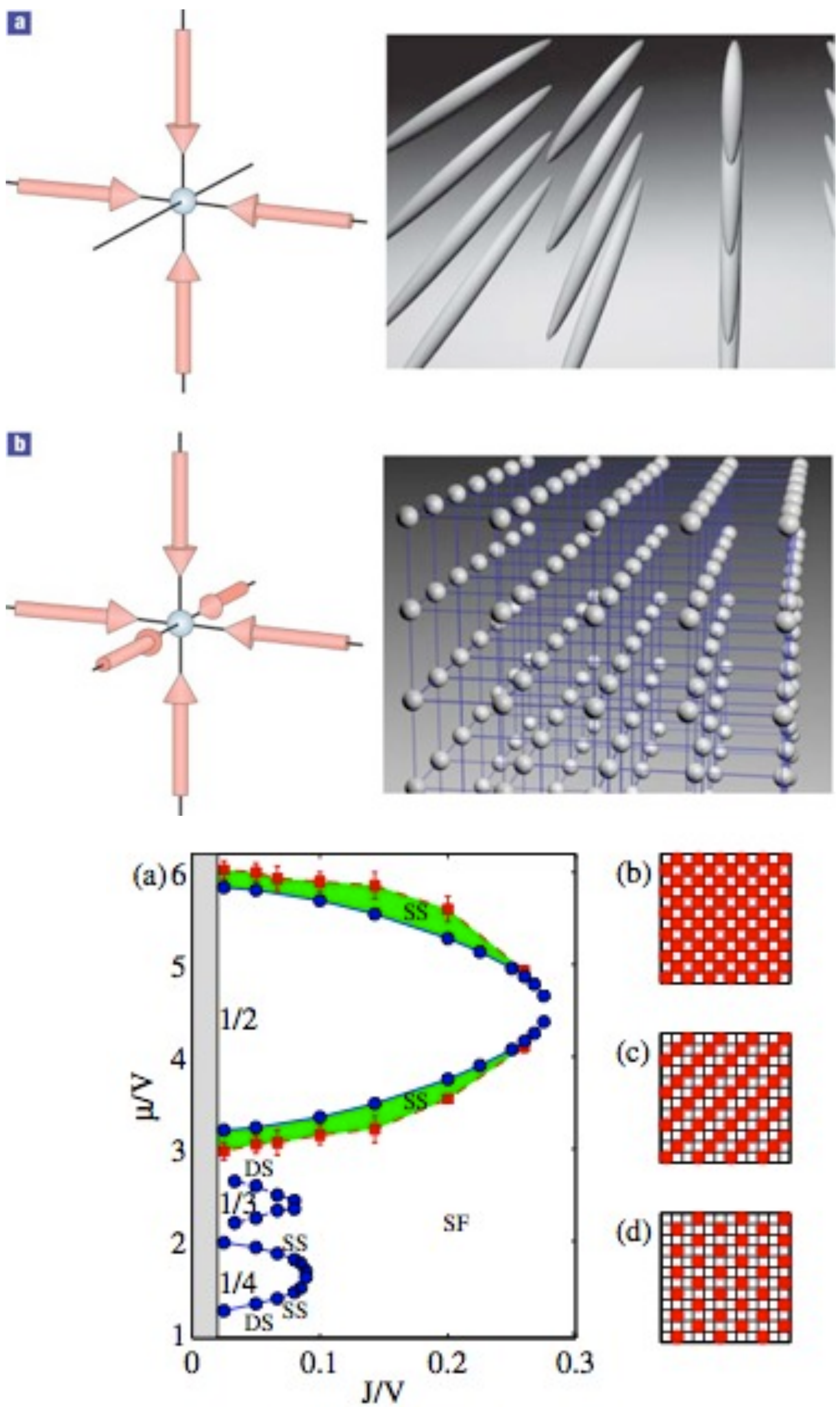
Dipoles in lattices

- Standing wave "Optical lattice"
- "Devil's staircase" of insulating phases
- Supersolidity (Pupillo,...)

- Are strong dipoles everything molecules have to offer for many-body physics?

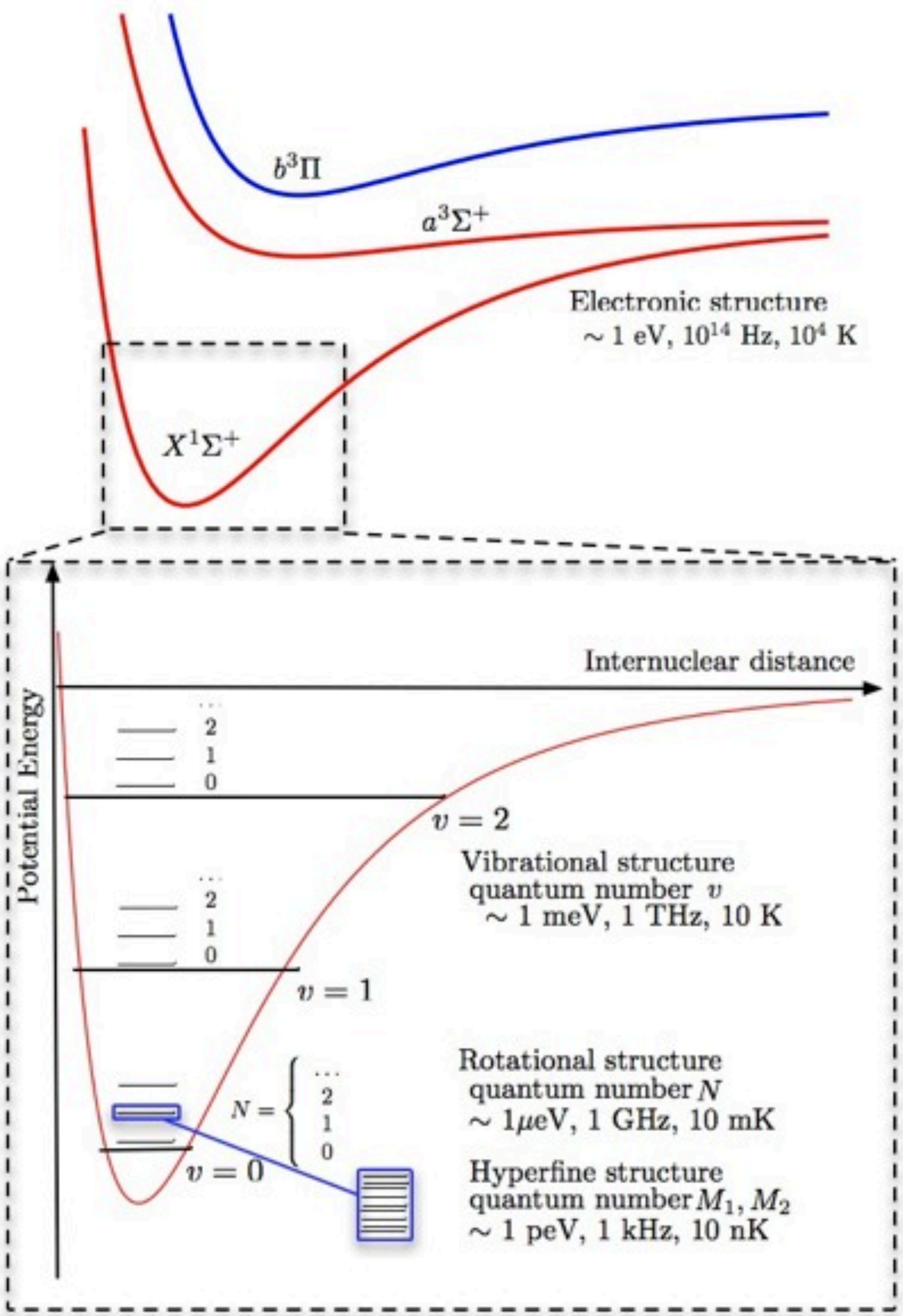
- Molecules are complex, tunable, multi-scale objects!

- Very different opportunities from solid state systems!



Capogrosso-Sansone *et al.* PRL **104** 125301

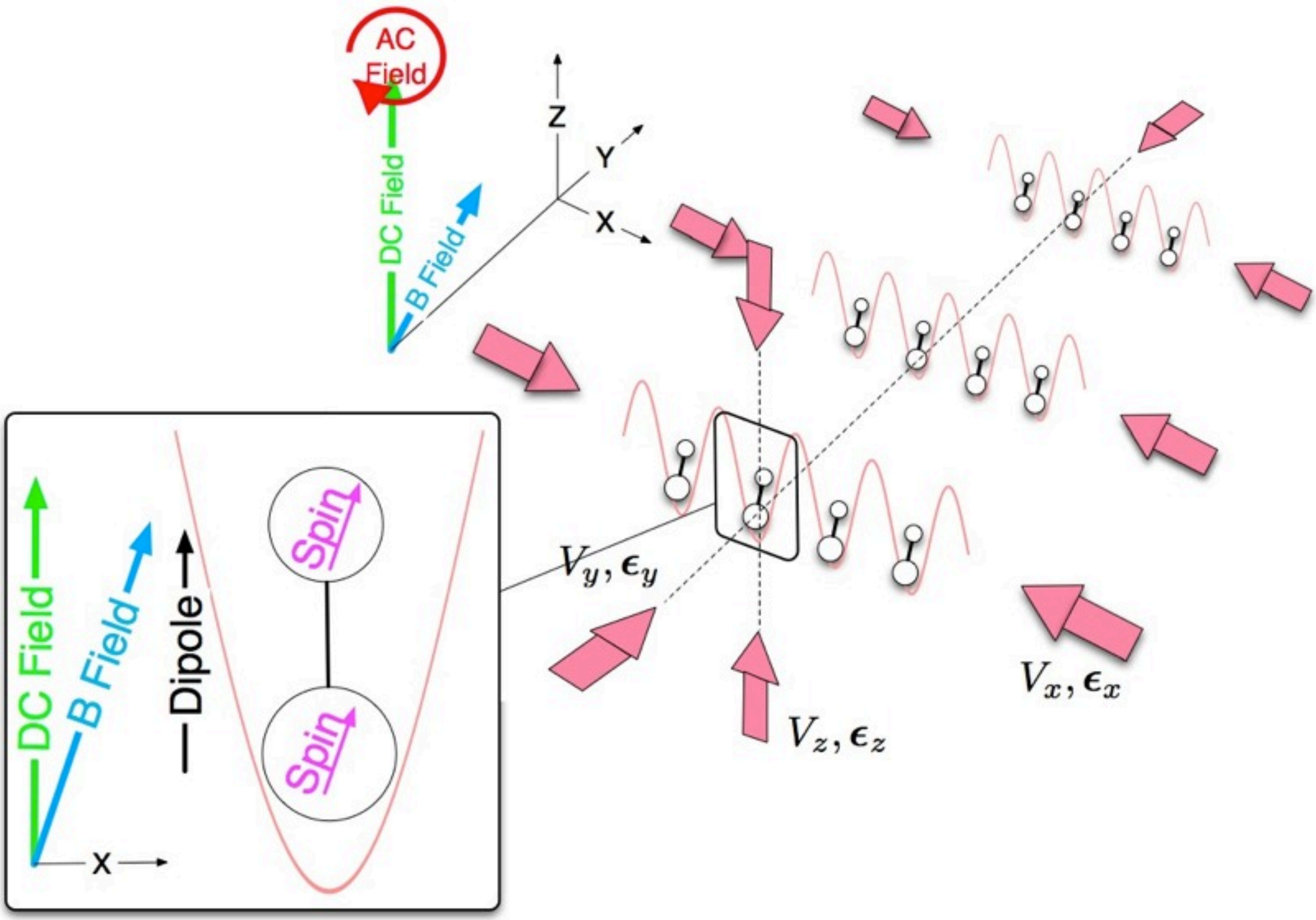
Characterization of $^1\Sigma$ molecules



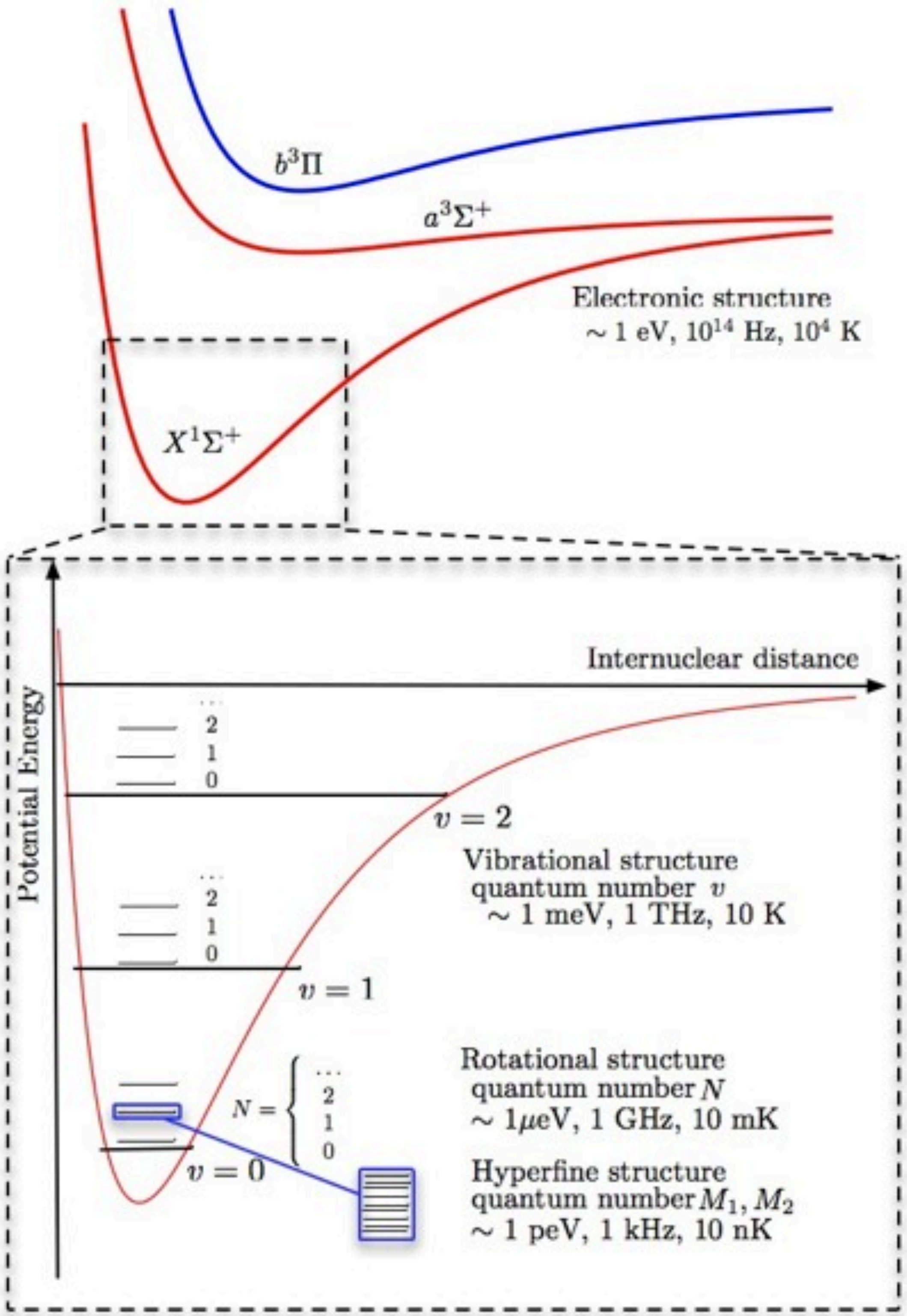
Multi-scale problem

- Electronic
  - Coupling to optical lattice
  - Anisotropic polarizability
- Rotational
  - Coupling to DC E-field
  - Dipole moments
  - Accessible with microwave field
- Hyperfine
  - Coupling to DC B-field
  - Quadrupole mixing with rotation
  - Large number of accessible internal states

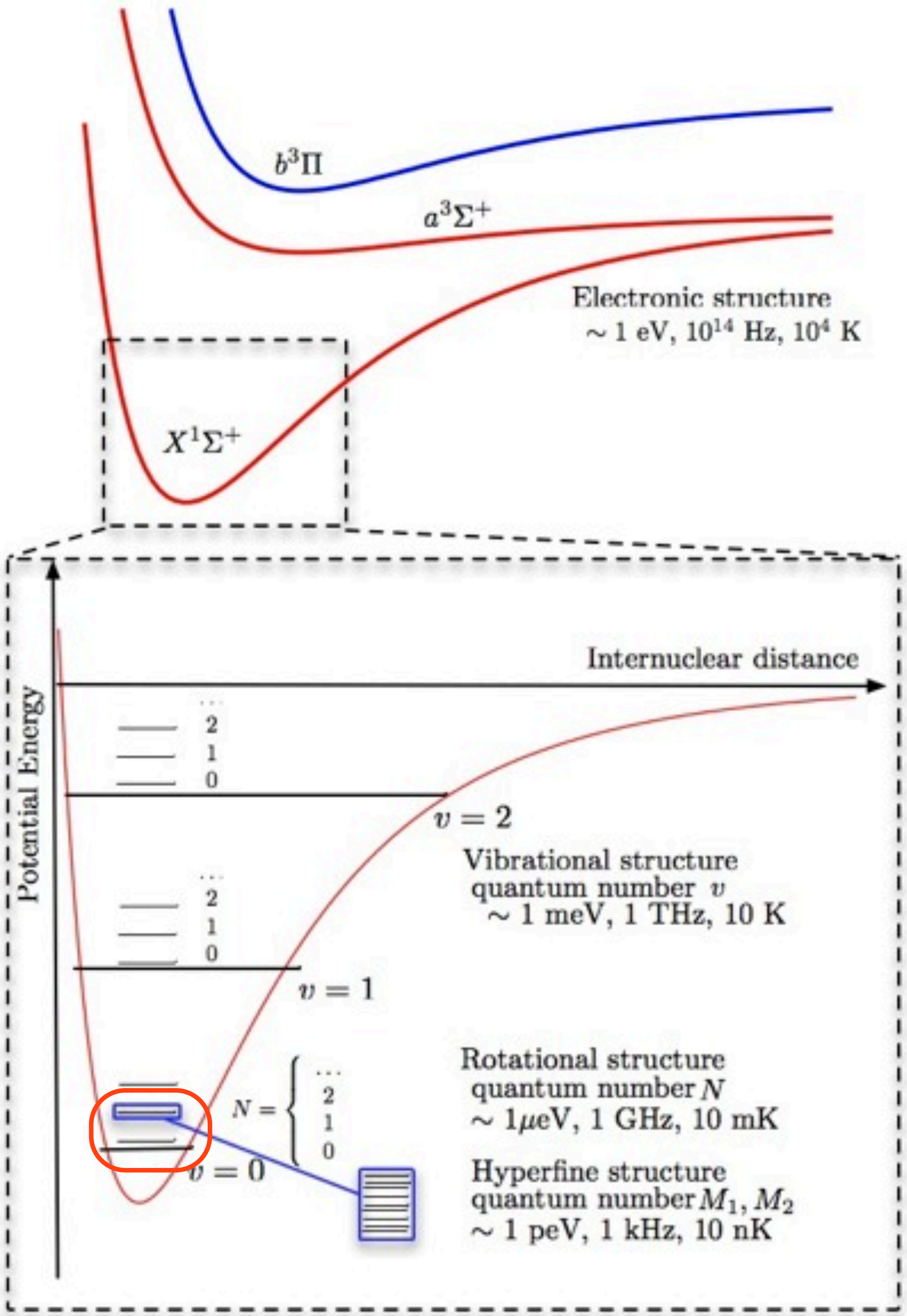
Experimental setup



Field Regimes

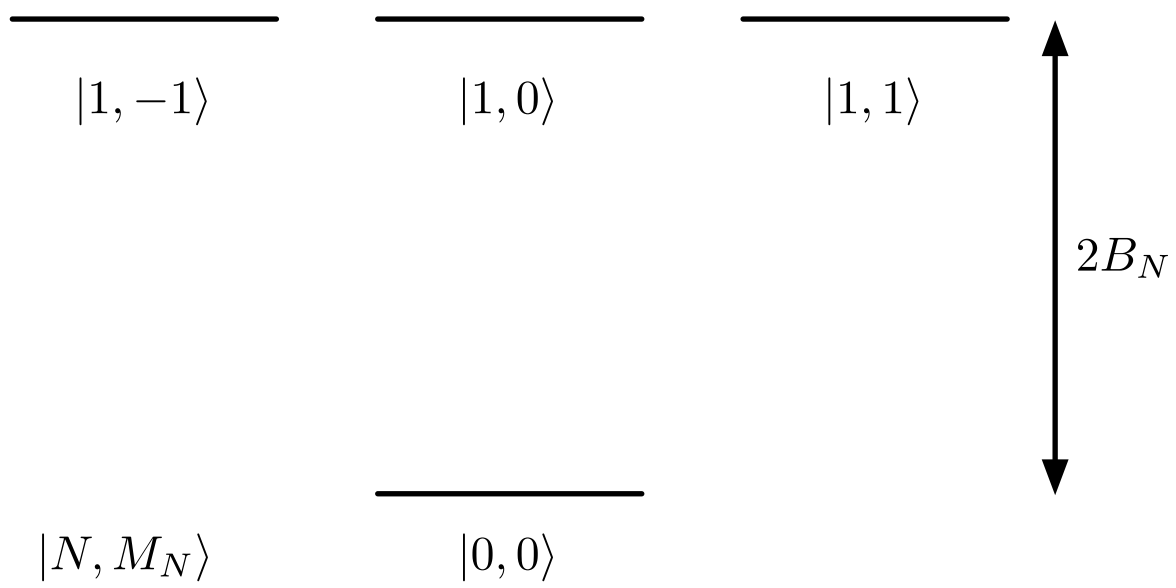


Field Regimes



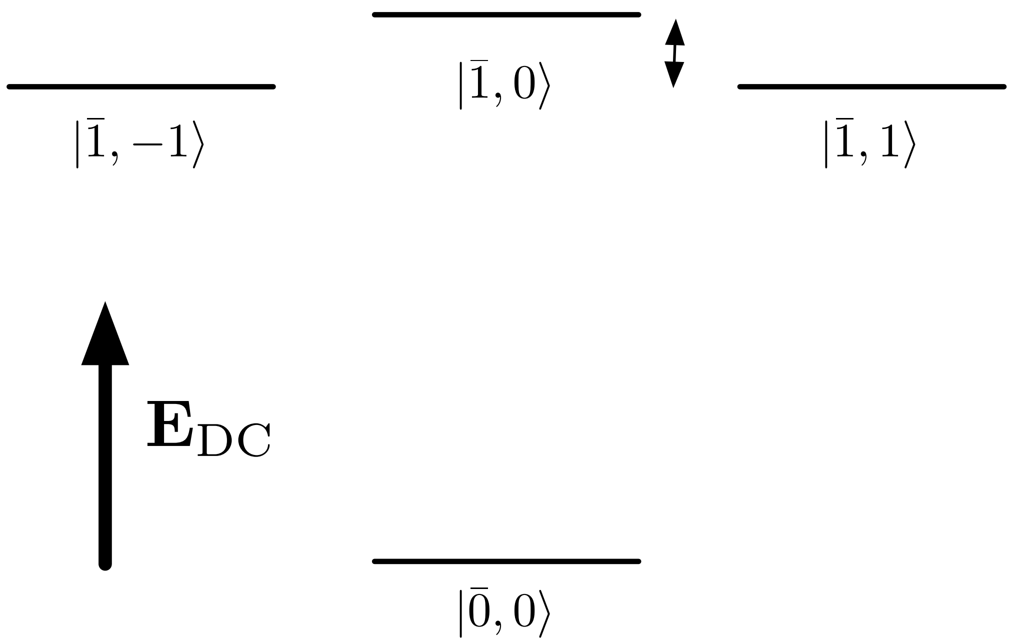
Field Regimes

- DC electric field
  - Splits N=1 degeneracy
  - Tunable dipole moments

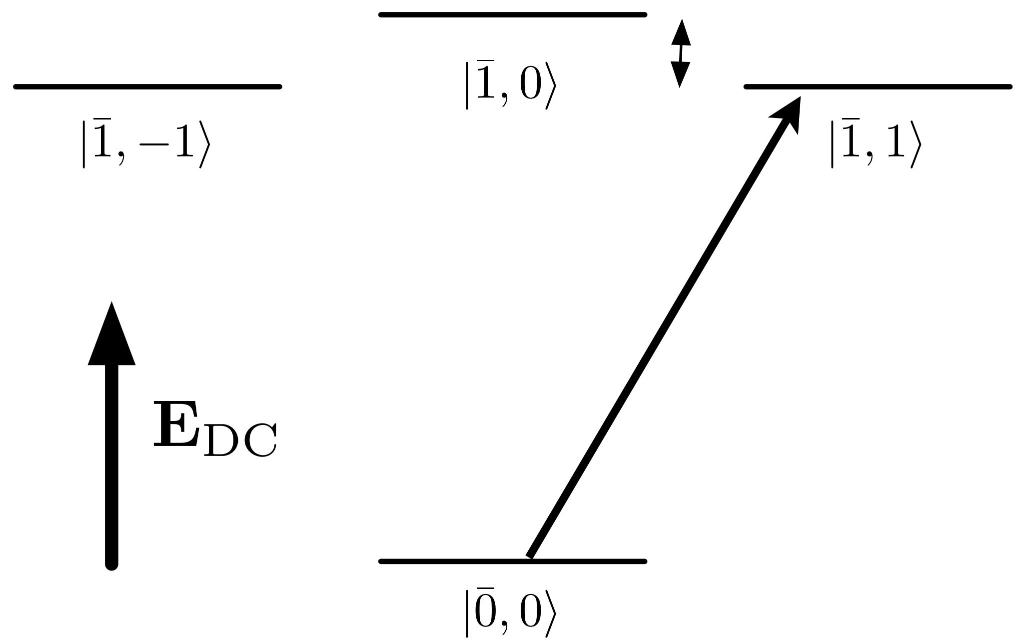


Field Regimes

- DC electric field
  - Splits N=1 degeneracy
  - Tunable dipole moments

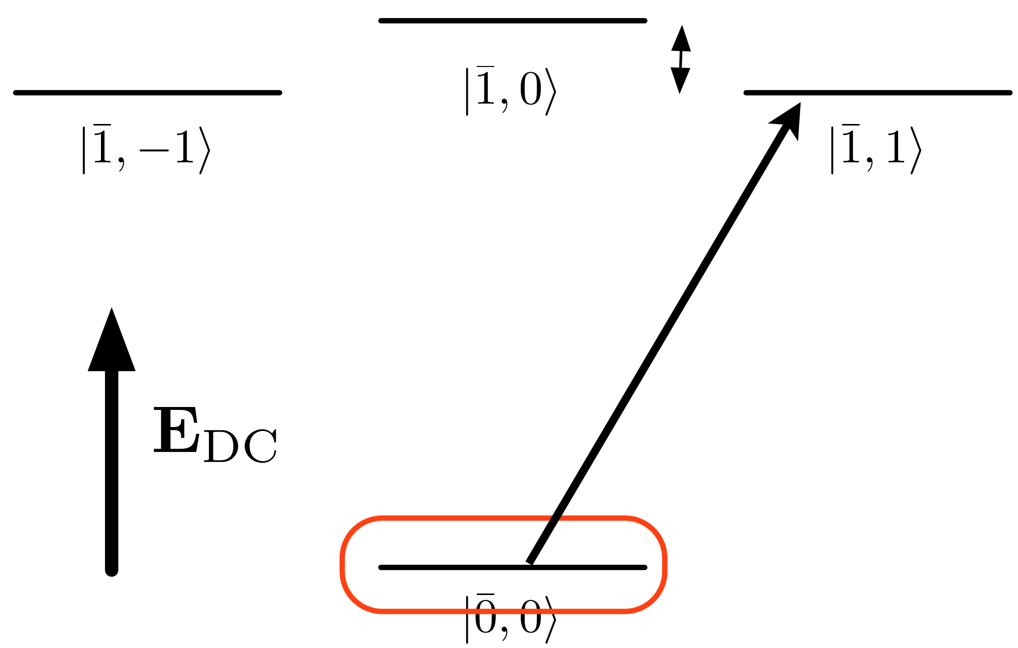


Field Regimes



- DC electric field
  - Splits N=1 degeneracy
  - Tunable dipole moments
- AC microwave field
  - Tunable access to internal states

Field Regimes

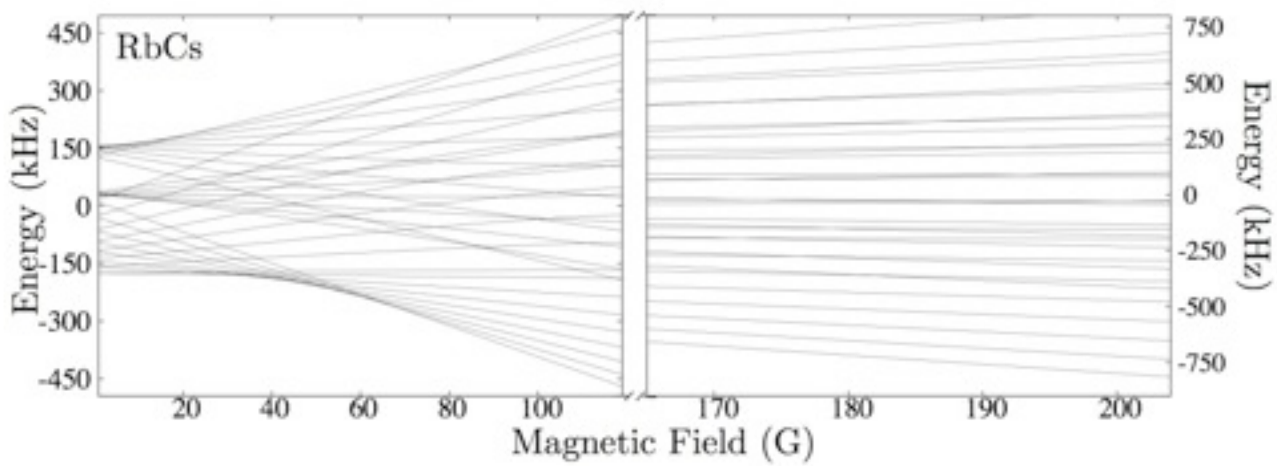


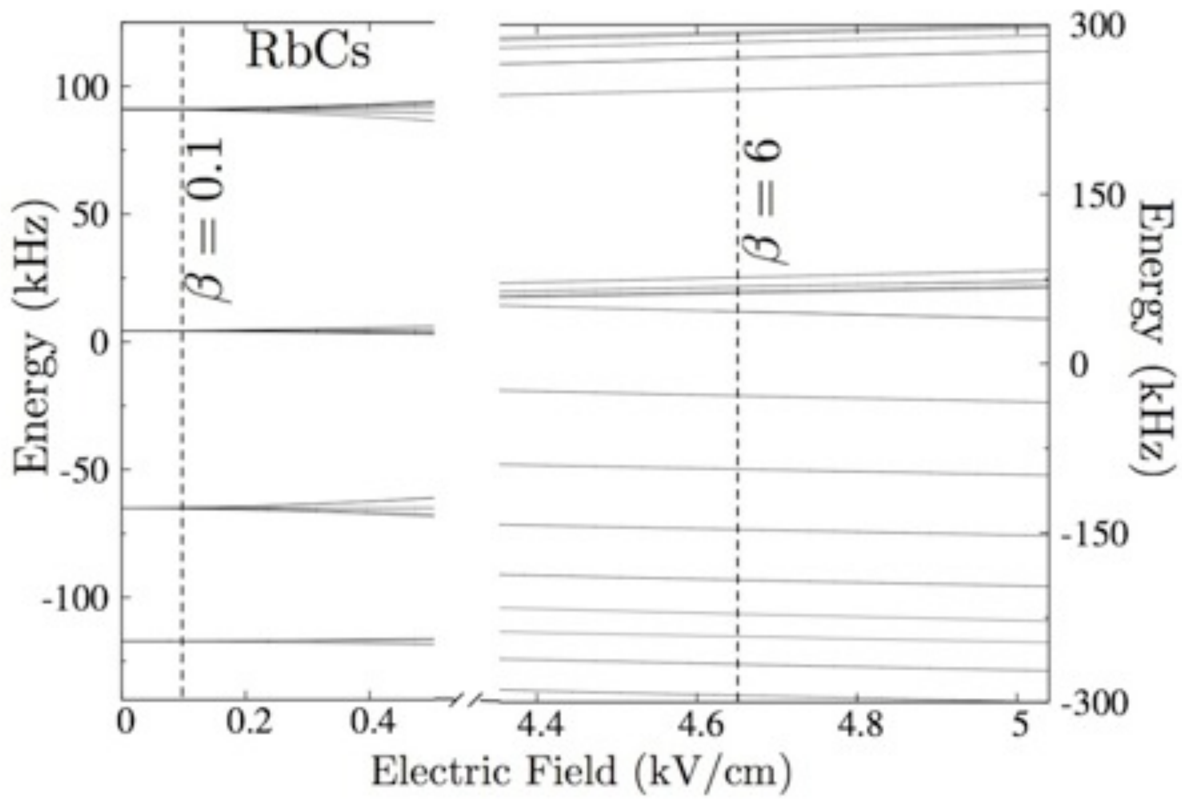
- DC electric field
  - Splits N=1 degeneracy
  - Tunable dipole moments
- AC microwave field
  - Tunable access to internal states

Field Regimes

- DC electric field
  - Splits N=1 degeneracy
  - Tunable dipole moments
- AC microwave field
  - Tunable access to internal states
- DC magnetic field
  - Splits hyperfine degeneracy
  - Tunable coupling of rotation and hyperfine spin
  - Large fields present for magneto-association

Field Regimes





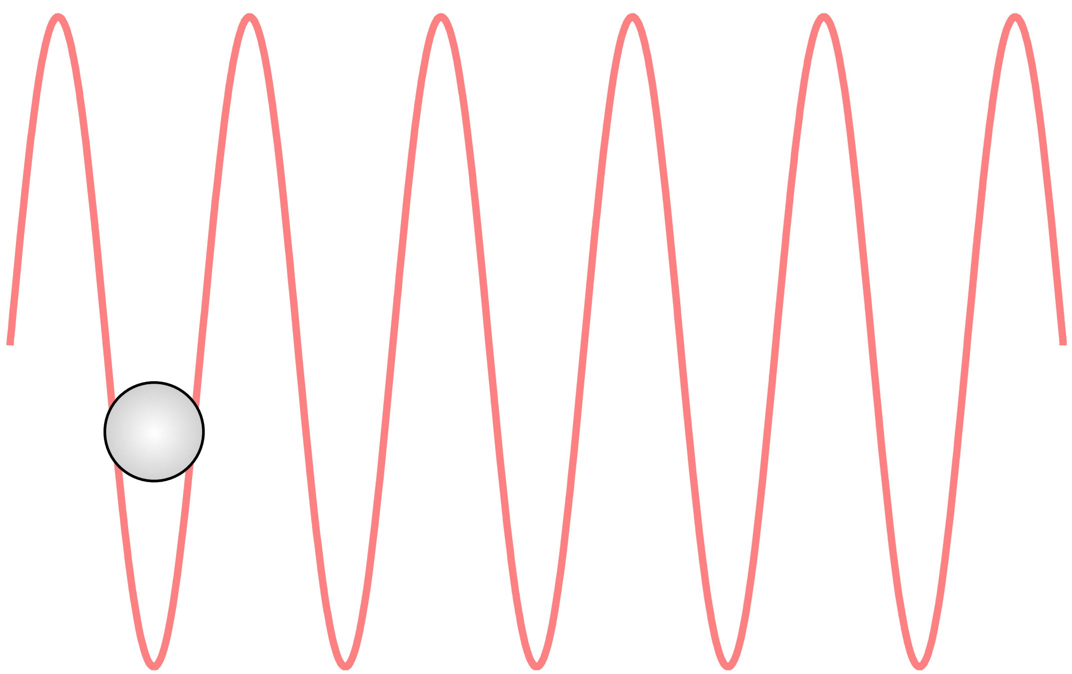
- DC electric field
  - Splits N=1 degeneracy
  - Tunable dipole moments
- AC microwave field
  - Tunable access to internal states
- DC magnetic field
  - Splits hyperfine degeneracy
  - Tunable coupling of rotation and hyperfine spin
  - Large fields present for magneto-association

Atoms in optical lattices

$$\hat{H} = -t \sum_{\langle i,j \rangle} \left[\hat{b}_i^\dagger \hat{b}_j + \text{h.c.} \right] + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right)$$

Atoms in optical lattices

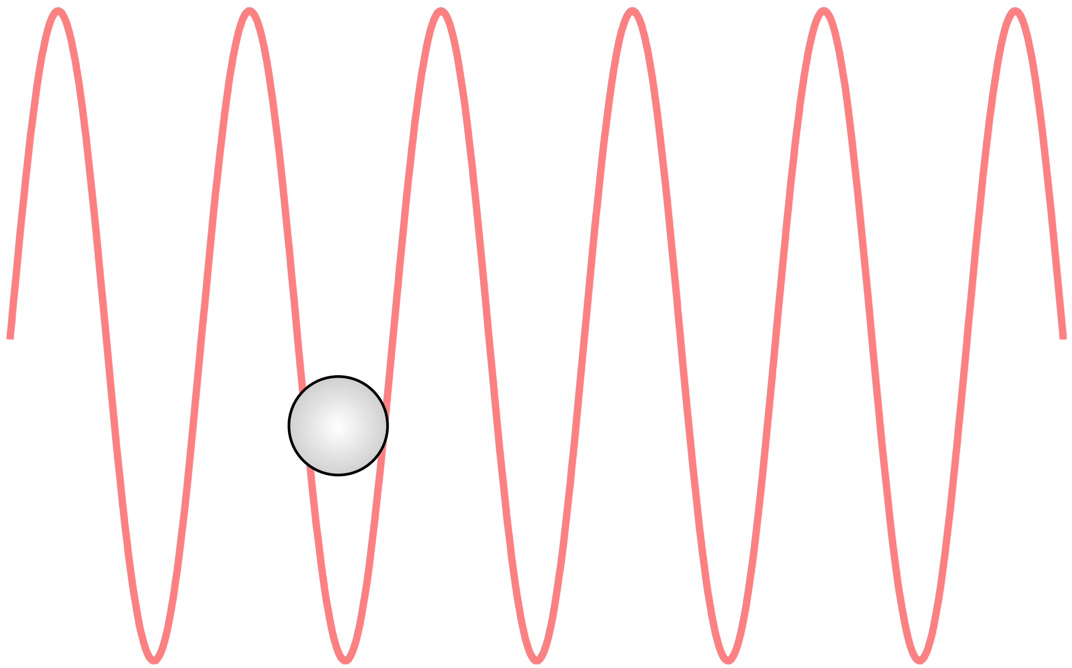
$$\hat{H} = -t \sum_{\langle i,j \rangle} \left[\hat{b}_i^\dagger \hat{b}_j + \text{h.c.} \right] + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right)$$



Atoms in optical lattices

tunneling

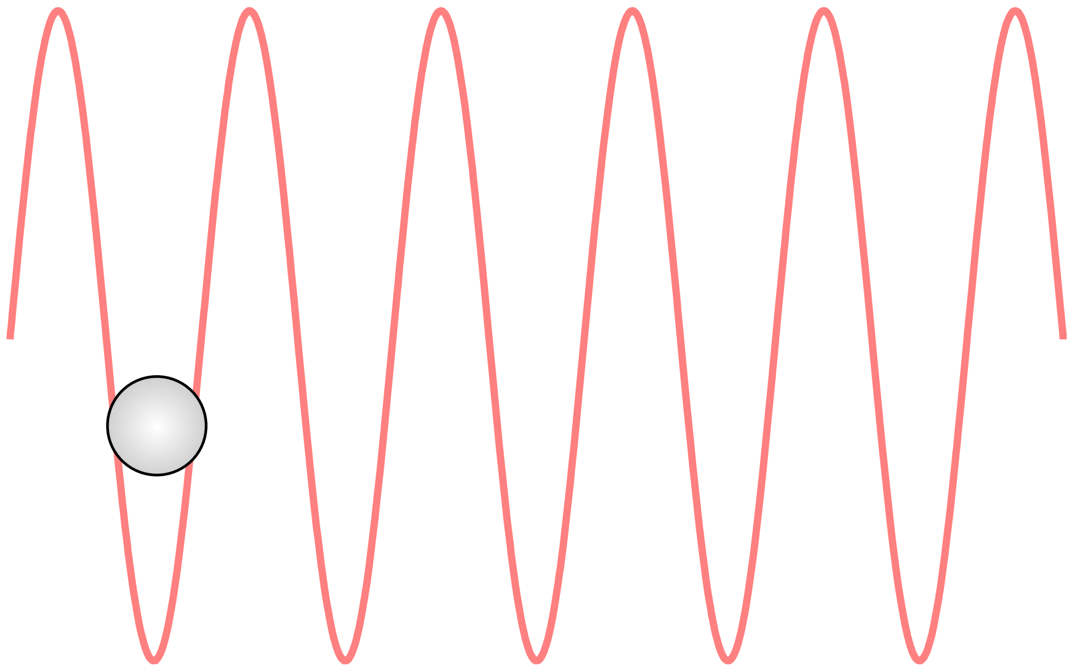
$$\hat{H} = -t \sum_{\langle i,j \rangle} \left[\hat{b}_i^{\dagger} \hat{b}_j + \text{h.c.} \right] + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right)$$



Atoms in optical lattices

tunneling

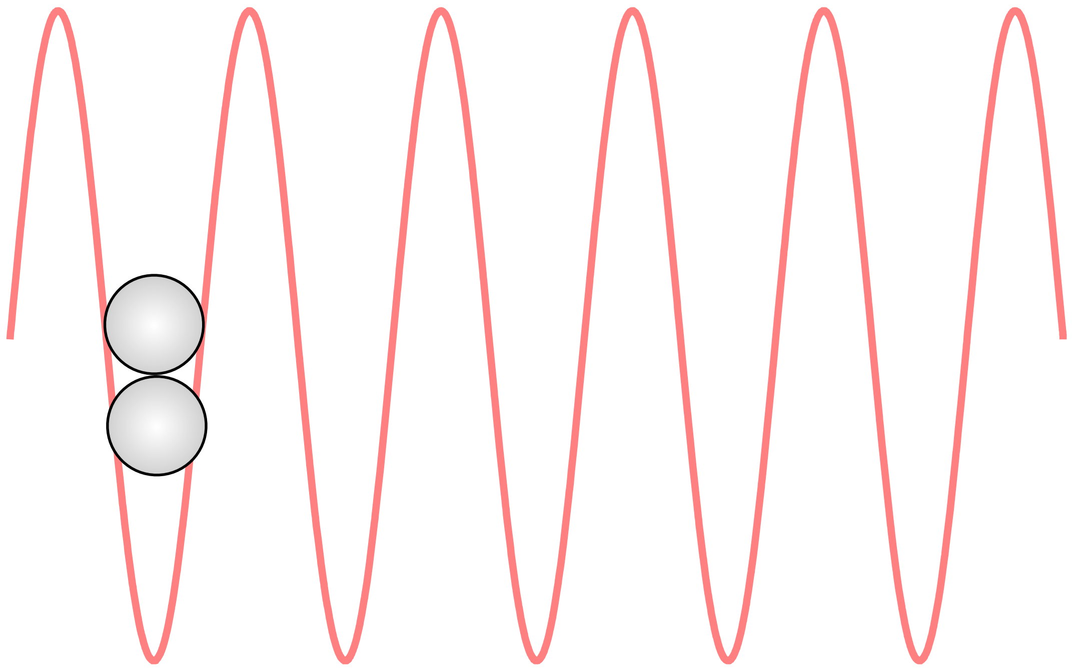
$$\hat{H} = -t \sum_{\langle i,j \rangle} \left[\hat{b}_i^\dagger \hat{b}_j + \text{h.c.} \right] + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right)$$



Atoms in optical lattices

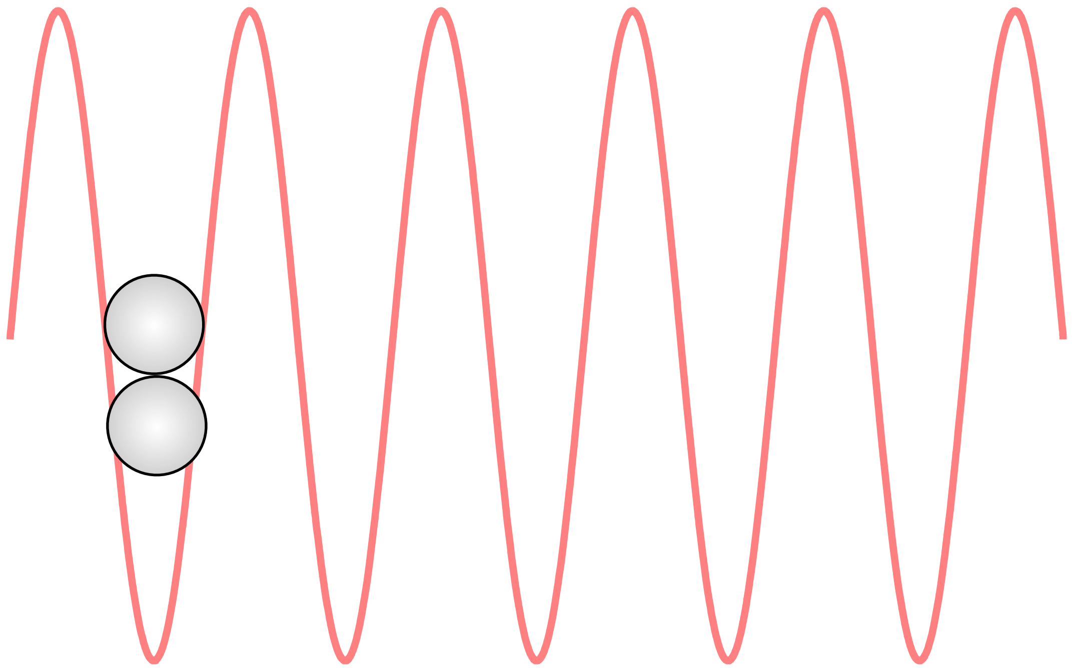
tunneling s-wave scattering

$$\hat{H} = -t \sum_{\langle i,j \rangle} \left[\hat{b}_i^\dagger \hat{b}_j + \text{h.c.} \right] + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right)$$



Atoms in optical lattices

$$\hat{H} = \overset{\text{tunneling}}{-t \sum_{\langle i,j \rangle} \left[\hat{b}_i^\dagger \hat{b}_j + \text{h.c.} \right]} + \overset{\text{s-wave scattering}}{\frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right)}$$



- "Quantum simulator"
- Also natural Hamiltonian for ultracold atoms
- What about molecules?

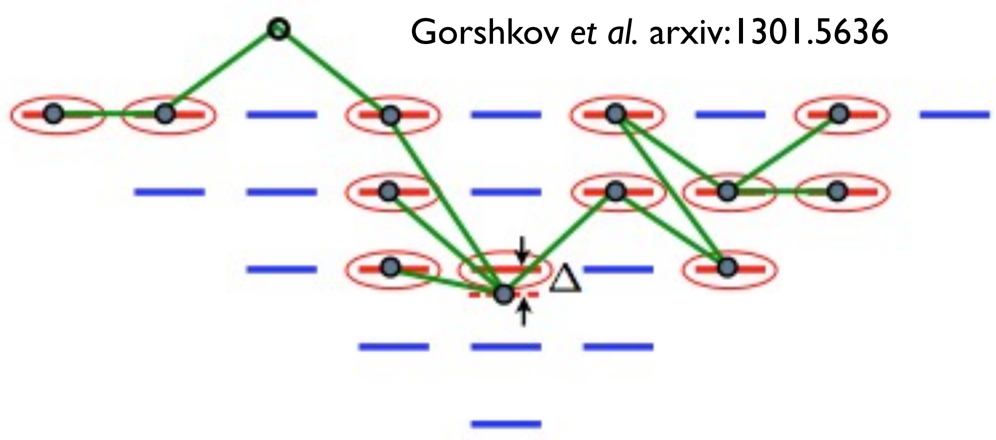
Molecules in optical lattices

- Two complementary questions:

Molecules in optical lattices

- Two complementary questions:

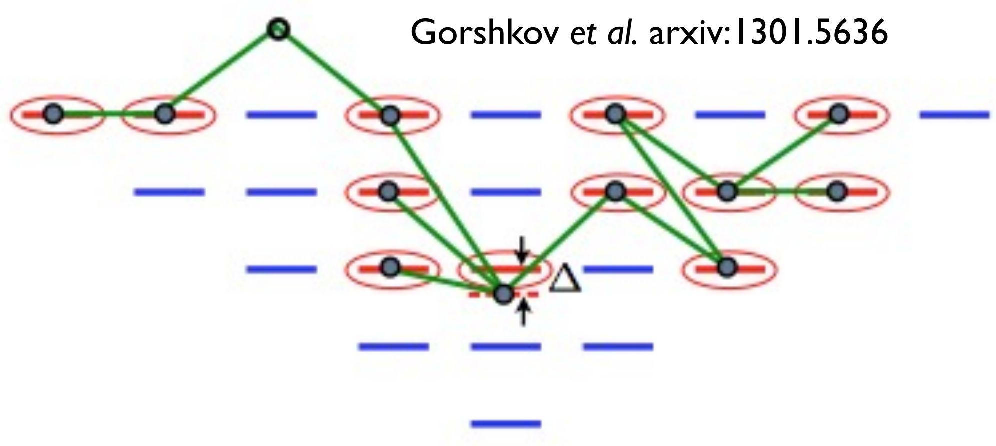
Gorshkov *et al.* arxiv:1301.5636



- Q1: What can we quantum simulate with ultracold molecules in optical lattices?
- A1: Quantum magnetism, topological phases, fractional Chern insulators,...

Molecules in optical lattices

- Two complementary questions:



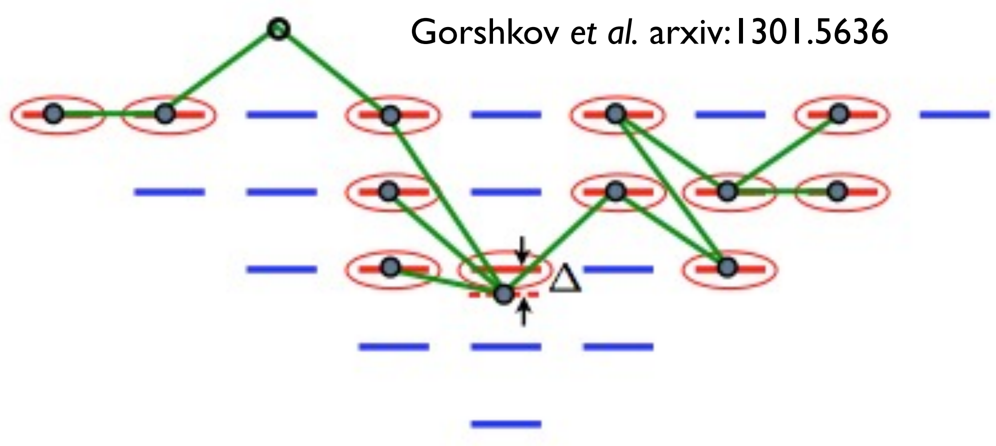
Gorshkov *et al.* arxiv:1301.5636

- Q1: What can we quantum simulate with ultracold molecules in optical lattices?
- A1: Quantum magnetism, topological phases, fractional Chern insulators,...

- Q2: What is the natural many-body Hamiltonian describing up-and-coming ultracold molecules in optical lattices?
- A2: The molecular Hubbard Hamiltonian

Molecules in optical lattices

- Two complementary questions:



Gorshkov *et al.* arxiv:1301.5636

- Q1: What can we quantum simulate with ultracold molecules in optical lattices?
- A1: Quantum magnetism, topological phases, fractional Chern insulators,...

- Q2: What is the natural many-body Hamiltonian describing up-and-coming ultracold molecules in optical lattices?
- A2: The molecular Hubbard Hamiltonian

Experimental Controls

Case Studies

Different molecules give different physics!

The molecular Hubbard Hamiltonian

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j;r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j;r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_{i} \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j;r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

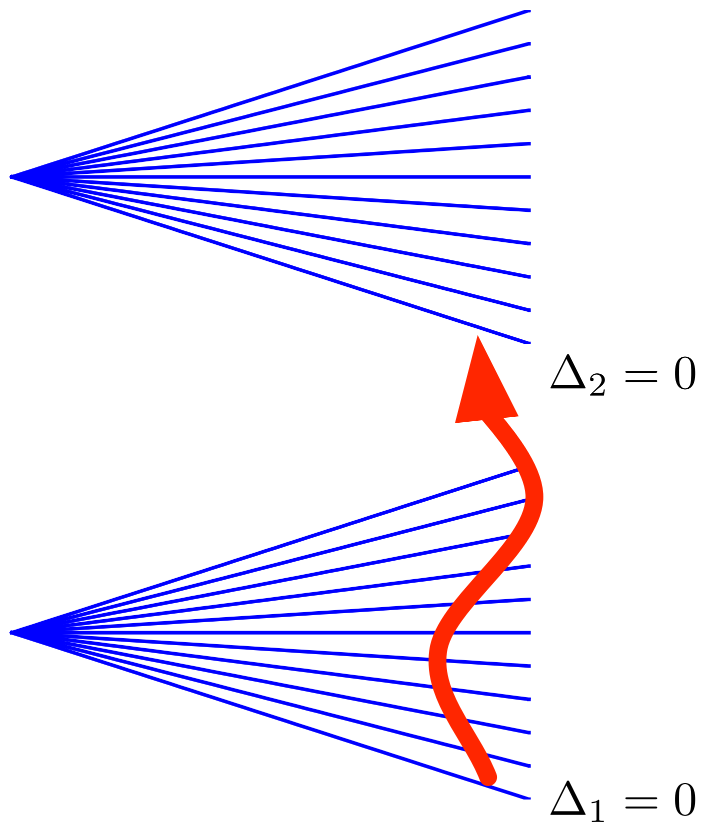
MLW and L.D.Carr NJP **11** 055027 MLW and L.D.Carr PRA **82** 013611 MLW, E Bekaroglu, and L. D. Carr arxiv:1212.3042

The molecular Hubbard Hamiltonian

Detuning

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j;r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j;r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j;r_E} \sum_{\sigma_1\sigma_2\sigma'_2\sigma'_1} E_{j-i,\sigma_1\sigma_2\sigma'_2\sigma'_1} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma'_2} \hat{a}_{i,\sigma'_1}$$

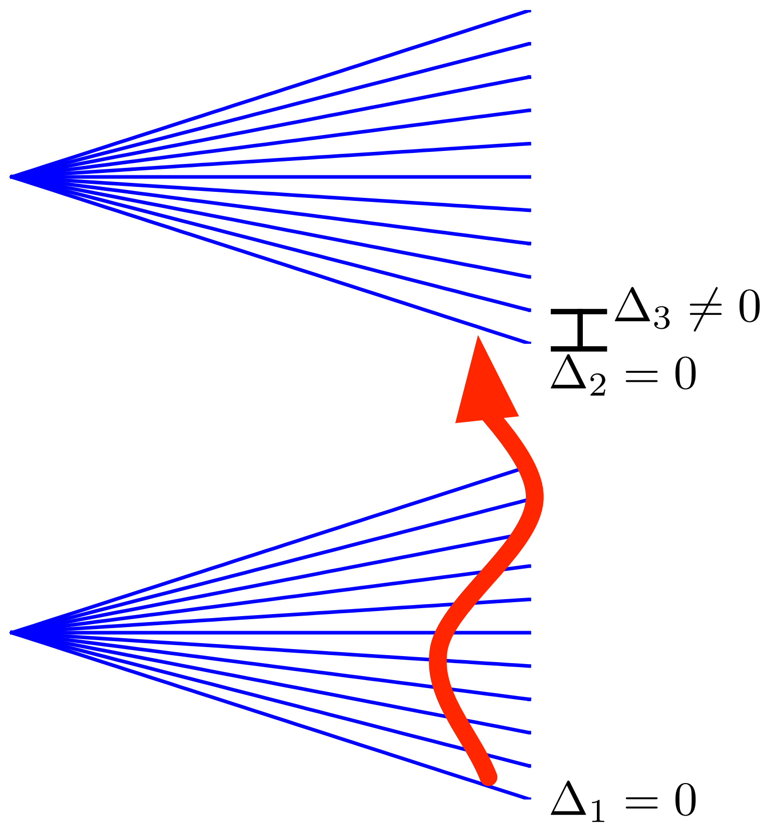


MLW and L.D.Carr NJP **11** 055027 MLW and L.D.Carr PRA **82** 013611 MLW, E Bekaroglu, and L. D. Carr arxiv:1212.3042

The molecular Hubbard Hamiltonian

Detuning

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j;r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j;r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$
$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_{i} \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j;r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$



MLW and L.D.Carr NJP **11** 055027 MLW and L.D.Carr PRA **82** 013611 MLW, E Bekaroglu, and L. D. Carr arxiv:1212.3042

The molecular Hubbard Hamiltonian

Detuning

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_{i} \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j; r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

$$\Delta_2 = 0$$

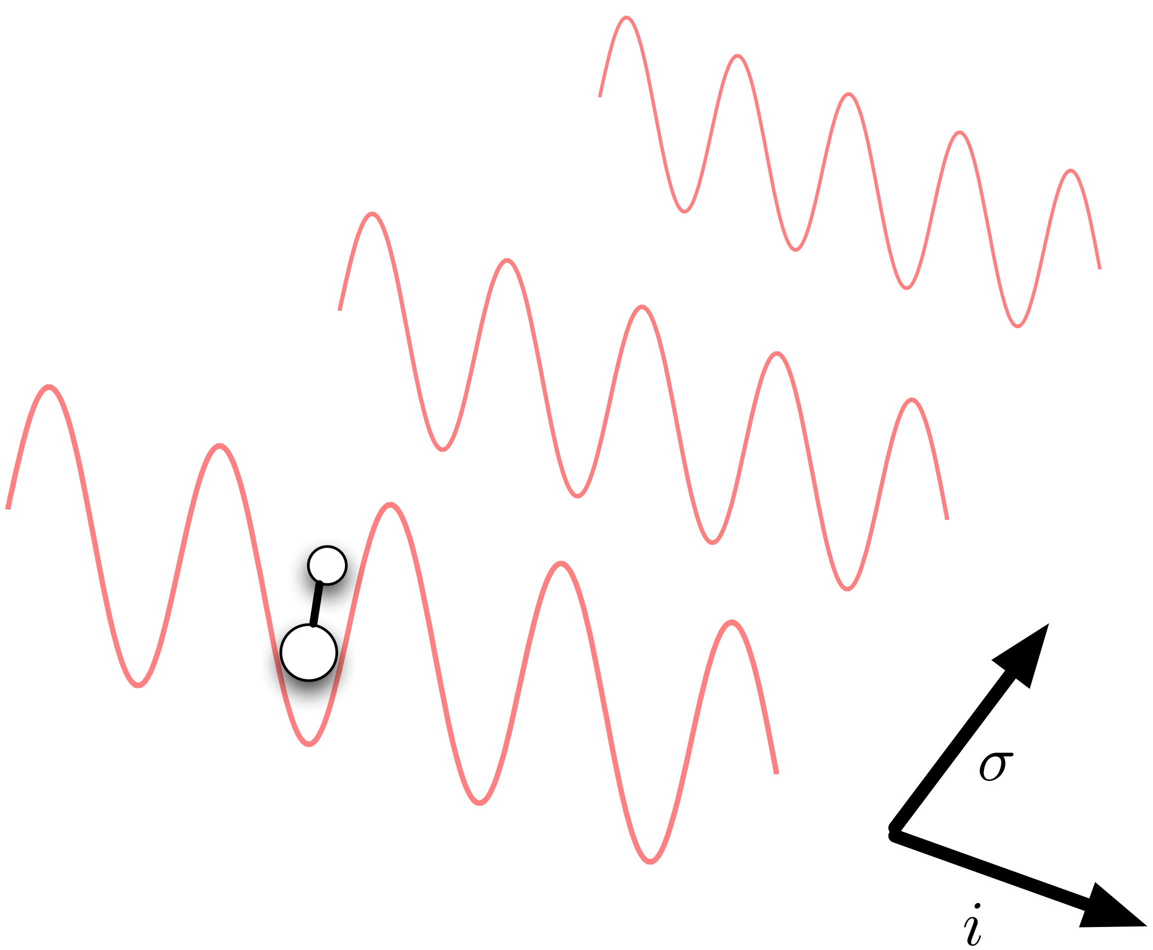
MLW and L.D.Carr NJP **11** 055027 MLW and L.D.Carr PRA **82** 013611 MLW, E Bekaroglu, and L. D. Carr arxiv:1212.3042

The molecular Hubbard Hamiltonian

Tunneling

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \boxed{\sum_{i\neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma}} + \frac{1}{2} \sum_{i\neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j; r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

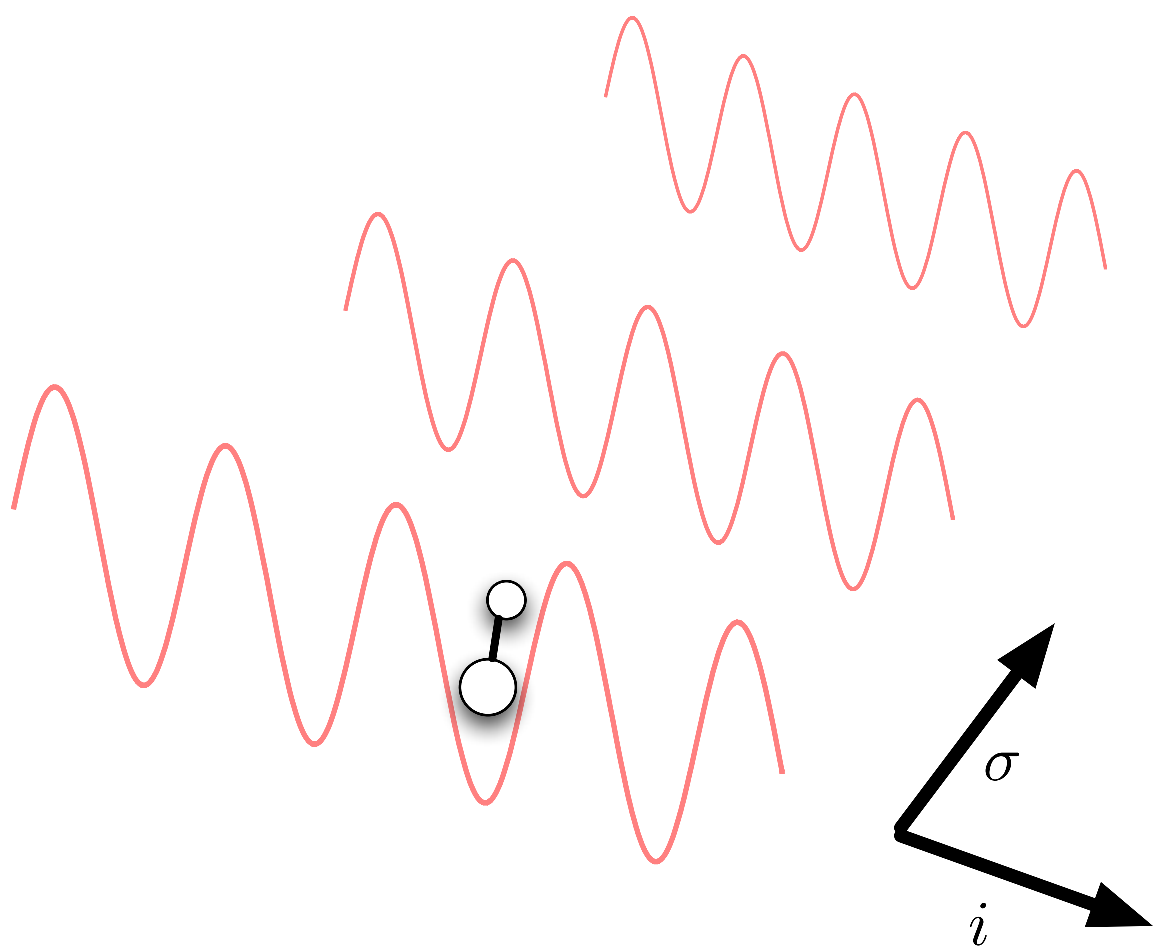


The molecular Hubbard Hamiltonian

Tunneling

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_{i} \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j; r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

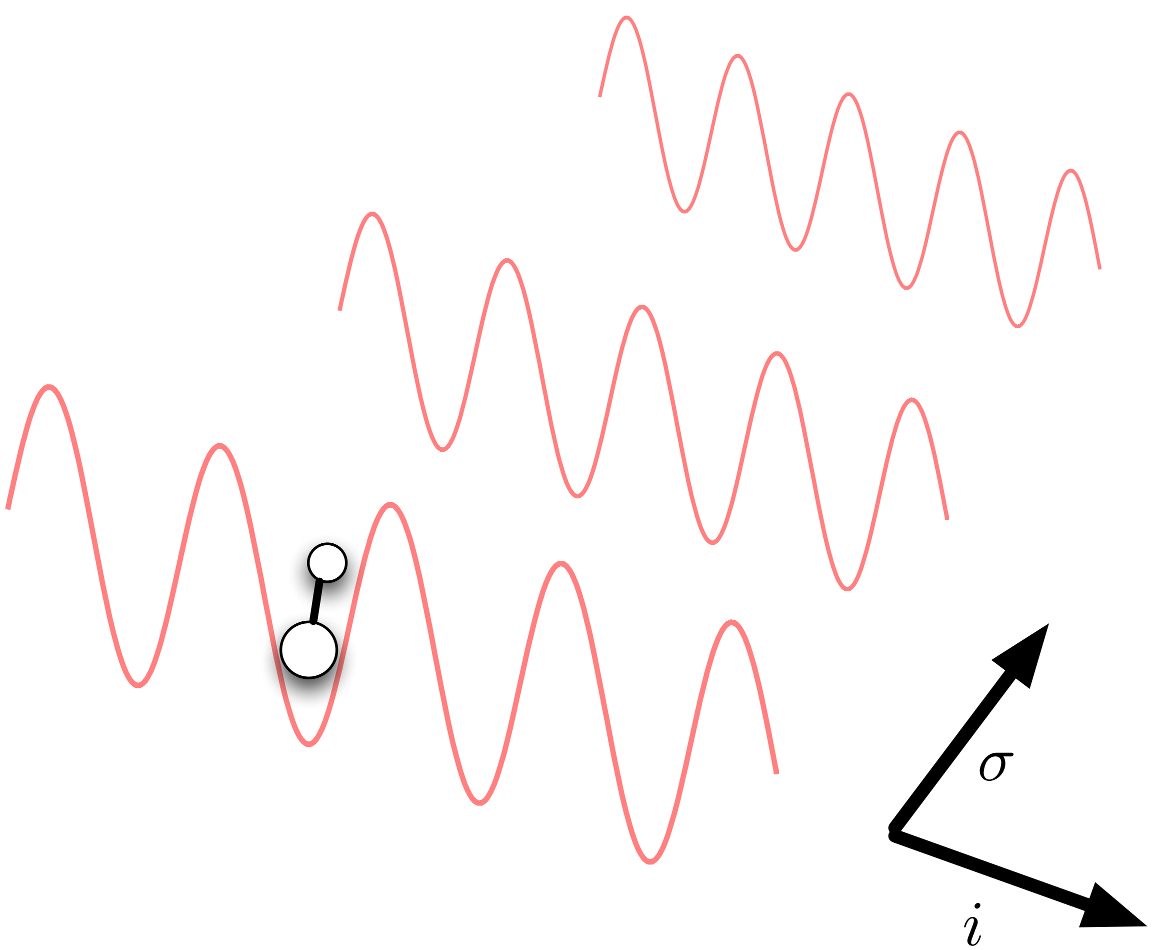


The molecular Hubbard Hamiltonian

Tunneling

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \boxed{\sum_{i\neq j;r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma}} + \frac{1}{2} \sum_{i\neq j;r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j;r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

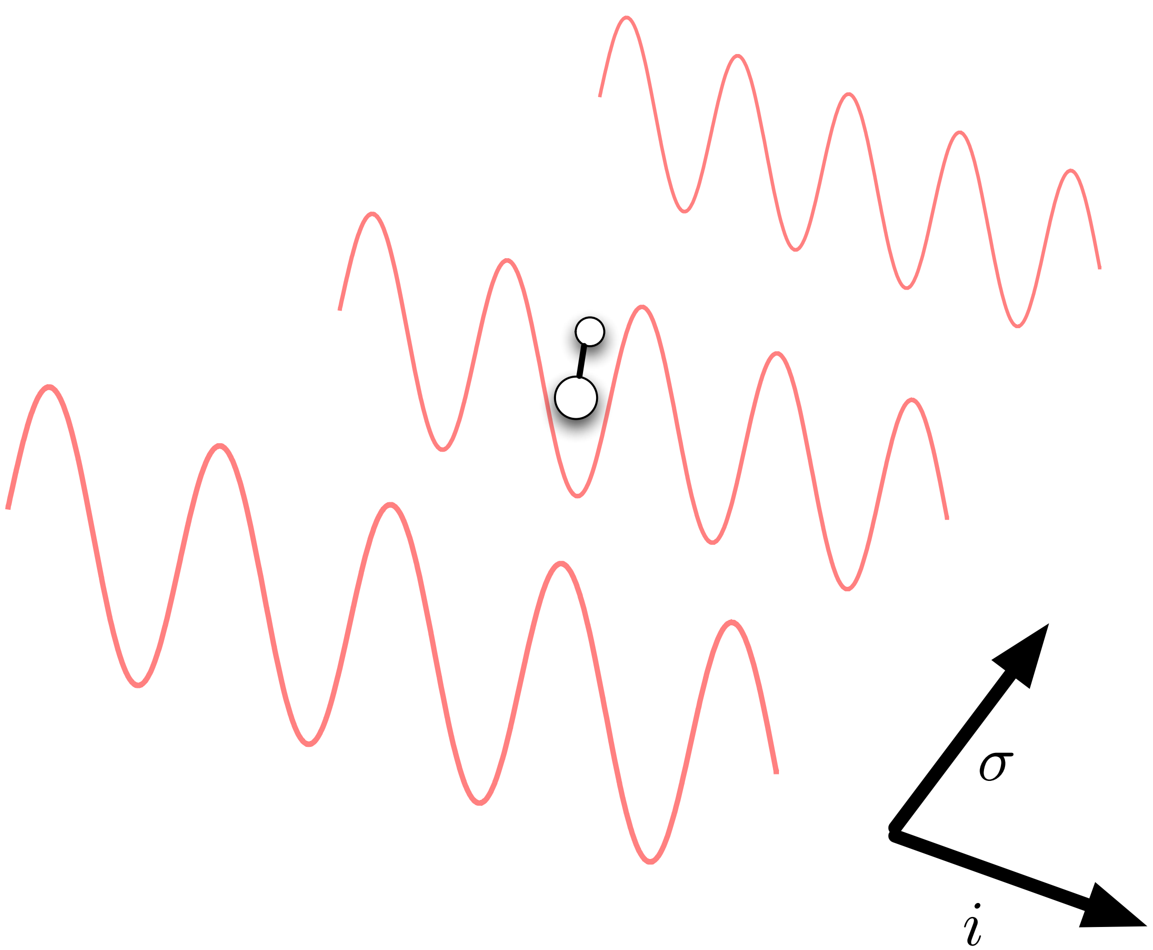


The molecular Hubbard Hamiltonian

Tunneling

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \boxed{\sum_{i\neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma}} + \frac{1}{2} \sum_{i\neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j; r_E} \sum_{\sigma_1\sigma_2\sigma'_2\sigma'_1} E_{j-i,\sigma_1\sigma_2\sigma'_2\sigma'_1} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma'_2} \hat{a}_{i,\sigma'_1}$$

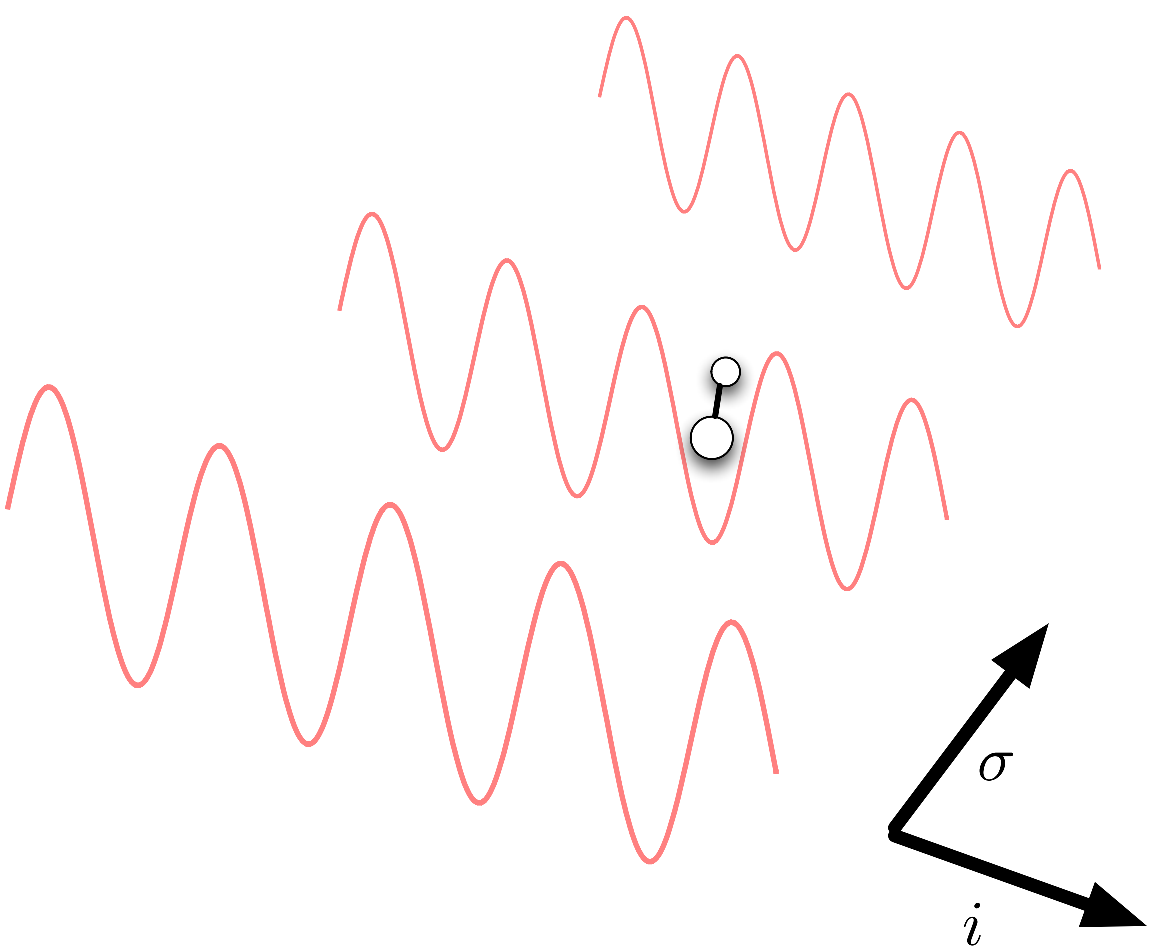


The molecular Hubbard Hamiltonian

Tunneling

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i \neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i \neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i \neq j; r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

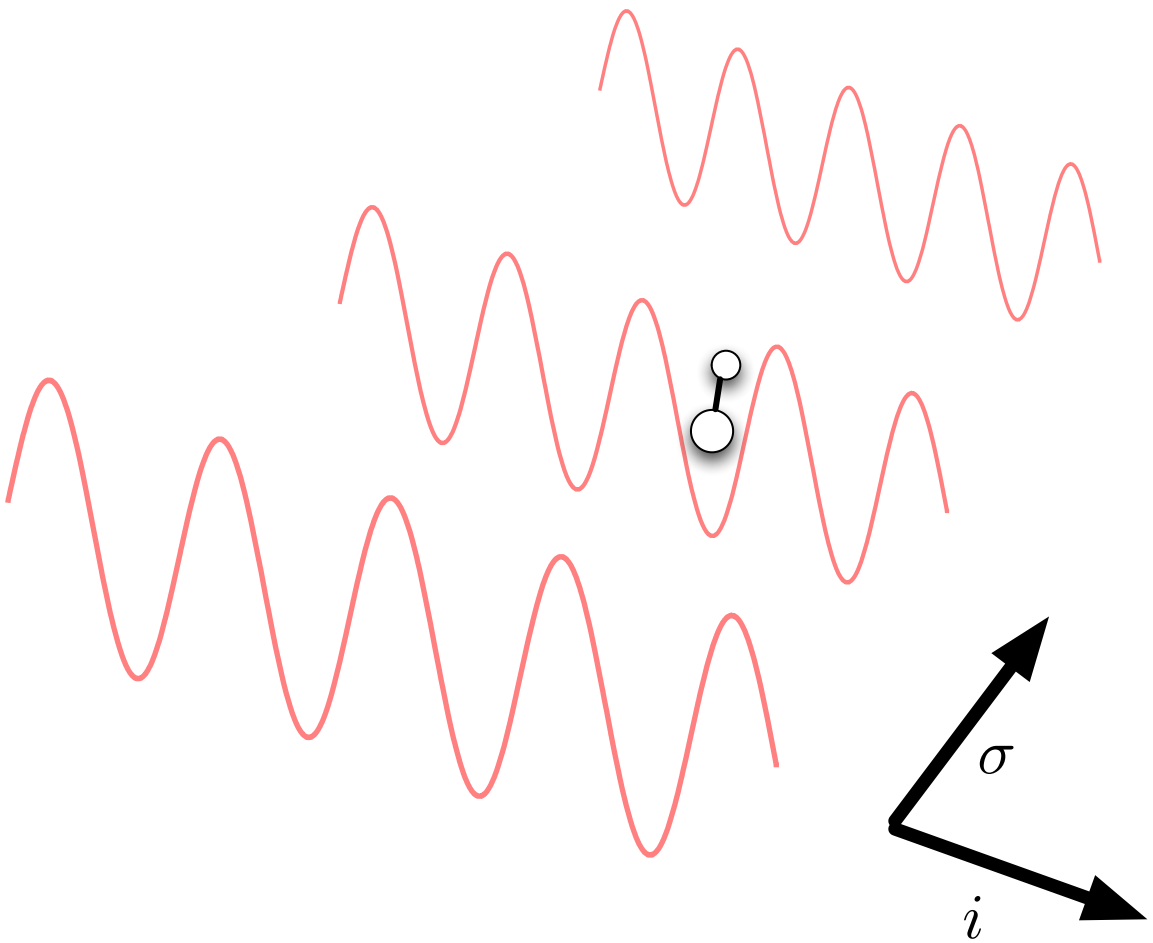


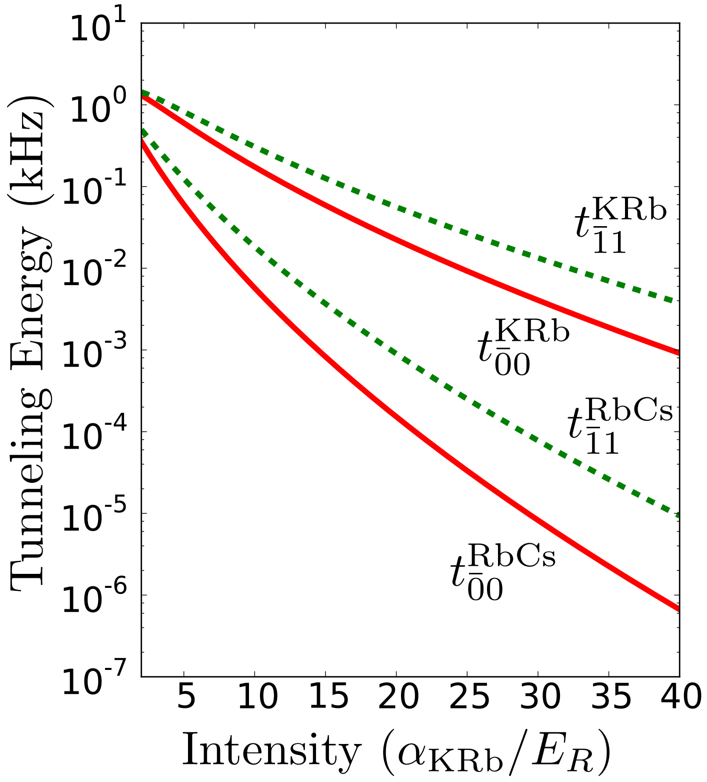
The molecular Hubbard Hamiltonian

Tunneling

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i \neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i \neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i \neq j; r_E} \sum_{\sigma_1\sigma_2\sigma'_2\sigma'_1} E_{j-i,\sigma_1\sigma_2\sigma'_2\sigma'_1} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma'_2} \hat{a}_{i,\sigma'_1}$$



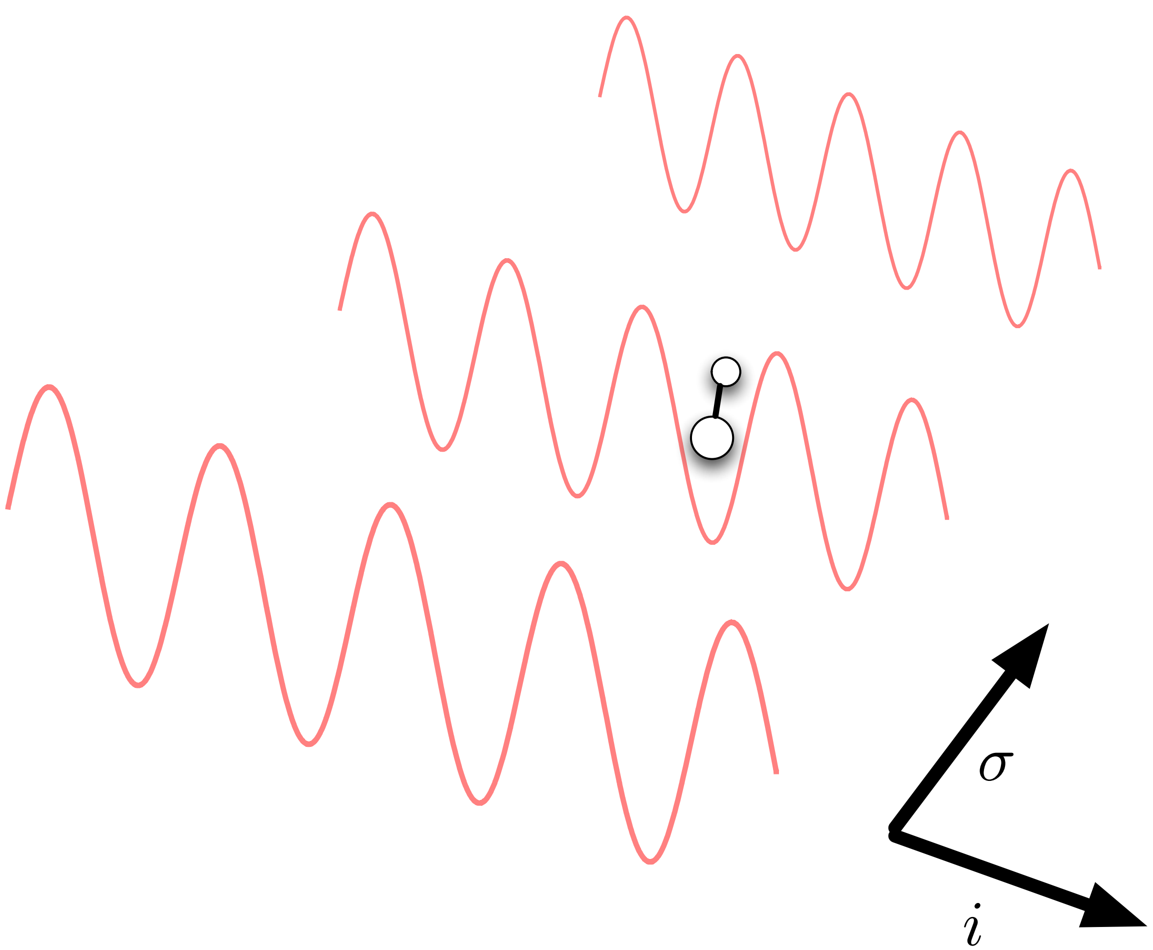


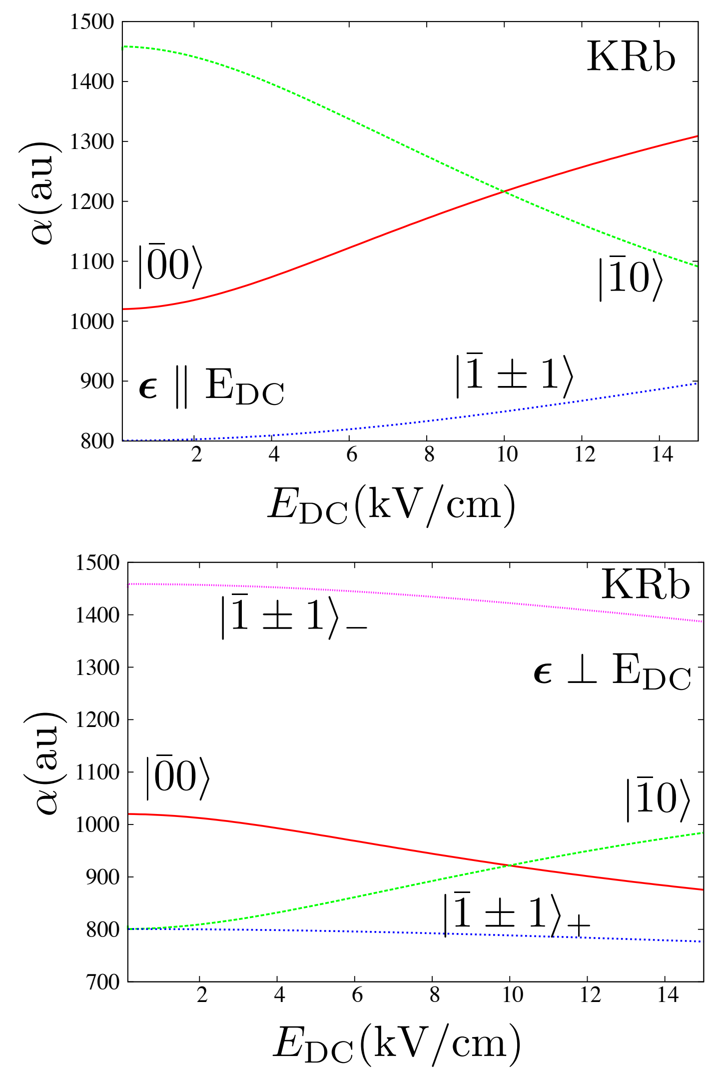
The molecular Hubbard Hamiltonian

Tunneling

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j;r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j;r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j;r_E} \sum_{\sigma_1\sigma_2\sigma'_2\sigma'_1} E_{j-i,\sigma_1\sigma_2\sigma'_2\sigma'_1} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma'_2} \hat{a}_{i,\sigma'_1}$$



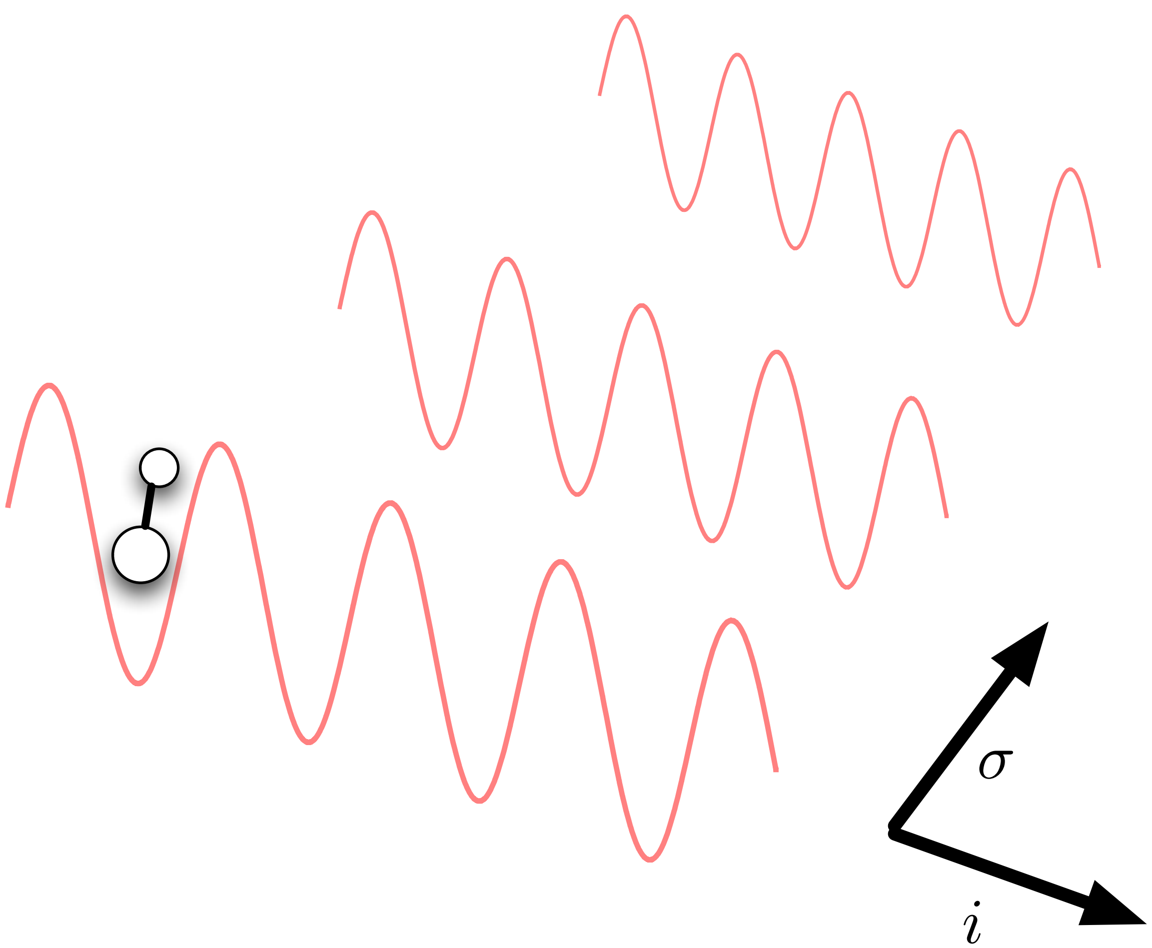


The molecular Hubbard Hamiltonian

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i \neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i \neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_{i} \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i \neq j; r_E} \sum_{\sigma_1\sigma_2\sigma'_2\sigma'_1} E_{j-i,\sigma_1\sigma_2\sigma'_2\sigma'_1} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma'_2} \hat{a}_{i,\sigma'_1}$$

Transitions

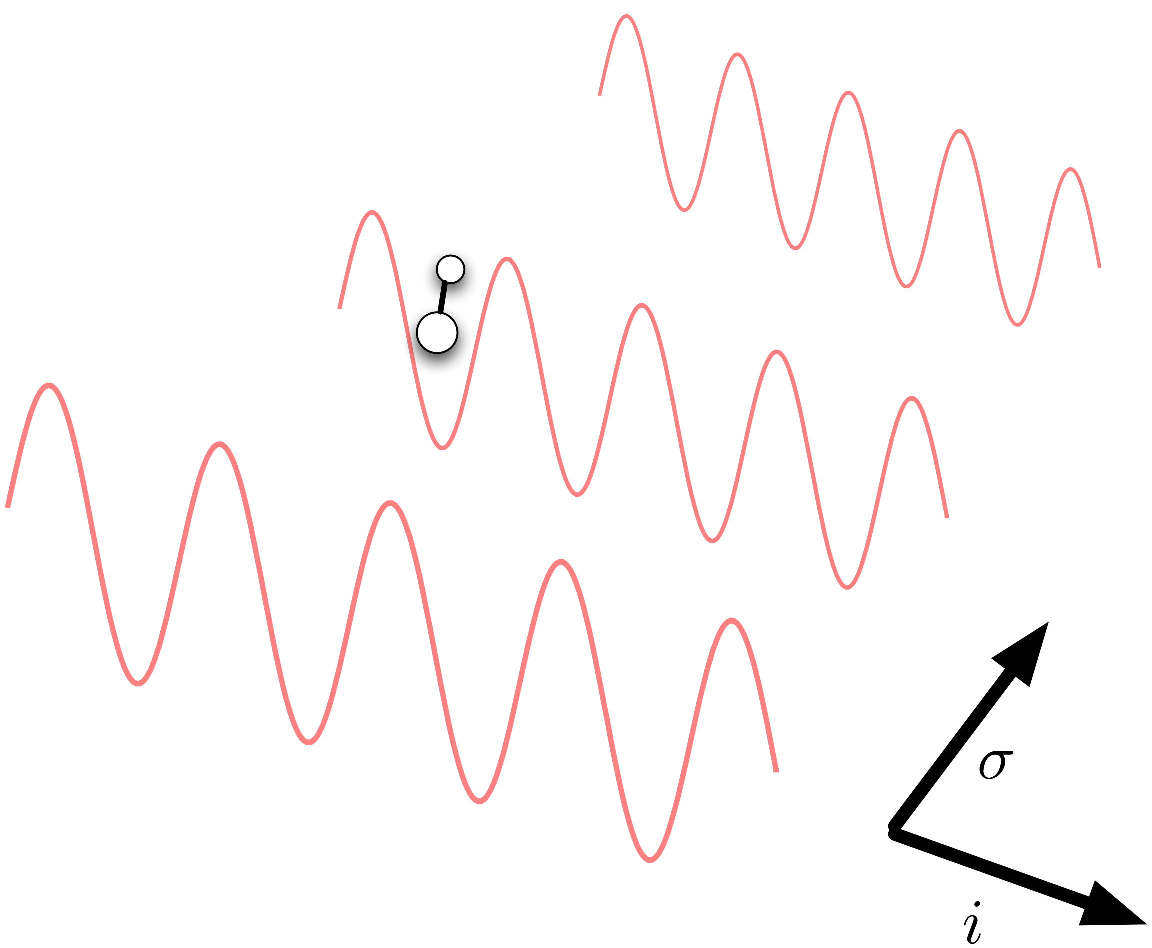


The molecular Hubbard Hamiltonian

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j; r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

Transitions



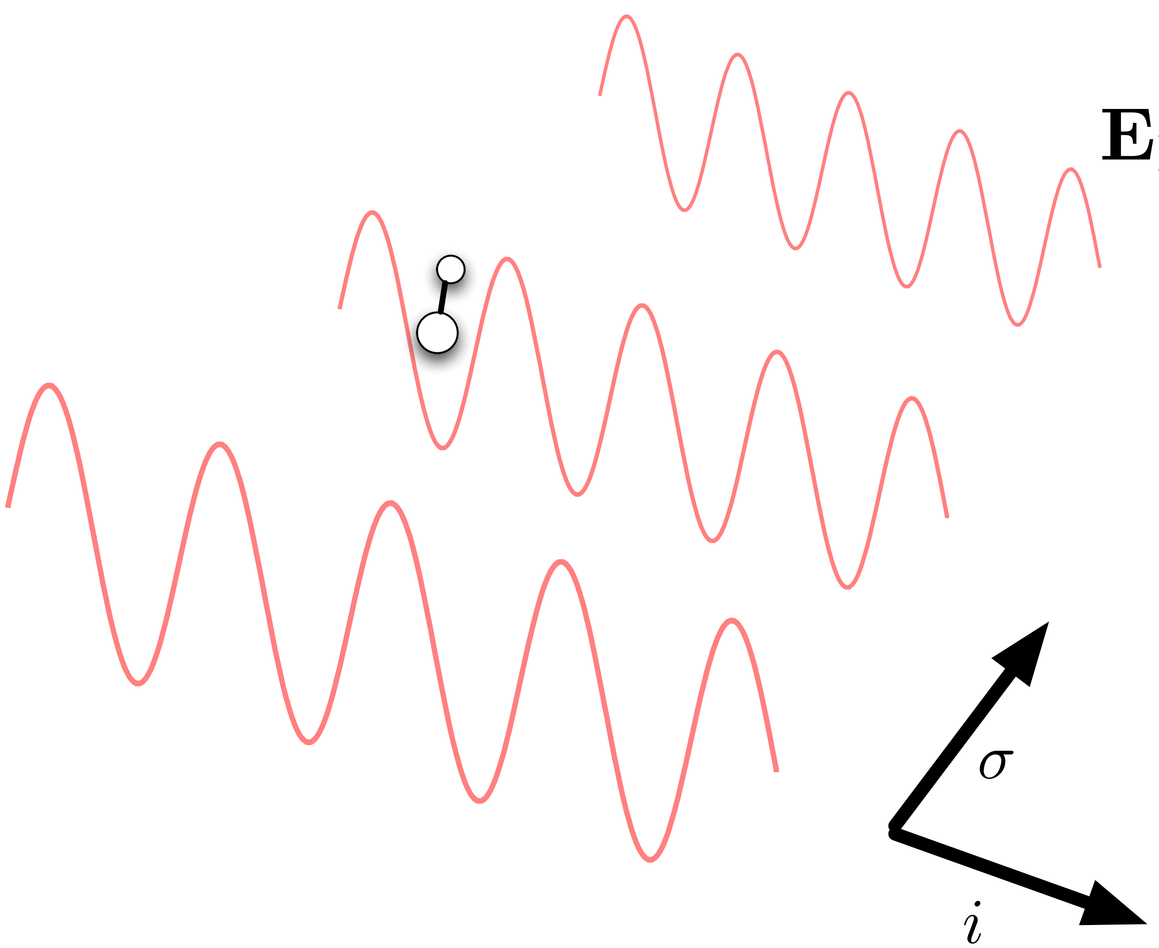
The molecular Hubbard Hamiltonian

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i \neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i \neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

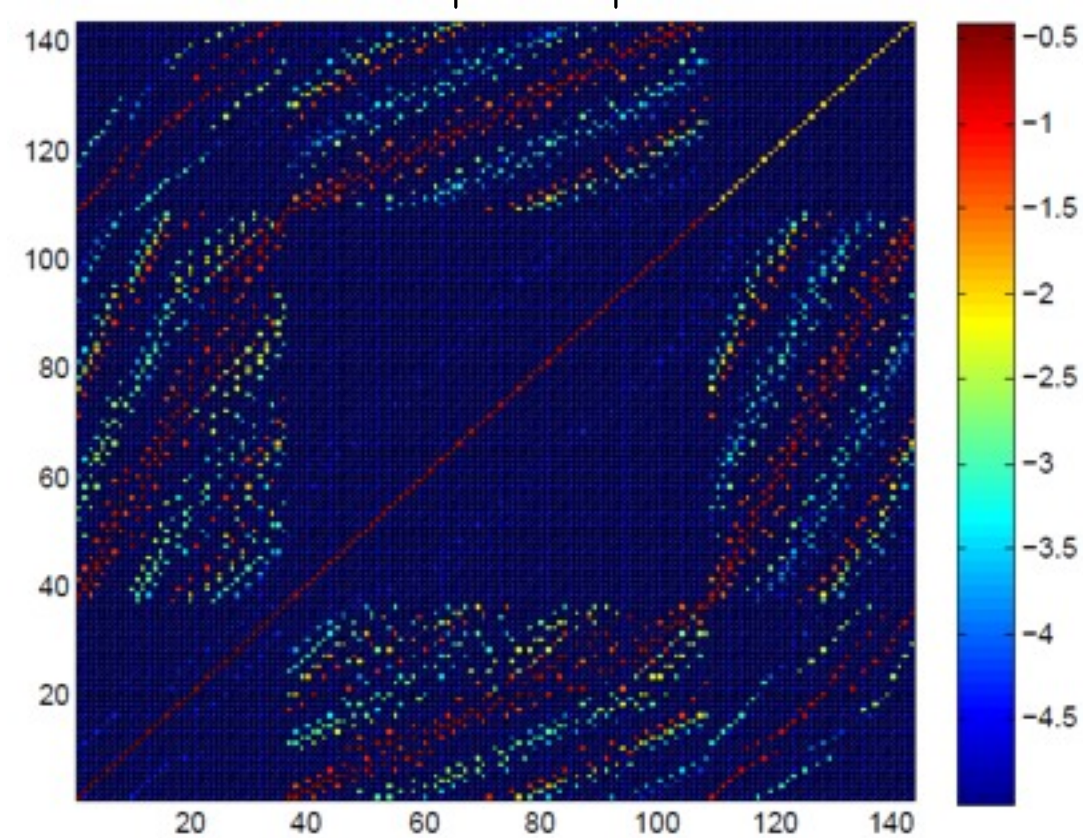
$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i \neq j; r_E} \sum_{\sigma_1 \sigma_2 \sigma_2' \sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

Transitions

$\mathbf{E}_{\mathrm{DC}} \parallel \mathbf{B}$



$\log \left| \hat{d}_{\sigma\sigma'} \right|$



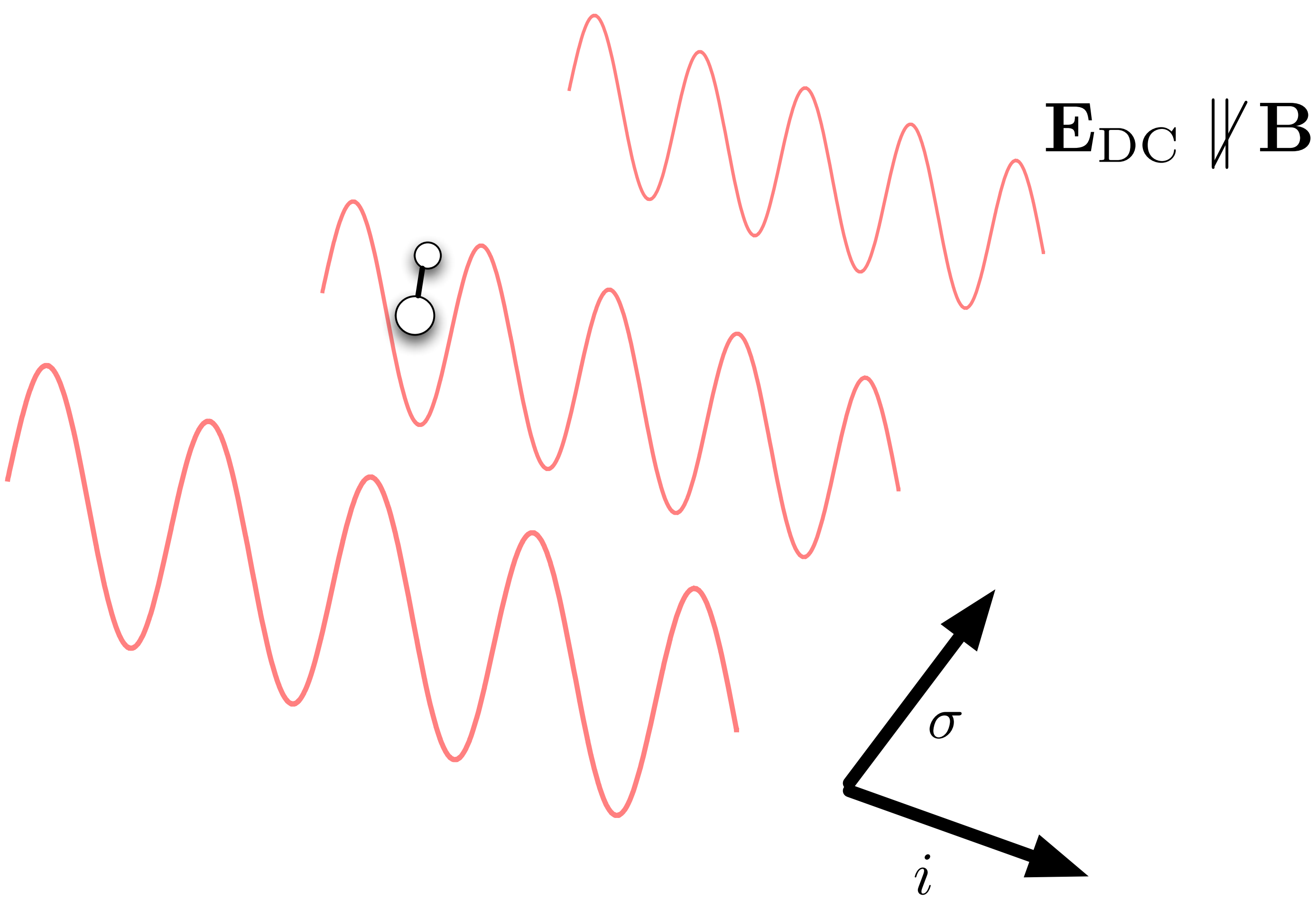
$\bar{N} = 0$ $\bar{N} = 1$

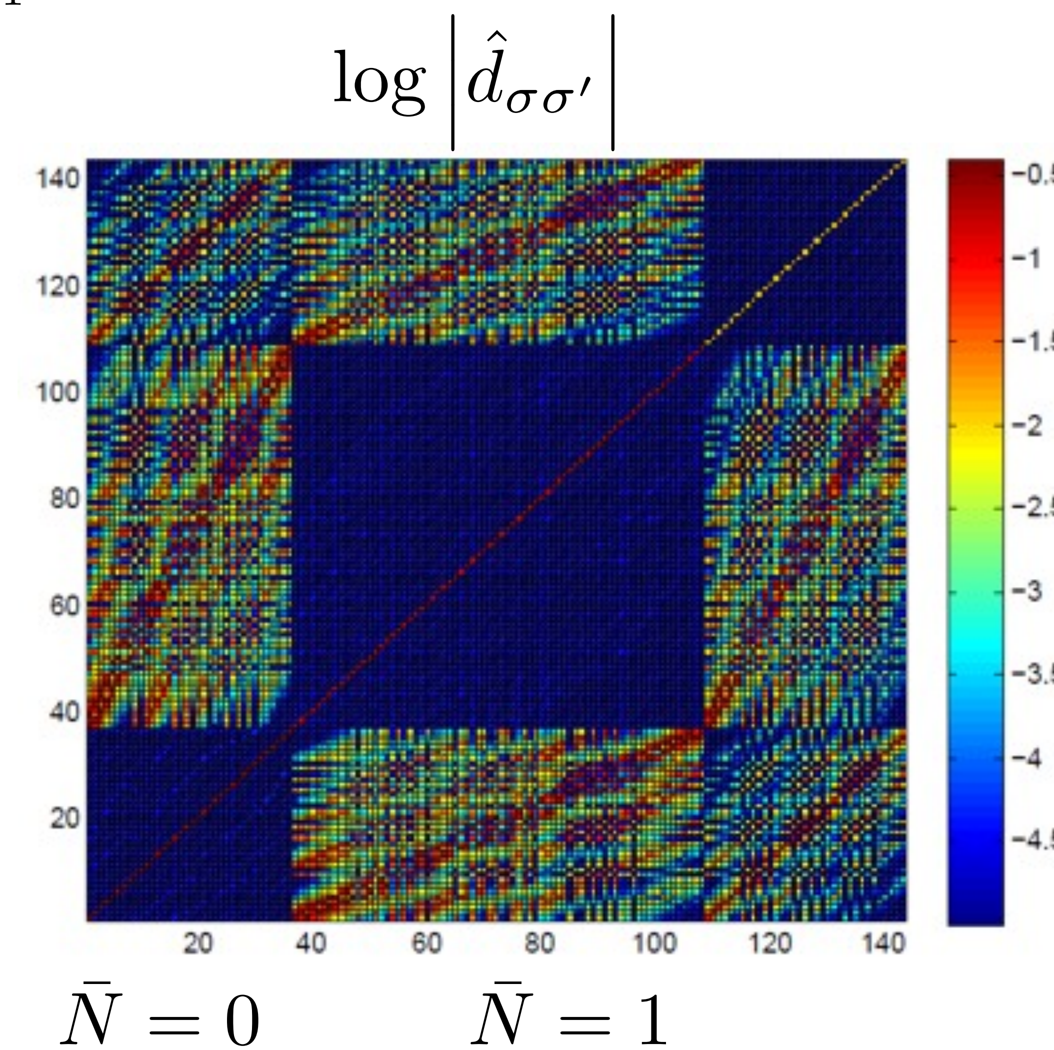
The molecular Hubbard Hamiltonian

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_{i} \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j; r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

Transitions



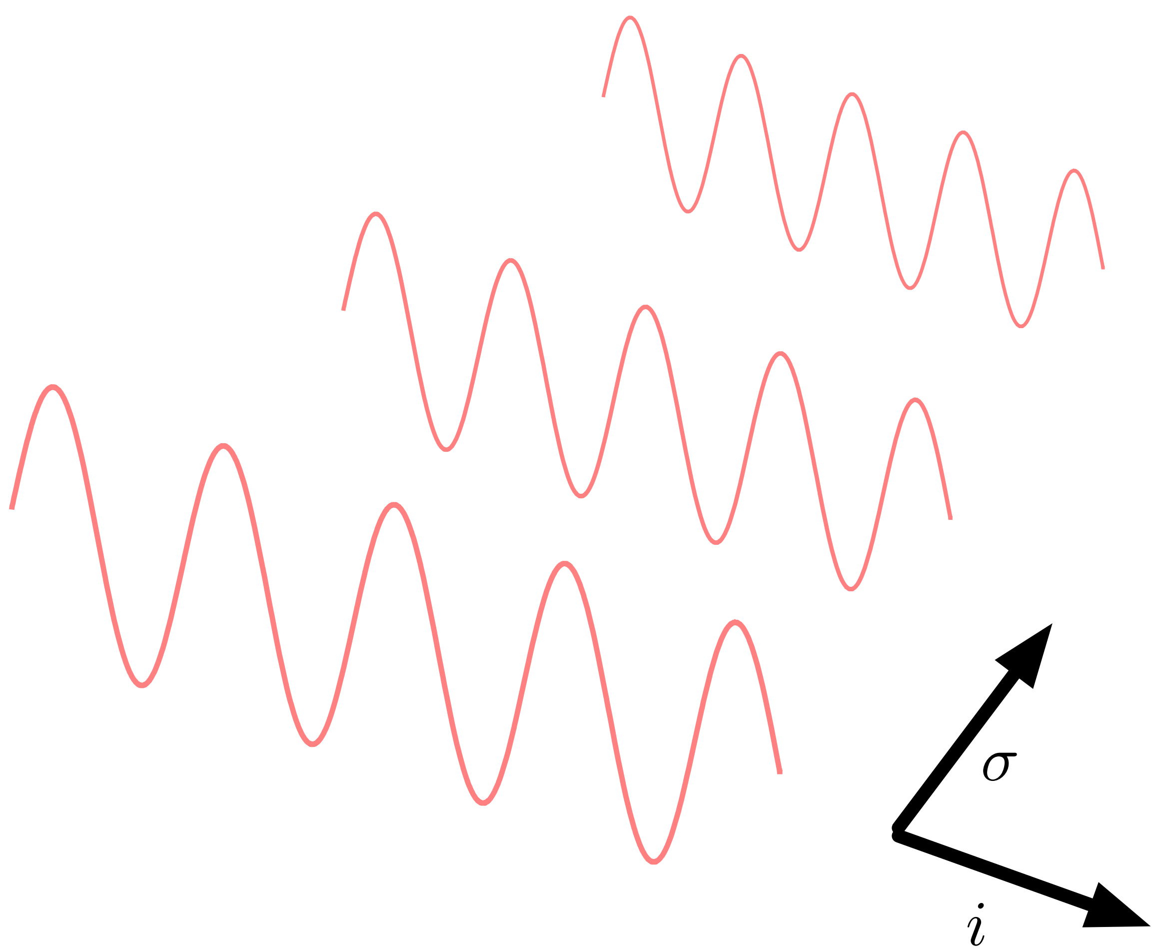


The molecular Hubbard Hamiltonian

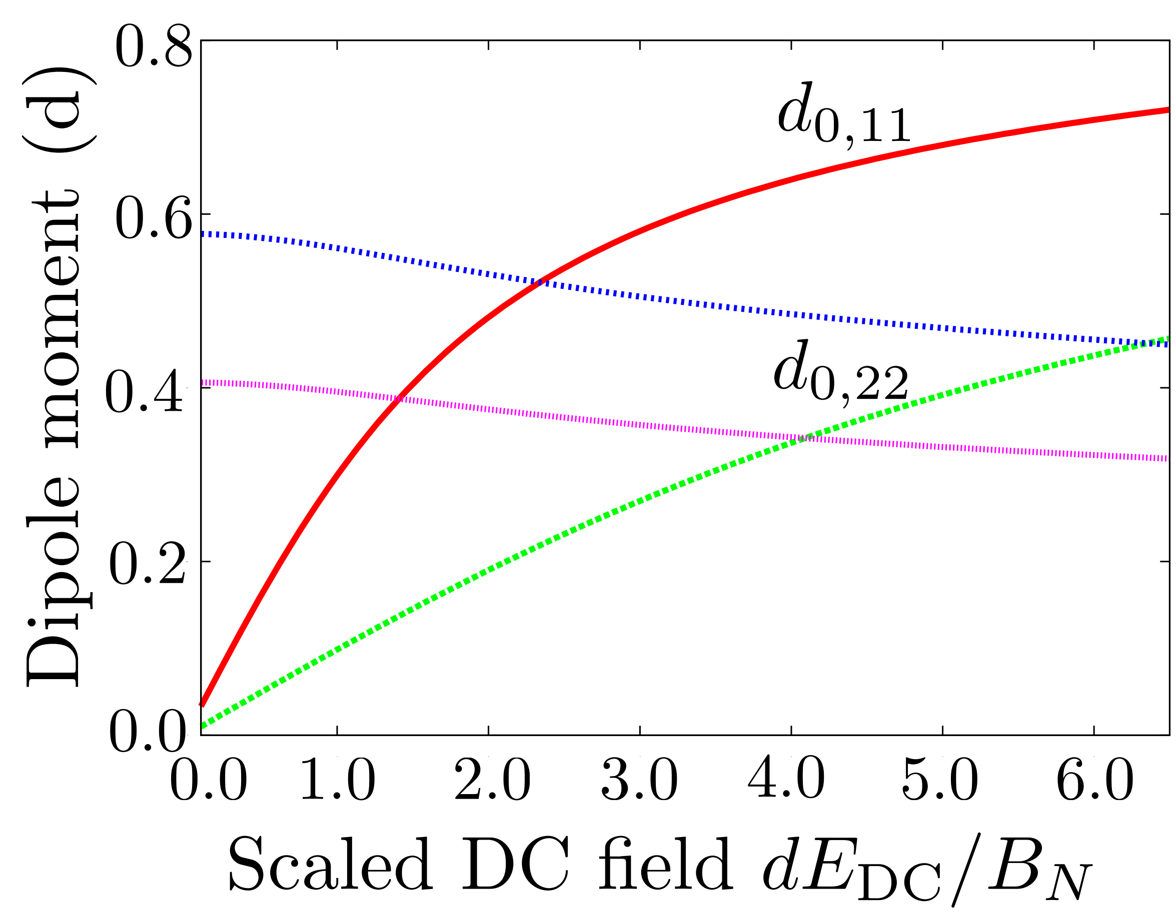
Direct interaction

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i \neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \boxed{\frac{1}{2} \sum_{i \neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_{i} \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i \neq j; r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$



$$d_{q,\sigma\sigma'} \equiv \langle \sigma | \hat{d}_q | \sigma' \rangle$$

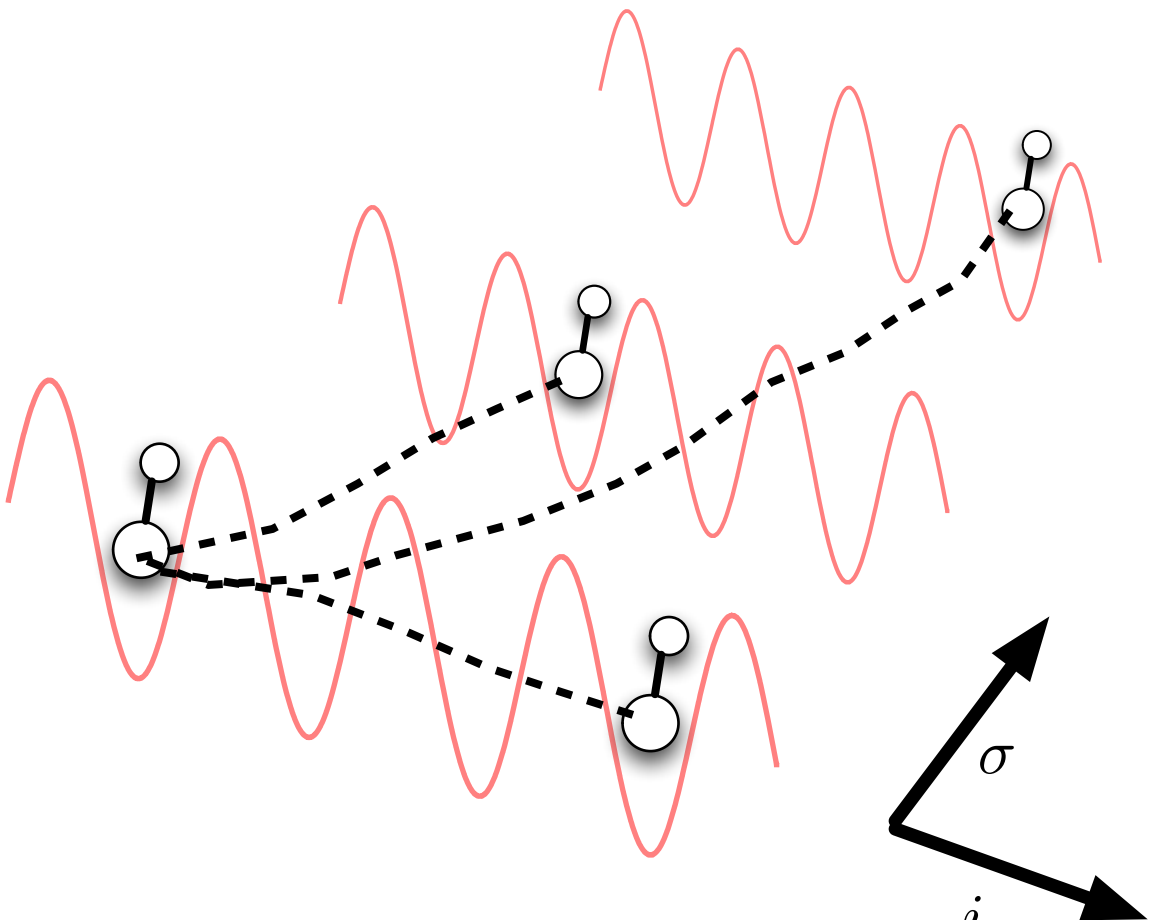


The molecular Hubbard Hamiltonian

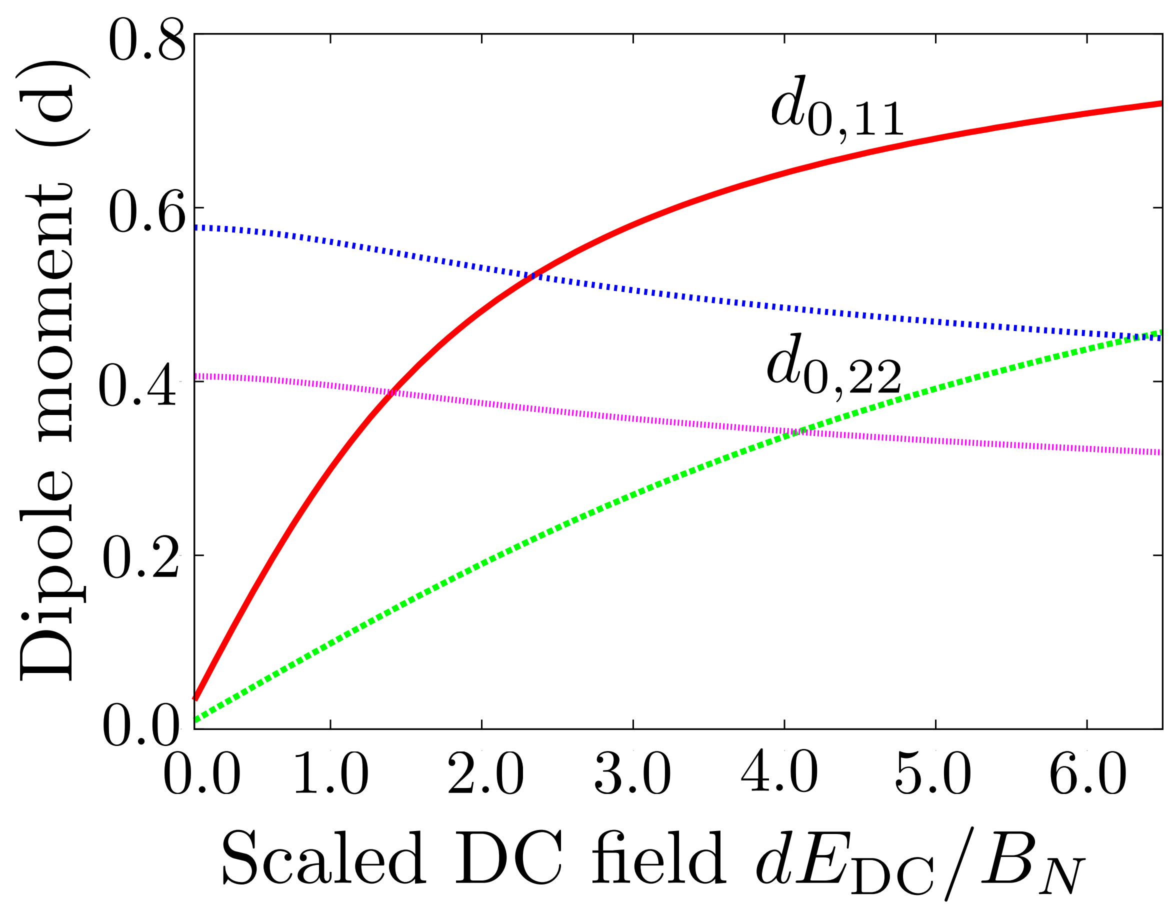
Direct interaction

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j;r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j;r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j;r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$



$$d_{q,\sigma\sigma'} \equiv \langle \sigma | \hat{d}_q | \sigma' \rangle$$



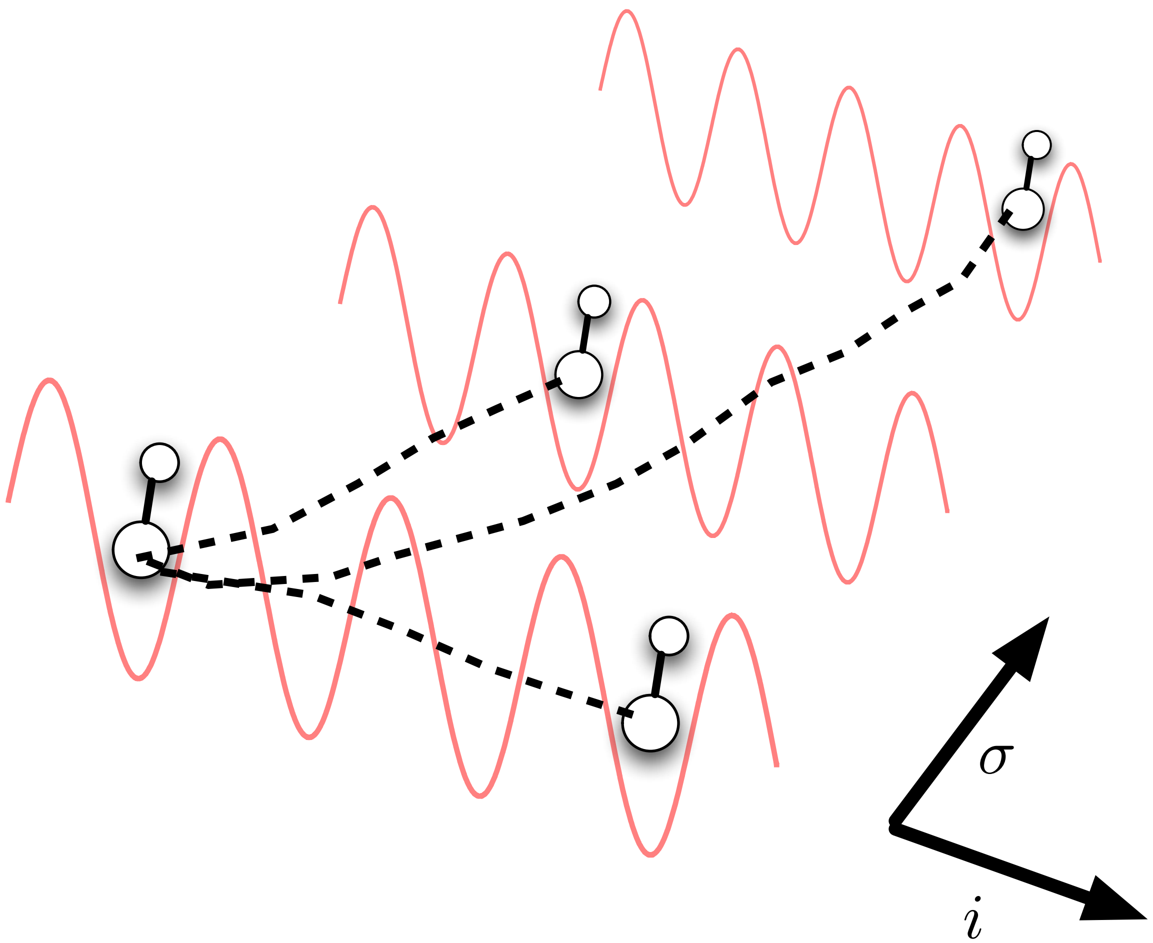
The molecular Hubbard Hamiltonian

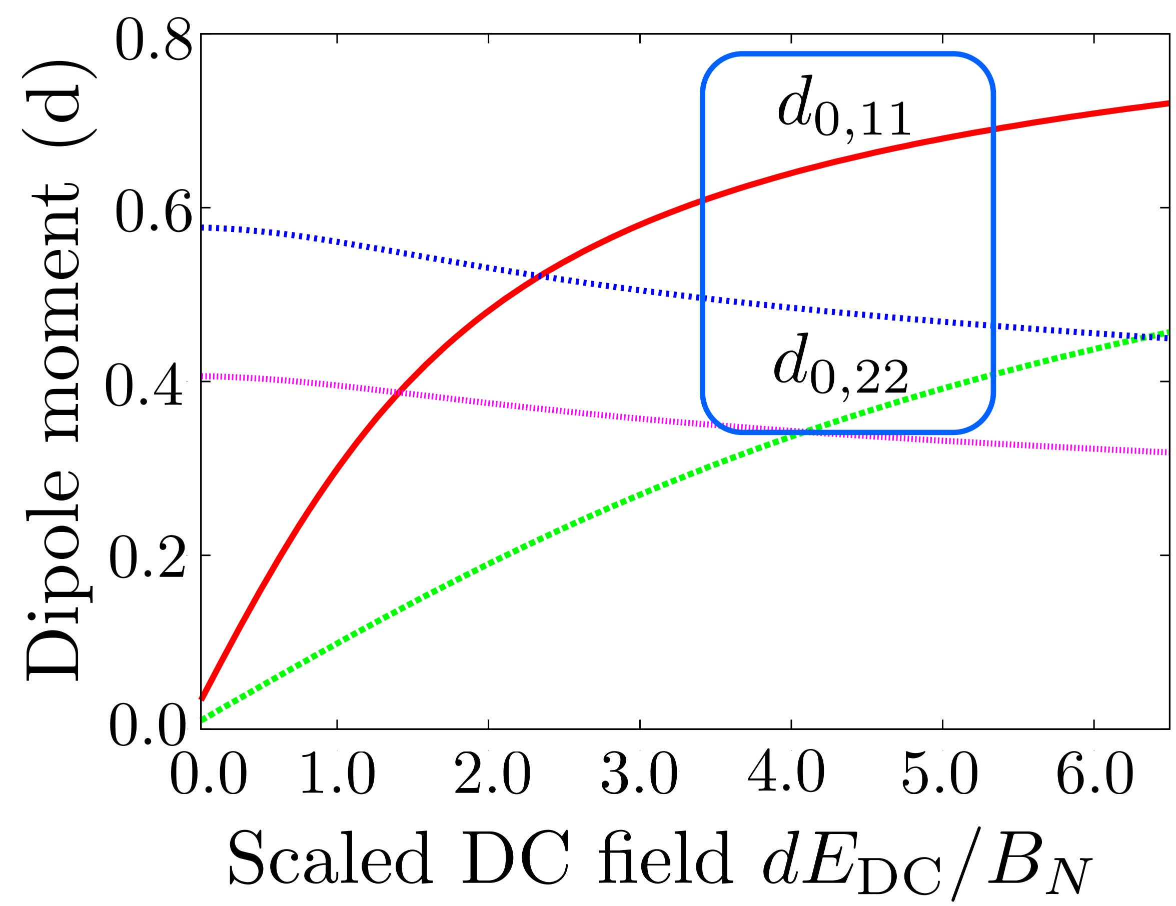
Direct interaction

$$\hat{H} = \sum_{i\sigma} \Delta_{\sigma} \hat{n}_{i,\sigma} - \sum_{i \neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^{\dagger}_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i \neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_{i} \hat{a}^{\dagger}_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i \neq j; r_E} \sum_{\sigma_1 \sigma_2 \sigma_2' \sigma_1'} E_{j-i,\sigma_1 \sigma_2 \sigma_2' \sigma_1'} \hat{a}^{\dagger}_{i,\sigma_1} \hat{a}^{\dagger}_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

$$d_{q,\sigma\sigma'} \equiv \langle \sigma | \hat{d}_q | \sigma' \rangle$$



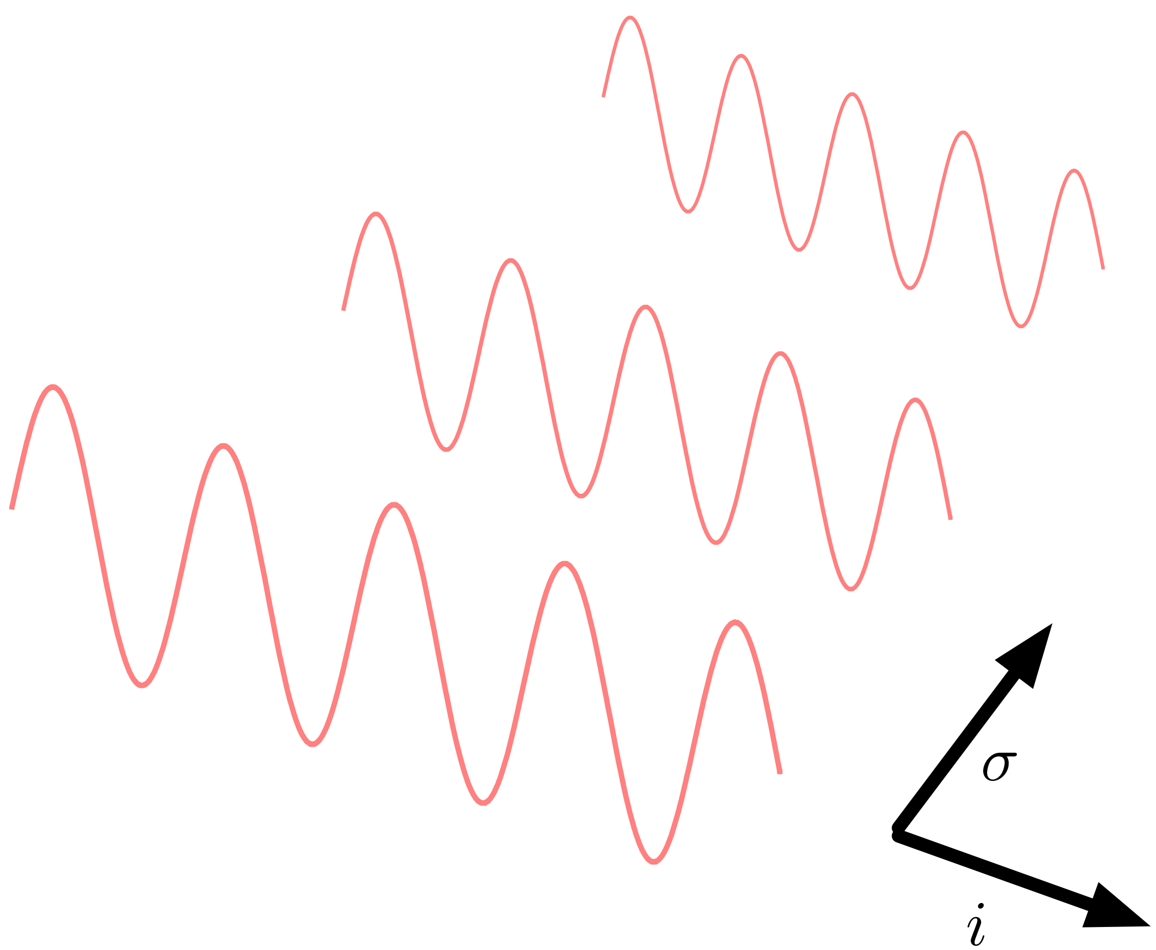


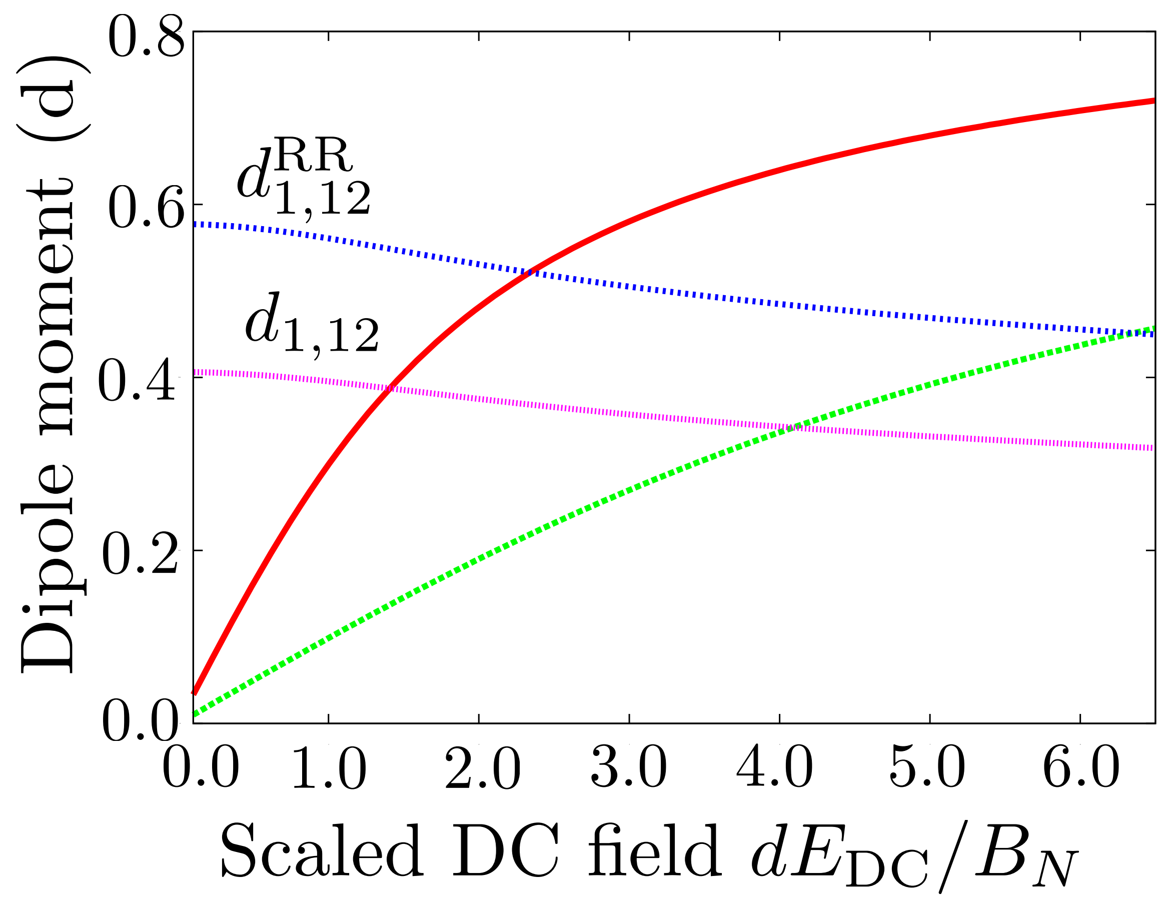
The molecular Hubbard Hamiltonian

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_{i} \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j; r_E} \sum_{\sigma_1\sigma_2\sigma'_2\sigma'_1} E_{j-i,\sigma_1\sigma_2\sigma'_2\sigma'_1} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma'_2} \hat{a}_{i,\sigma'_1}$$

Exchange interaction



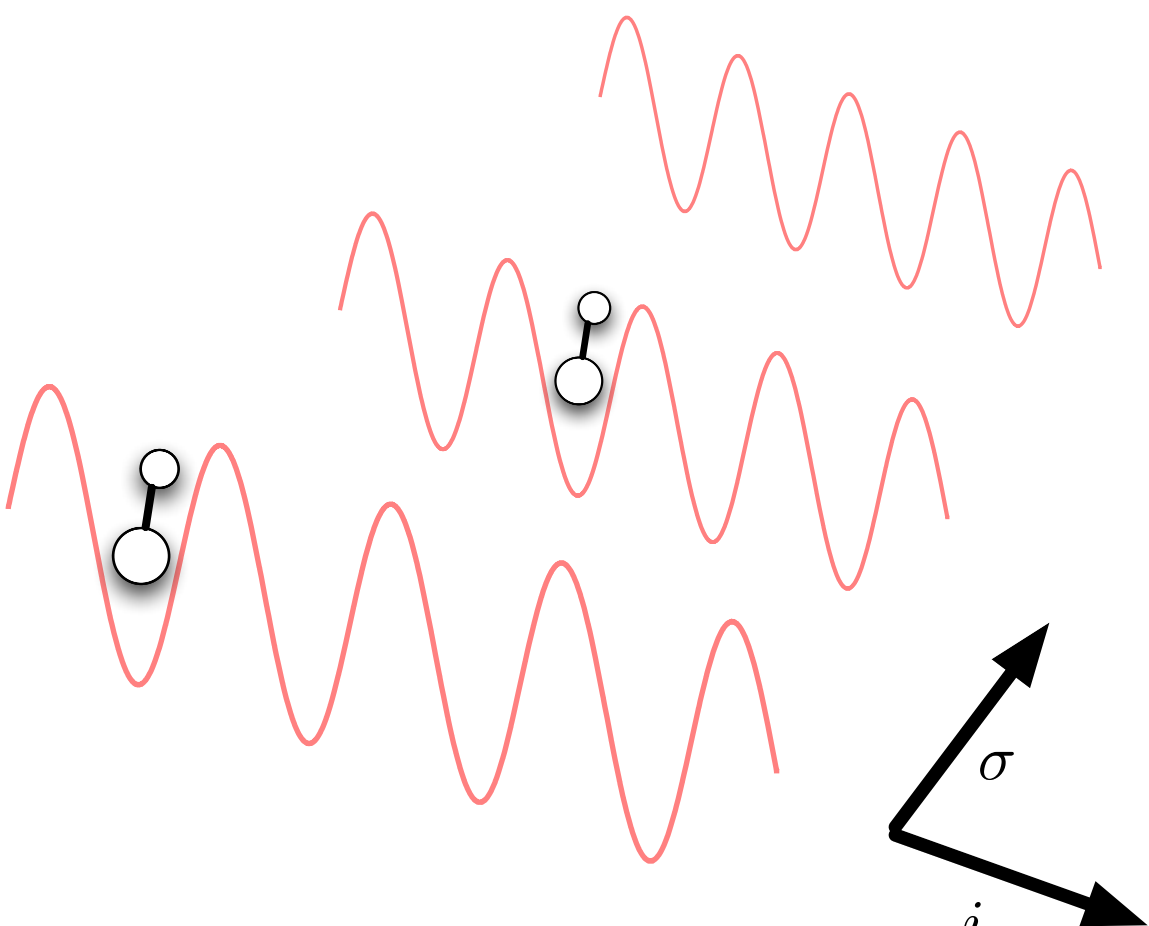


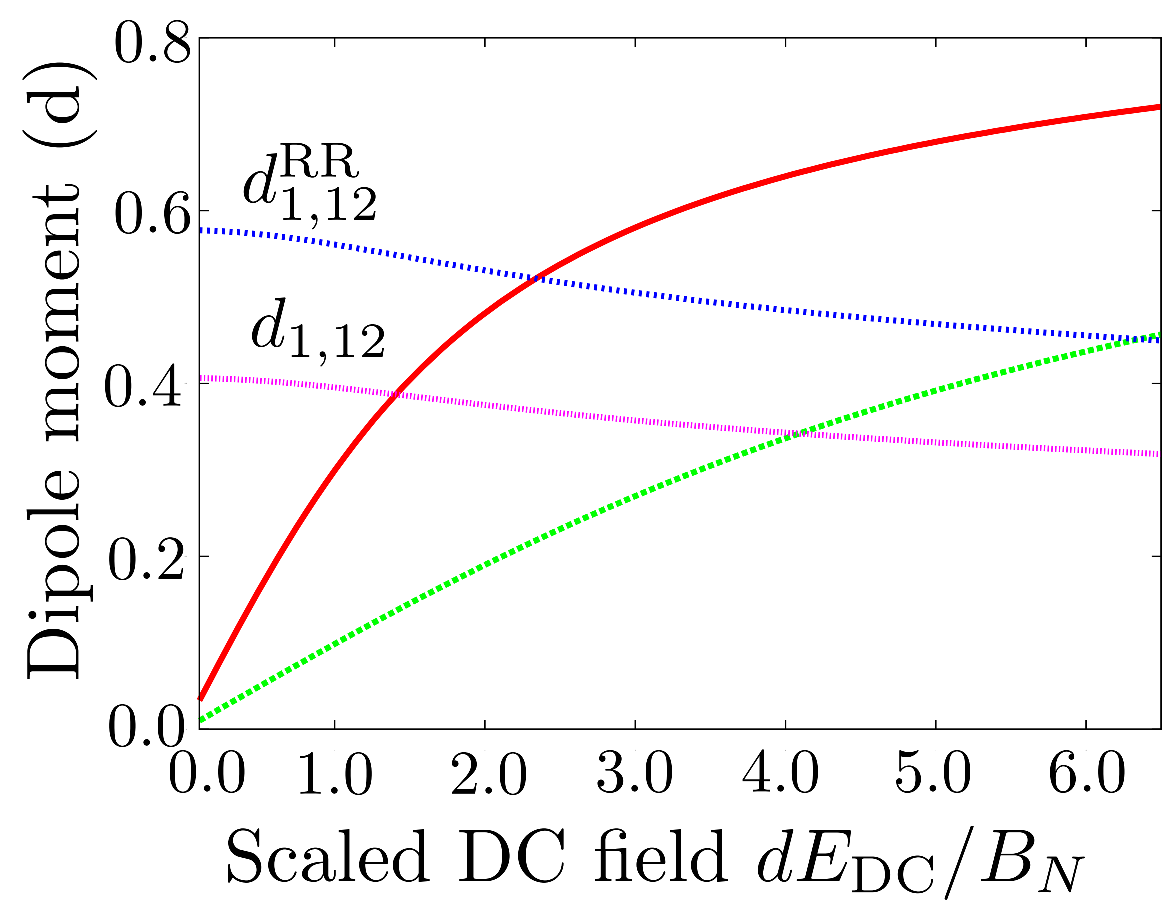
The molecular Hubbard Hamiltonian

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_{i} \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j; r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

Exchange interaction



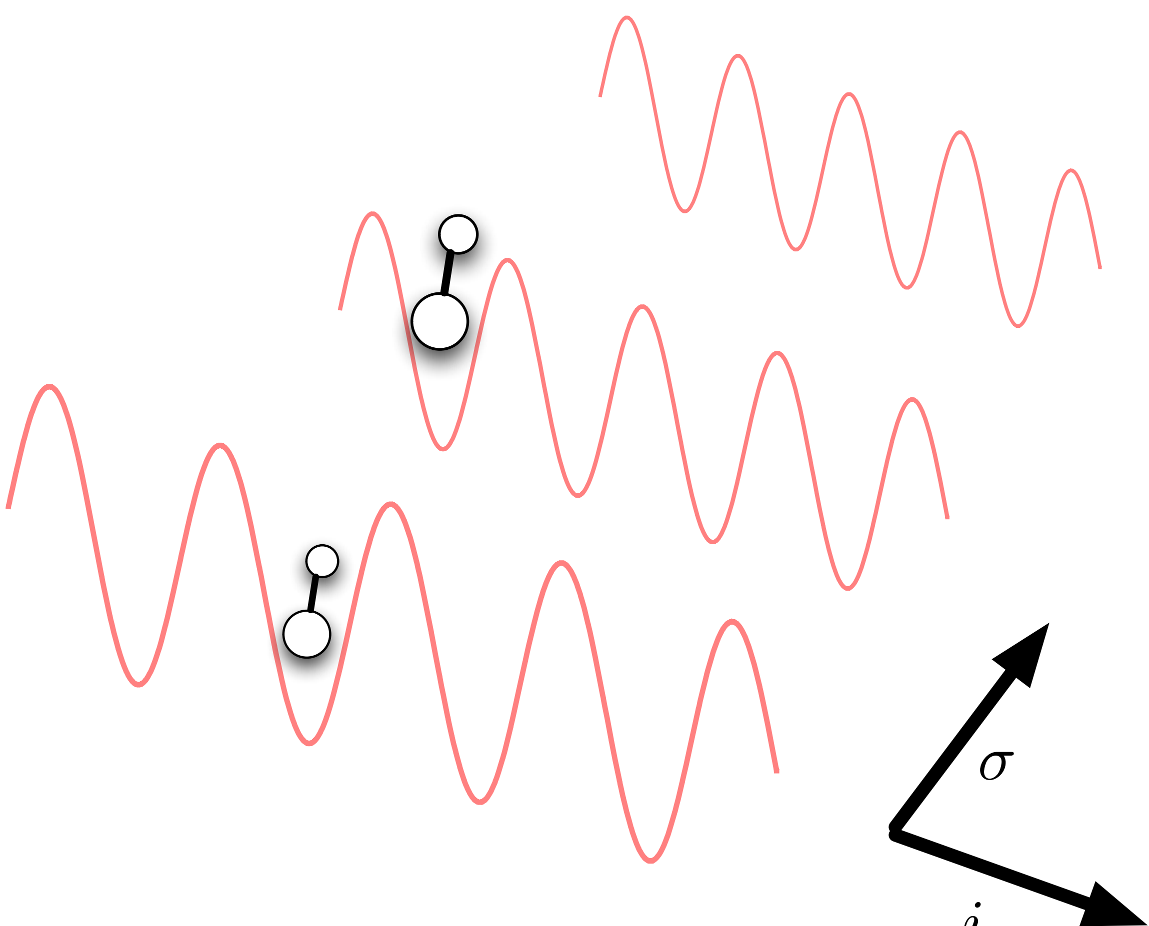


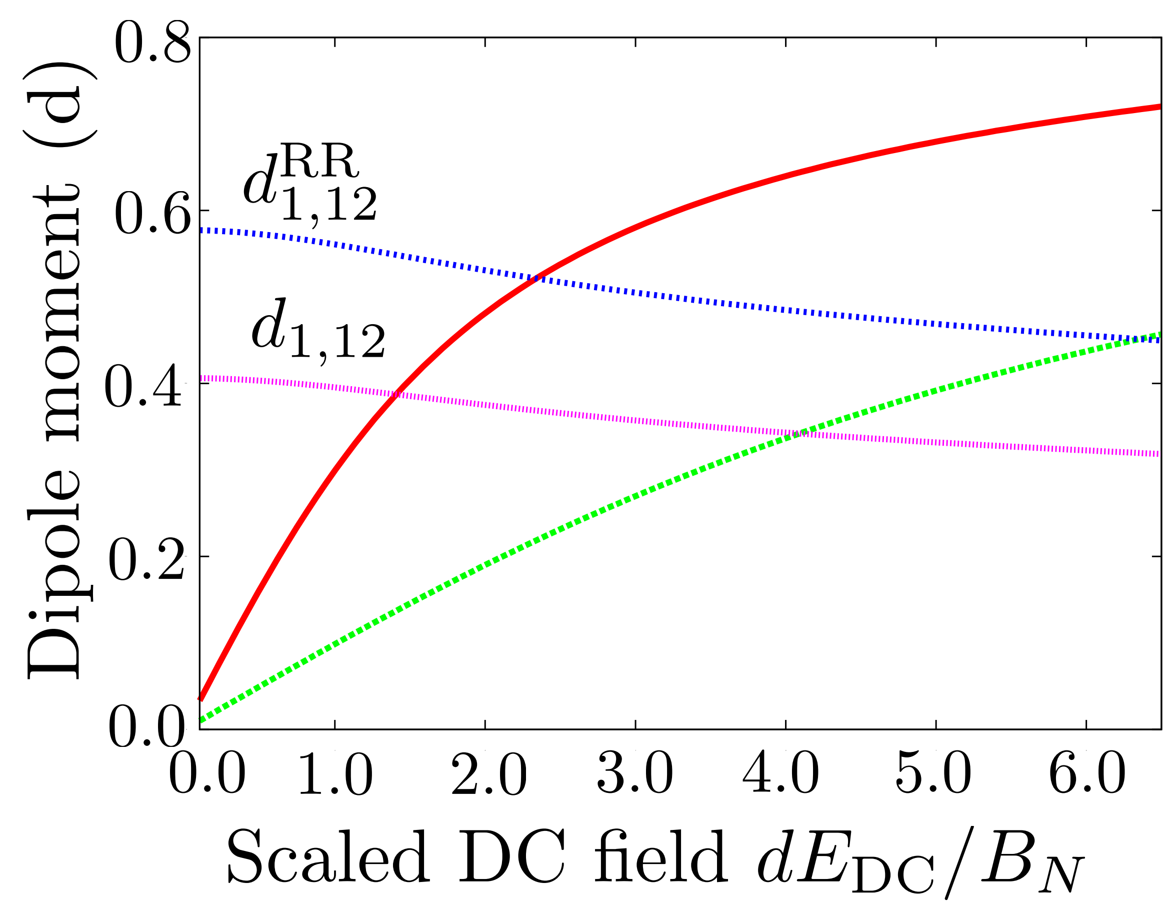
The molecular Hubbard Hamiltonian

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j; r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

Exchange interaction



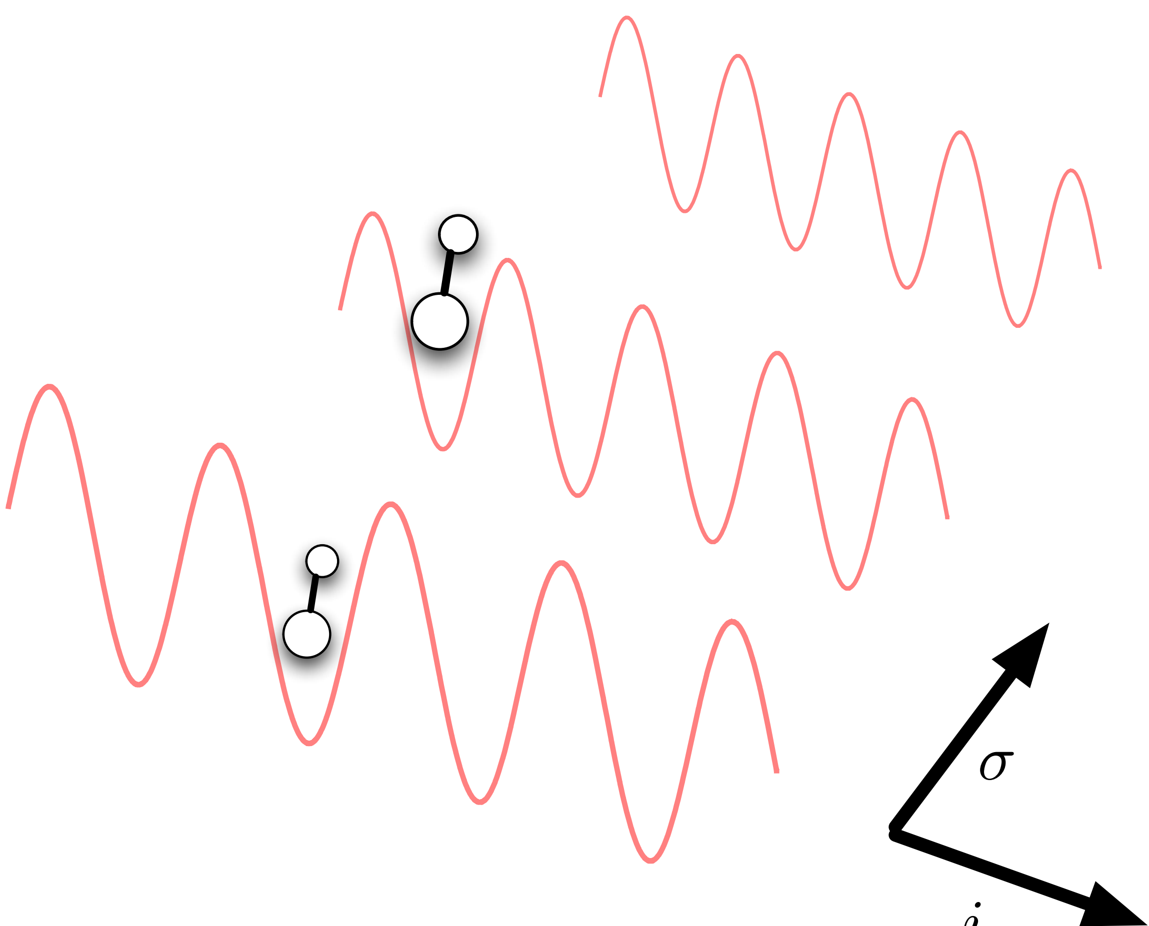


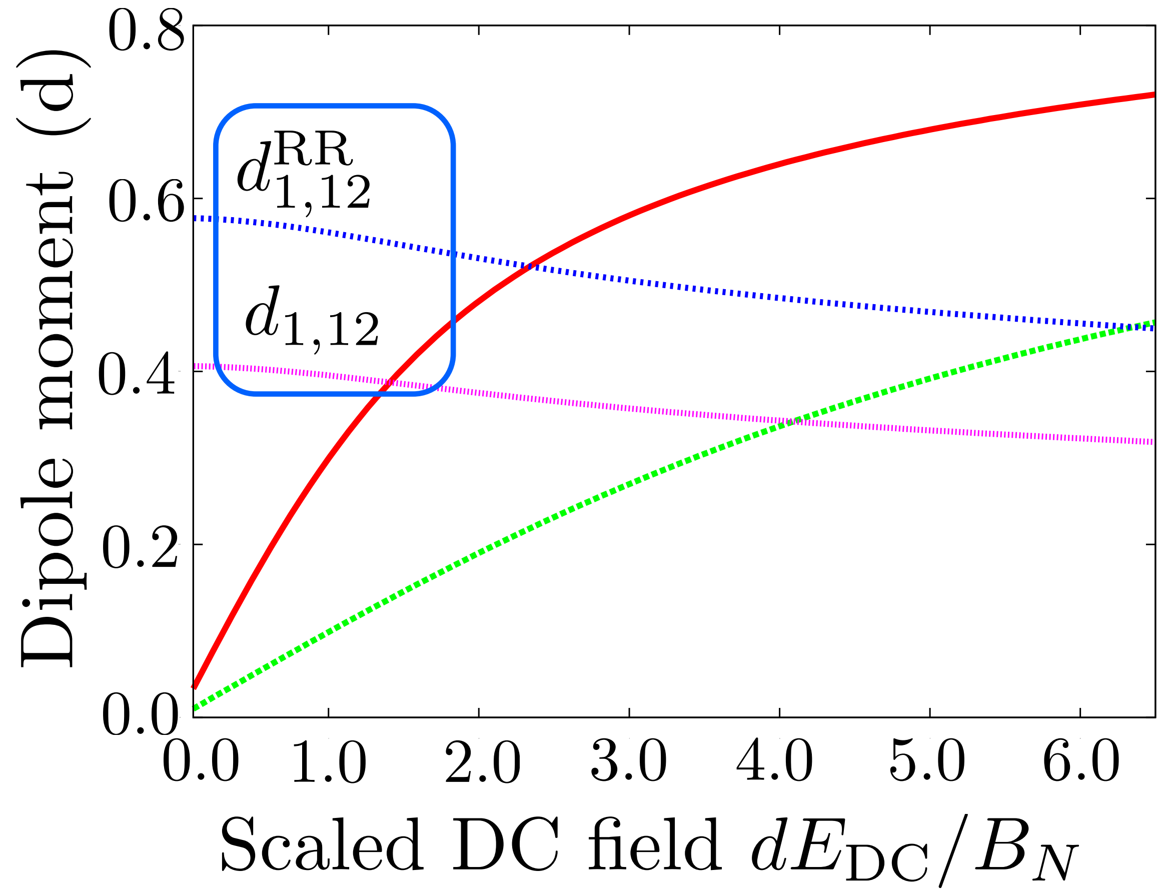
The molecular Hubbard Hamiltonian

$$\hat{H} = \sum_{i\sigma} \Delta_\sigma \hat{n}_{i,\sigma} - \sum_{i\neq j; r_t} \sum_{\sigma} t_{j-i,\sigma} \hat{a}^\dagger_{i,\sigma} \hat{a}_{j,\sigma} + \frac{1}{2} \sum_{i\neq j; r_U} \sum_{\sigma\sigma'} U_{j-i,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}$$

$$- \sum_{\sigma\sigma'} \Omega_{\sigma\sigma'} \sum_i \hat{a}^\dagger_{i,\sigma} \hat{a}_{i,\sigma'} + \frac{1}{4} \sum_{i\neq j; r_E} \sum_{\sigma_1\sigma_2\sigma_2'\sigma_1'} E_{j-i,\sigma_1\sigma_2\sigma_2'\sigma_1'} \hat{a}^\dagger_{i,\sigma_1} \hat{a}^\dagger_{j,\sigma_2} \hat{a}_{j,\sigma_2'} \hat{a}_{i,\sigma_1'}$$

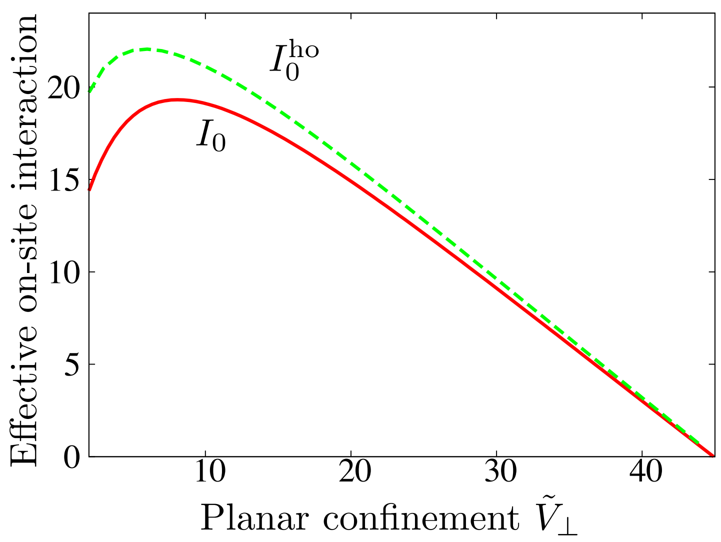
Exchange interaction





Confinement effects

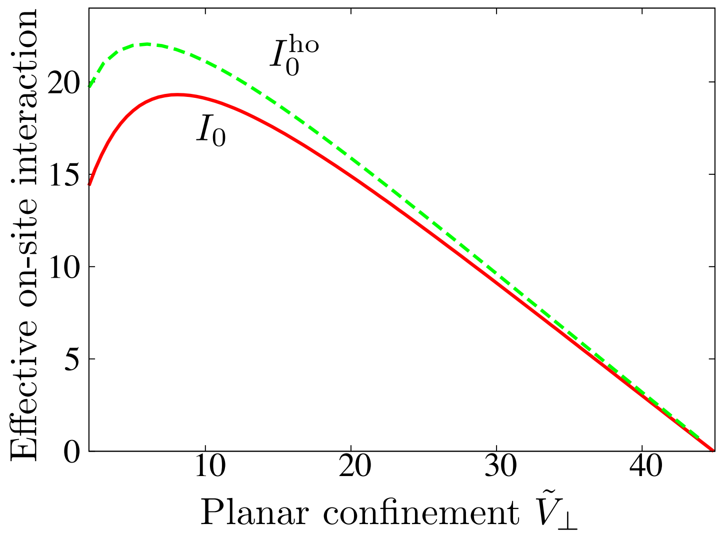
- Harmonic oscillator: anisotropy affects energy



MLW and L.D.Carr arxiv:1303.1230

Confinement effects

- Harmonic oscillator: anisotropy affects energy



- Lattice: Long-ranged interactions also affected!
- Dipolar interactions are different in a lattice!

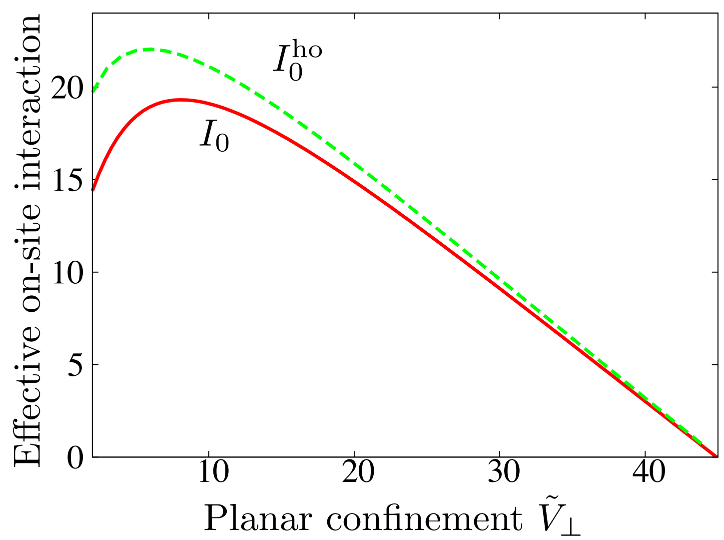
$$U_r \neq \frac{d^2}{a^3}\frac{1}{r^3} \qquad U_r \sim \frac{d^2}{a^3}\left[\frac{1}{r^3} + a_e \exp\left(-b_e r\right)\right]$$

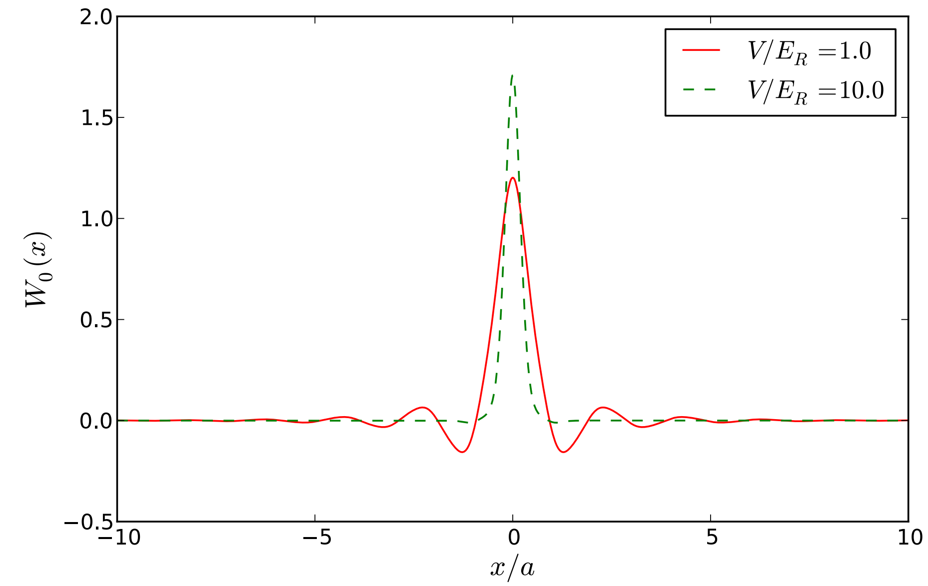
- 30-50% corrections at nearest-neighbor distance in quasi-low dimensional scenarios

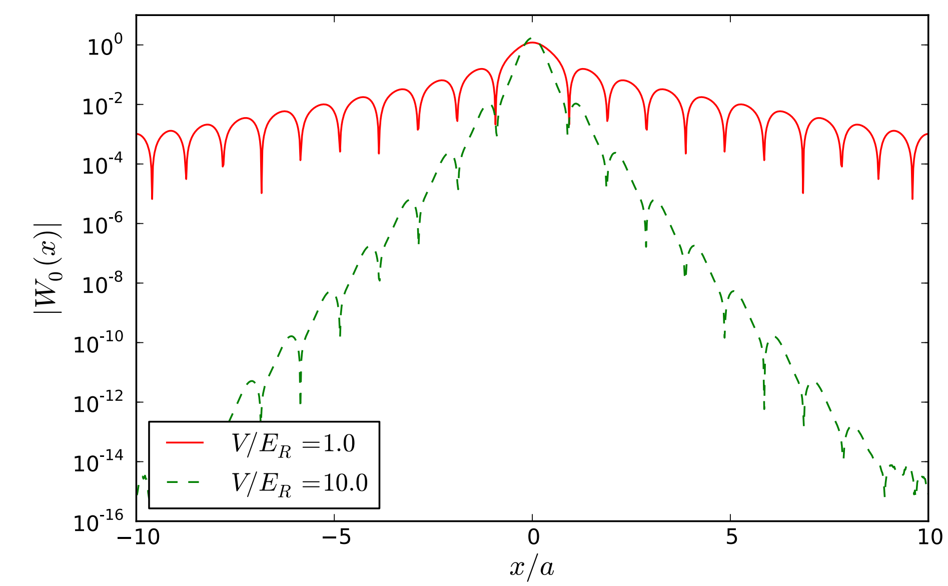
MLW and L.D.Carr arxiv:1303.1230

Confinement effects

- Harmonic oscillator: anisotropy affects energy







- Lattice: Long-ranged interactions also affected!
- Dipolar interactions are different in a lattice!

$$U_r \neq \frac{d^2}{a^3}\frac{1}{r^3} \qquad U_r \sim \frac{d^2}{a^3}\left[\frac{1}{r^3} + a_e \exp\left(-b_e r\right)\right]$$

- 30-50% corrections at nearest-neighbor distance in quasi-low dimensional scenarios

MLW and L.D.Carr arxiv:1303.1230

Comparisons of molecules

	$^{6}Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^{6}Li^{23}Na$
d/Debye	5.52	2.76	1.25	0.566	0.56
I_1	1	3/2	3/2	4	1
I_2	7/2	4	7/2	3/2	3/2
B_N/GHz	6.5202	2.8268	0.504	1.114	12.7355
$\frac{(eQq)_1}{\text{MHz}}$	3×10^{-4}	-0.167	-0.872	0.45	8×10^{-4}
$\frac{(eQq)_2}{\text{MHz}}$	0.187	0.796	0.051	-1.41	0.687
g_1	0.822	1.479	1.834	-0.324	0.822
g_2	0.738	-0.324	0.738	1.834	1.479
c_1/Hz	15.2	110.6	98.4	-24.1	83.2
c_2/Hz	3476.0	-90.9	194.1	420.1	802.2
c_3/Hz	53.1	-46.5	192.4	-48.2	196.2
c_4/Hz	620.8	-466.2	17345.4	-2030.4	212.3
B/Gauss	843.5	139.7	181.7	545.9	745
$\bar{a}$/nm	25	23.5	23.5	6	2.5

Comparisons of molecules

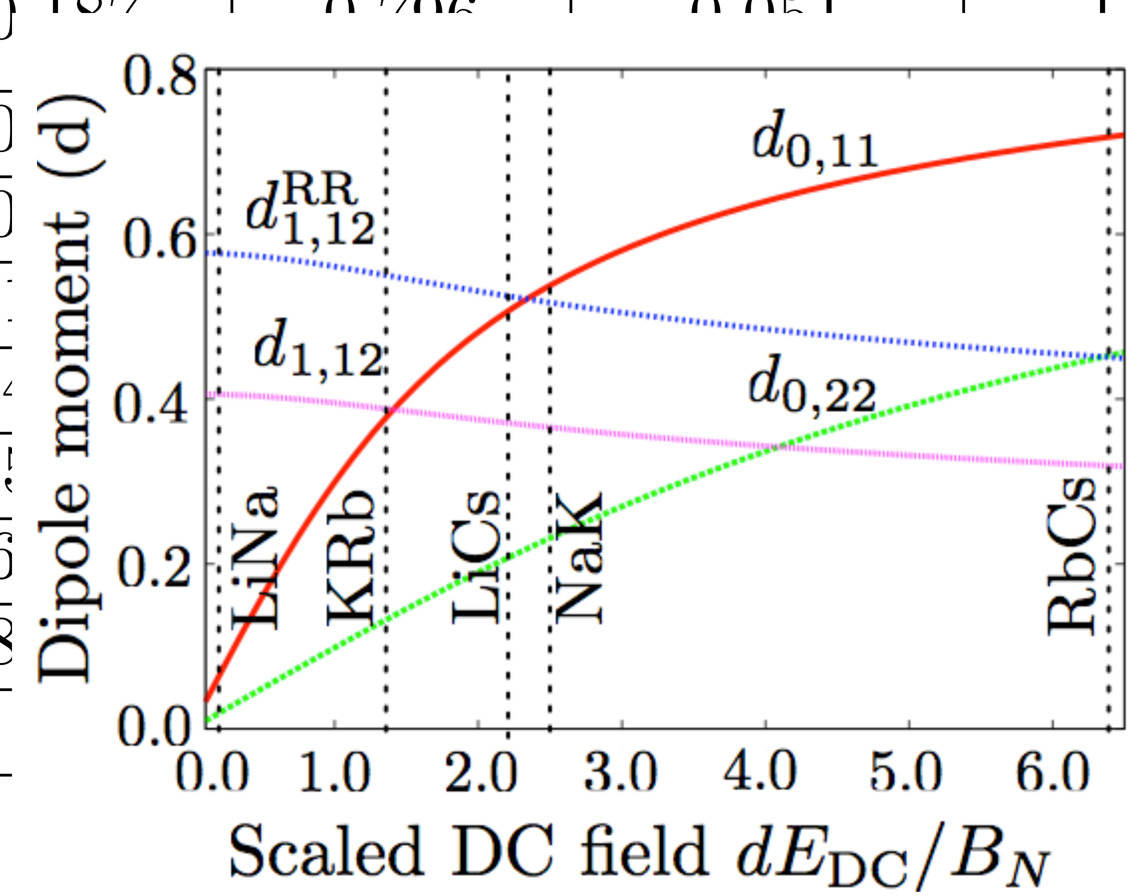
	$^6Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^6Li^{23}Na$
d/Debye	5.52	2.76	1.25	0.566	0.56
I_1	1	3/2	3/2	4	1
I_2	7/2	4	7/2	3/2	3/2
B_N/GHz	6.5202	2.8268	0.504	1.114	12.7355
$\frac{(eQq)_1}{\text{MHz}}$	3×10^{-4}	-0.167	-0.872	0.45	8×10^{-4}
$\frac{(eQq)_2}{\text{MHz}}$	0.187	0.796	0.051	-1.41	0.687
g_1	0.822	1.479	1.834	-0.324	0.822
g_2	0.738	-0.324	0.738	1.834	1.479
c_1/Hz	15.2	110.6	98.4	-24.1	83.2
c_2/Hz	3476.0	-90.9	194.1	420.1	802.2
c_3/Hz	53.1	-46.5	192.4	-48.2	196.2
c_4/Hz	620.8	-466.2	17345.4	-2030.4	212.3
B/Gauss	843.5	139.7	181.7	545.9	745
$\bar{a}$/nm	25	23.5	23.5	6	2.5

Comparisons of molecules

	^{6}Li^{133}Cs	^{23}Na^{40}K	^{87}Rb^{133}Cs	^{40}K^{87}Rb	^{6}Li^{23}Na
d/Debye	5.52	2.76	1.25	0.566	0.56
I_1	1	3/2	3/2	4	1
I_2	7/2	4	7/2	3/2	3/2
B_N/GHz	6.5202	2.8268	0.504	1.114	12.7355
$\frac{(eQq)_1}{\text{MHz}}$	3×10^{-4}	-0.167	-0.872	0.45	8×10^{-4}
$\frac{(eQq)_2}{\text{MHz}}$	0.187	0.796	0.051	-1.41	0.687
g_1	0.822	1.479	1.834	-0.324	0.822
g_2	0.738	-0.324	0.738	1.834	1.479
c_1/Hz	15.2	110.6	98.4	-24.1	83.2
c_2/Hz	3476.0	-90.9	194.1	420.1	802.2
c_3/Hz	53.1	-46.5	192.4	-48.2	196.2
c_4/Hz	620.8	-466.2	17345.4	-2030.4	212.3
B/Gauss	843.5	139.7	181.7	545.9	745
$\bar{a}$/nm	25	23.5	23.5	6	2.5

Comparisons of molecules

	$^6Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^6Li^{23}Na$
d/Debye	5.52	2.76	1.25	0.566	0.56
I_1	1	3/2	3/2	4	1
I_2	7/2	4	7/2	3/2	3/2
B_N/GHz	6.5202	2.8268	0.504	1.114	12.7355
$\frac{(eQq)_1}{\text{MHz}}$	3×10^{-4}	-0.167	-0.872	0.45	8×10^{-4}
$\frac{(eQq)_2}{\text{MHz}}$	[illegible]	[illegible]	[illegible]	[illegible]	0.687
g_1	[illegible]	[illegible]	[illegible]	[illegible]	0.822
g_2	[illegible]	[illegible]	[illegible]	[illegible]	1.479
c_1/Hz	[illegible]	[illegible]	[illegible]	[illegible]	83.2
c_2/Hz	[illegible]	[illegible]	[illegible]	[illegible]	802.2
c_3/Hz	[illegible]	[illegible]	[illegible]	[illegible]	196.2
c_4/Hz	[illegible]	[illegible]	[illegible]	[illegible]	212.3
B/Gauss	[illegible]	[illegible]	[illegible]	[illegible]	745
$\bar{a}$/nm	[illegible]	[illegible]	[illegible]	[illegible]	2.5

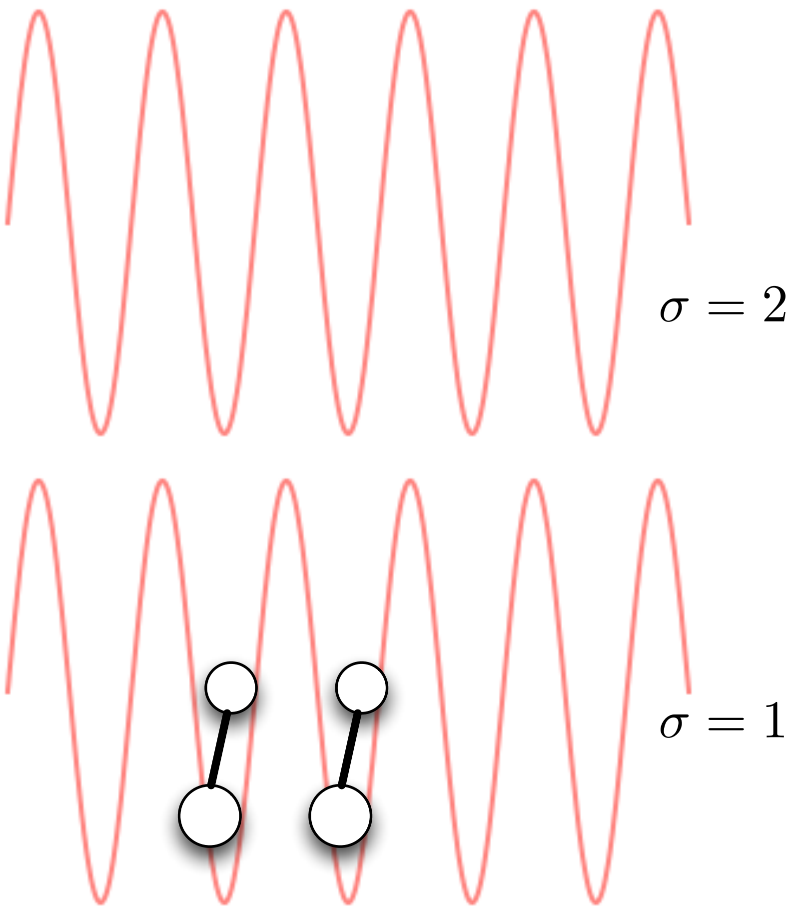


Comparisons of molecules

	$^6Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^6Li^{23}Na$
d/Debye	5.52	2.76	1.25	0.566	0.56
I_1	1	3/2	3/2	4	1
I_2	7/2	4	7/2	3/2	3/2
B_N/GHz	6.5202	2.8268	0.504	1.114	12.7355
$\frac{(eQq)_1}{\text{MHz}}$	3×10^{-4}	-0.167	-0.872	0.45	8×10^{-4}
$\frac{(eQq)_2}{\text{MHz}}$	0.187	0.796	0.051	-1.41	0.687
g_1	0.822	1.479	1.834	-0.324	0.822
g_2	0.738	-0.324	0.738	1.834	1.479
c_1/Hz	15.2	110.6	98.4	-24.1	83.2
c_2/Hz	3476.0	-90.9	194.1	420.1	802.2
c_3/Hz	53.1	-46.5	192.4	-48.2	196.2
c_4/Hz	620.8	-466.2	17345.4	-2030.4	212.3
B/Gauss	843.5	139.7	181.7	545.9	745
$\bar{a}$/nm	25	23.5	23.5	6	2.5

Many-body case studies

	$^{6}Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^{6}Li^{23}Na$
E_{DC}= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	2×10^{-5}
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	5×10^{5}
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	3×10^{6}
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	2×10^{3}
E_{DC}= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	5×10^{-4}
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	2×10^{3}
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	1.2×10^{5}
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114

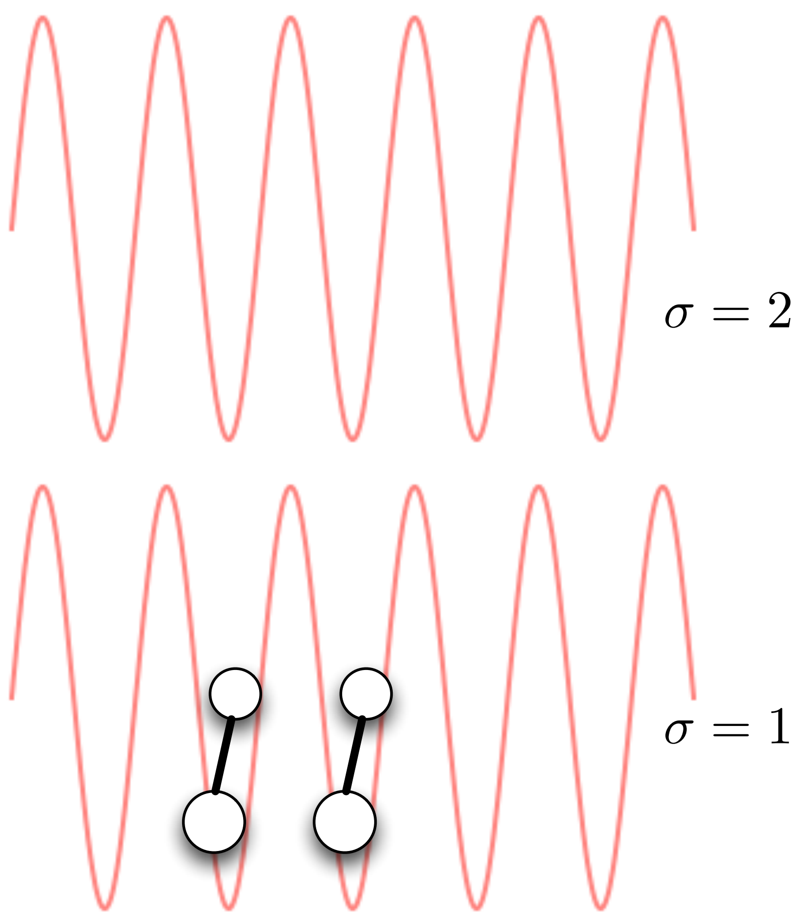


Quasi-1D, 2 internal states
r, distance
σ, internal state

Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma_2'\sigma_1'}$

Many-body case studies

	$^{6}Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^{6}Li^{23}Na$
E_{DC}= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	2×10^{-5}
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	5×10^{5}
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	3×10^{6}
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	2×10^{3}
E_{DC}= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	5×10^{-4}
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	2×10^{3}
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	1.2×10^{5}
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114

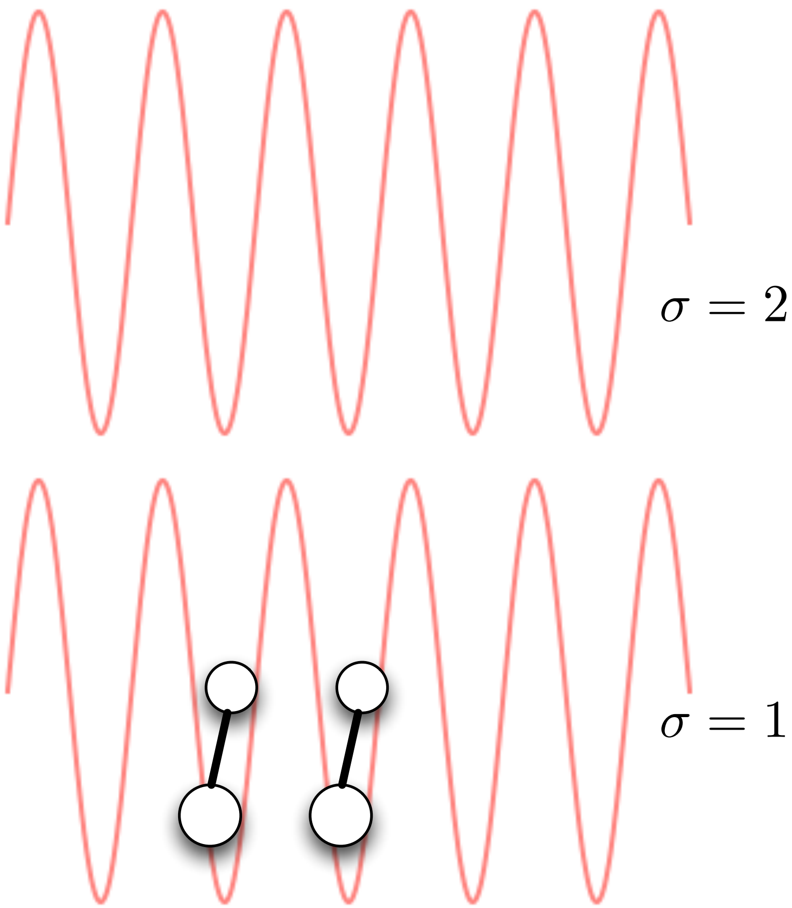


Quasi-1D, 2 internal states
r, distance
σ, internal state

Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma_2'\sigma_1'}$

Many-body case studies

	$^{6}Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^{6}Li^{23}Na$
E_{DC}= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	2×10^{-5}
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	5×10^{5}
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	3×10^{6}
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	2×10^{3}
E_{DC}= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	5×10^{-4}
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	2×10^{3}
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	1.2×10^{5}
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114

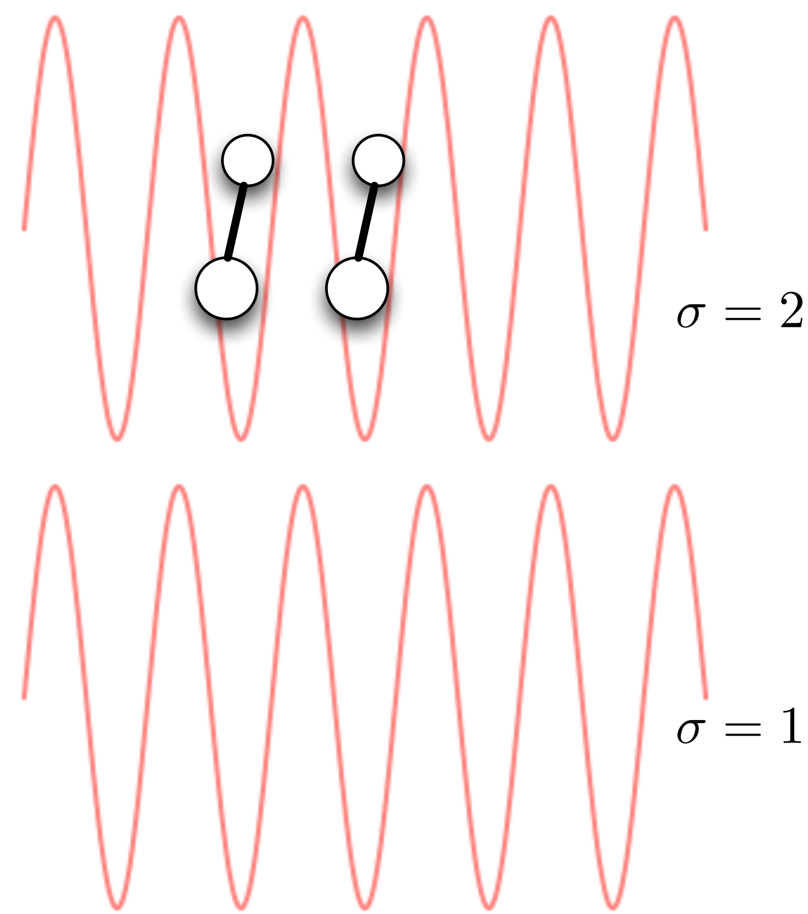


Quasi-1D, 2 internal states
r, distance
σ, internal state

Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma_2'\sigma_1'}$

Many-body case studies

	^{6}Li^{133}Cs	^{23}Na^{40}K	^{87}Rb^{133}Cs	^{40}K^{87}Rb	^{6}Li^{23}Na
E_{DC}= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	$2{\times}10^{-5}$
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	$5{\times}10^{5}$
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	$3{\times}10^{6}$
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	$2{\times}10^{3}$
E_{DC}= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	$5{\times}10^{-4}$
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	$2{\times}10^{3}$
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	$1.2{\times}10^{5}$
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114

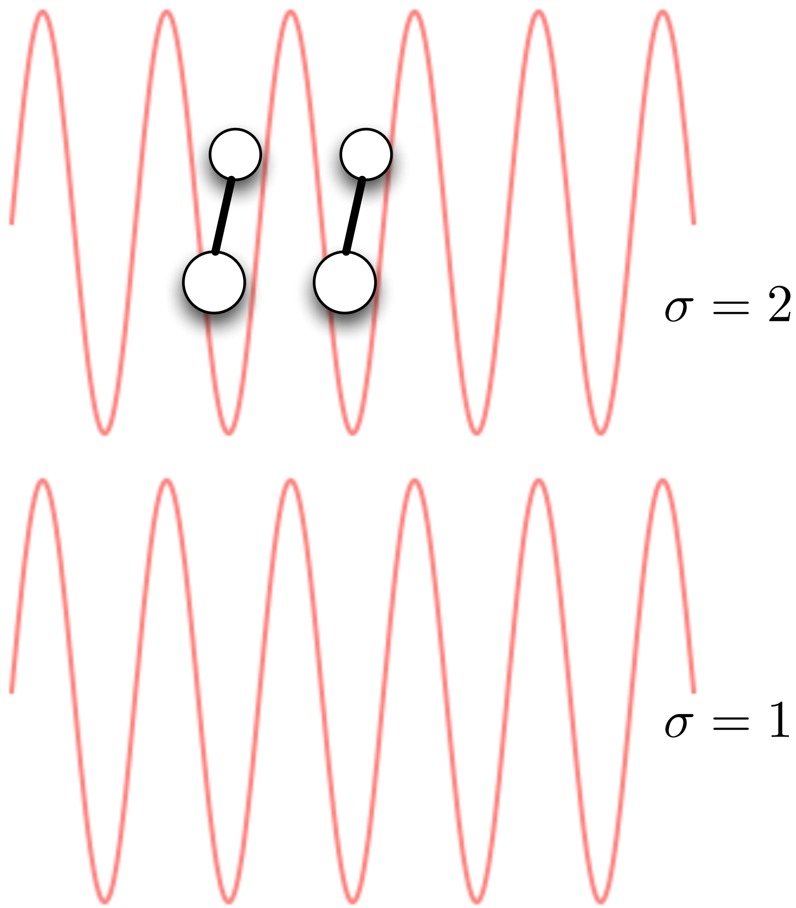


Quasi-1D, 2 internal states
r, distance
σ, internal state

Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma_2'\sigma_1'}$

Many-body case studies

	^{6}Li^{133}Cs	^{23}Na^{40}K	^{87}Rb^{133}Cs	^{40}K^{87}Rb	^{6}Li^{23}Na
$E_{\rm DC}$= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	2×10^{-5}
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	5×10^{5}
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	3×10^{6}
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	2×10^{3}
$E_{\rm DC}$= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	5×10^{-4}
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	2×10^{3}
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	1.2×10^{5}
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114

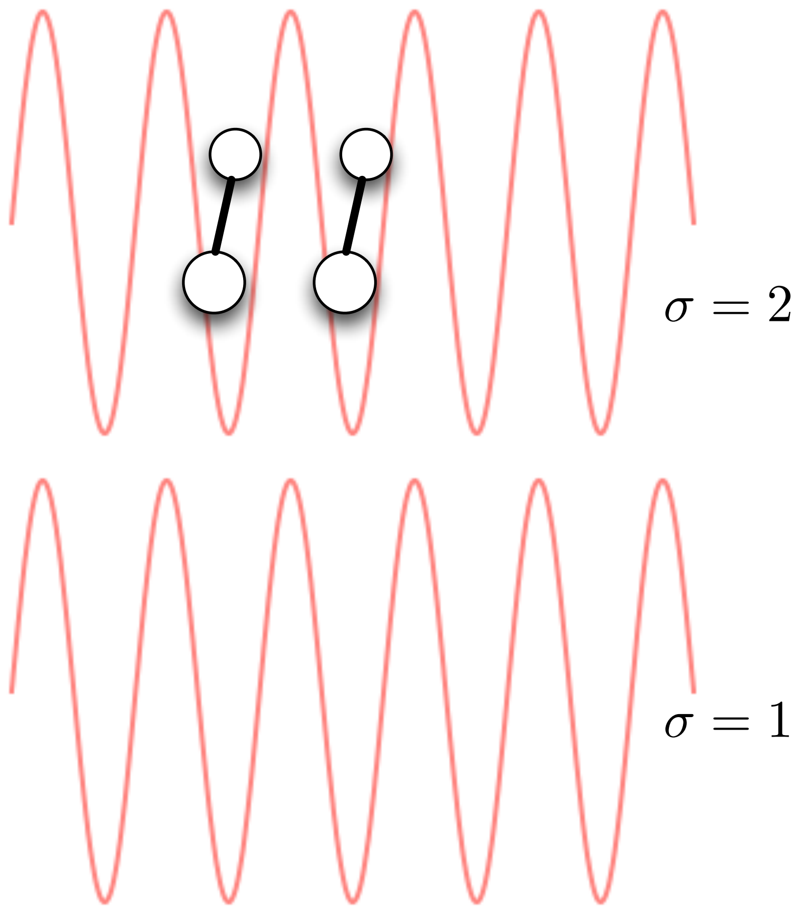


Quasi-1D, 2 internal states
r, distance
σ, internal state

Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma'_2\sigma'_1}$

Many-body case studies

	$^6Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^6Li^{23}Na$
E_{DC}= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	2×10^{-5}
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	5×10^5
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	3×10^6
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	2×10^3
E_{DC}= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	5×10^{-4}
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	2×10^3
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	1.2×10^5
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114

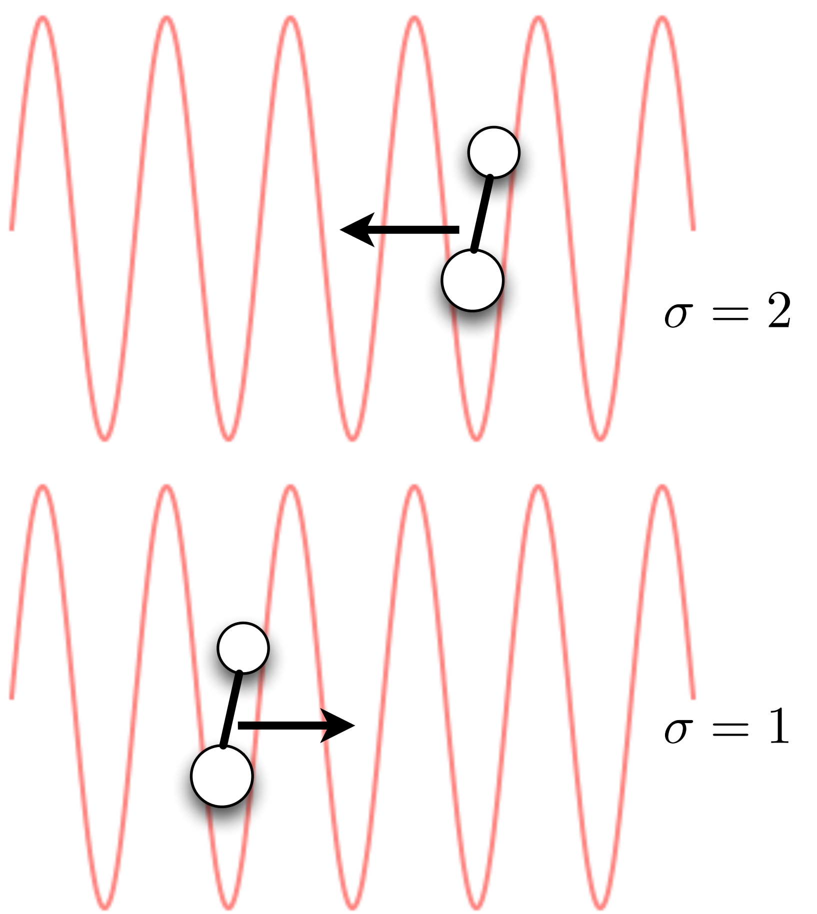


Quasi-1D, 2 internal states
r, distance
σ, internal state

Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma_2'\sigma_1'}$

Many-body case studies

	$^{6}Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^{6}Li^{23}Na$
E_{DC}= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	2×10^{-5}
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	5×10^{5}
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	3×10^{6}
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	2×10^{3}
E_{DC}= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	5×10^{-4}
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	2×10^{3}
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	1.2×10^{5}
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114

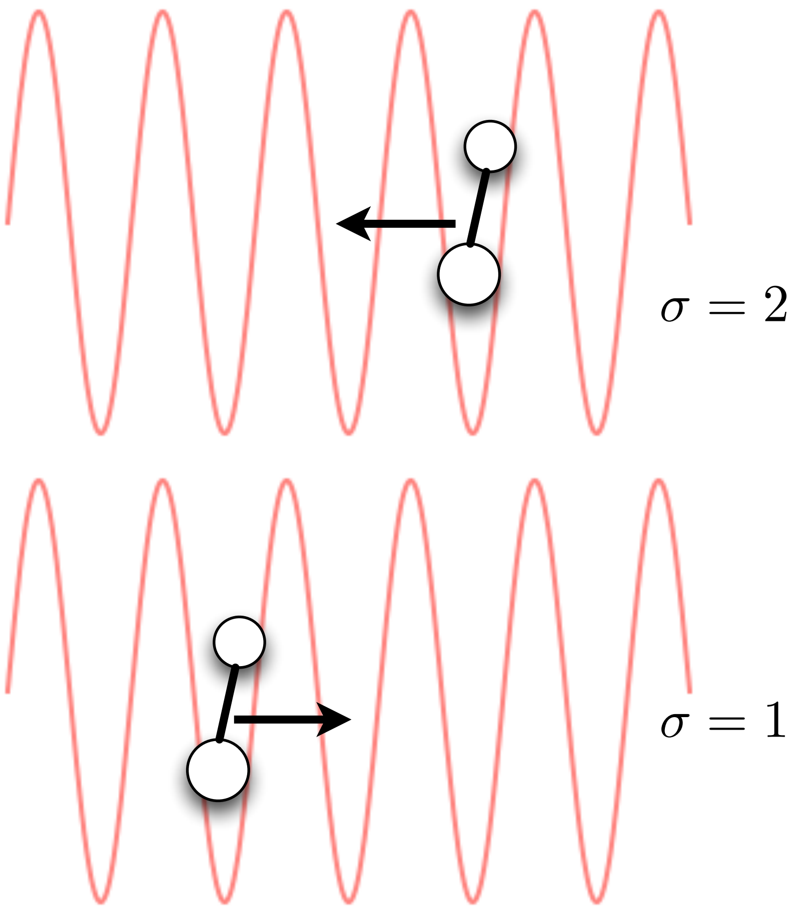


Quasi-1D, 2 internal states
r, distance
σ, internal state

Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma_2'\sigma_1'}$

Many-body case studies

	^{6}Li^{133}Cs	^{23}Na^{40}K	^{87}Rb^{133}Cs	^{40}K^{87}Rb	^{6}Li^{23}Na
$E_{\rm DC}$= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	2×10^{-5}
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	5×10^5
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	3×10^6
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	2×10^3
$E_{\rm DC}$= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	5×10^{-4}
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	2×10^3
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	1.2×10^5
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114

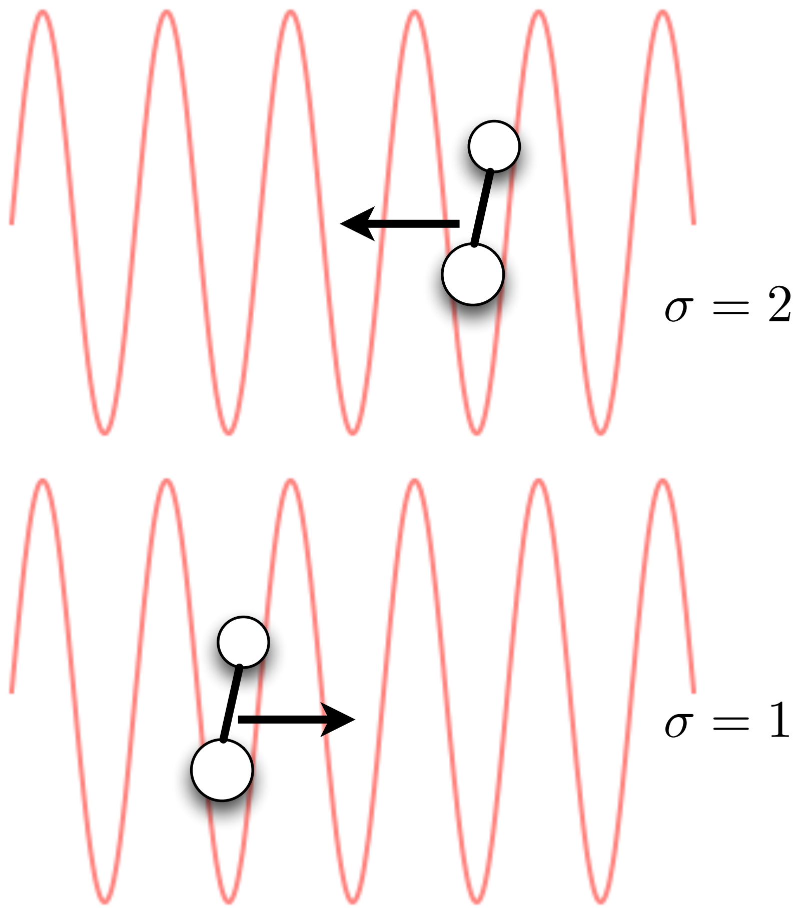


Quasi-1D, 2 internal states
r, distance
σ, internal state

Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma_2'\sigma_1'}$

Many-body case studies

	^{6}Li^{133}Cs	^{23}Na^{40}K	^{87}Rb^{133}Cs	^{40}K^{87}Rb	^{6}Li^{23}Na
E_{DC}= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	2×10^{-5}
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	5×10^{5}
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	3×10^{6}
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	2×10^{3}
E_{DC}= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	5×10^{-4}
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	2×10^{3}
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	1.2×10^{5}
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114

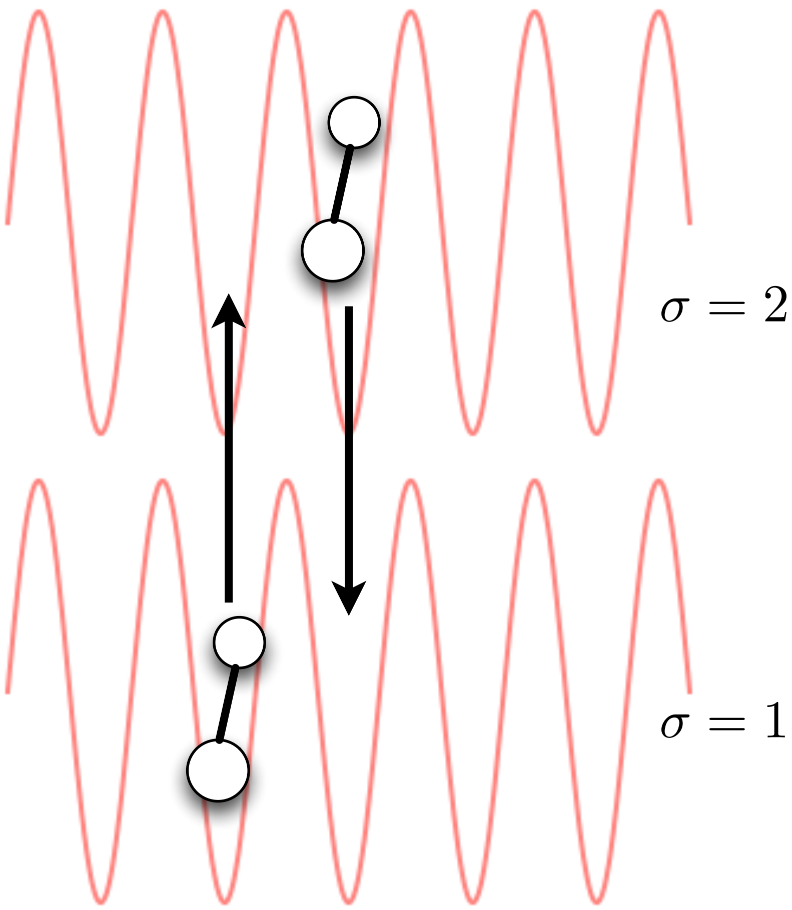


Quasi-1D, 2 internal states
r, distance
σ, internal state

Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma_2'\sigma_1'}$

Many-body case studies

	$^6Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^6Li^{23}Na$
E_{DC}= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	2×10^{-5}
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	5×10^5
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	3×10^6
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	2×10^3
E_{DC}= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	5×10^{-4}
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	2×10^3
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	1.2×10^5
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114

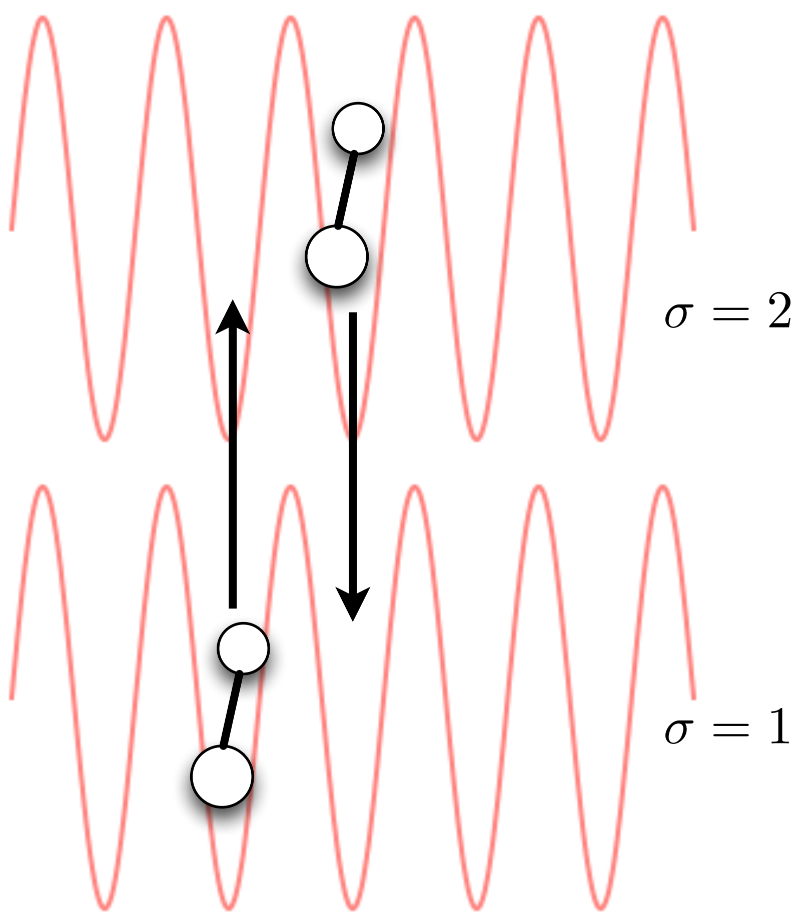


Quasi-1D, 2 internal states
r, distance
σ, internal state

Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma_2'\sigma_1'}$

Many-body case studies

	$^6Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^6Li^{23}Na$
E_{DC}= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	2×10^{-5}
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	5×10^5
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	3×10^6
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	2×10^3
E_{DC}= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	5×10^{-4}
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	2×10^3
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	1.2×10^5
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114

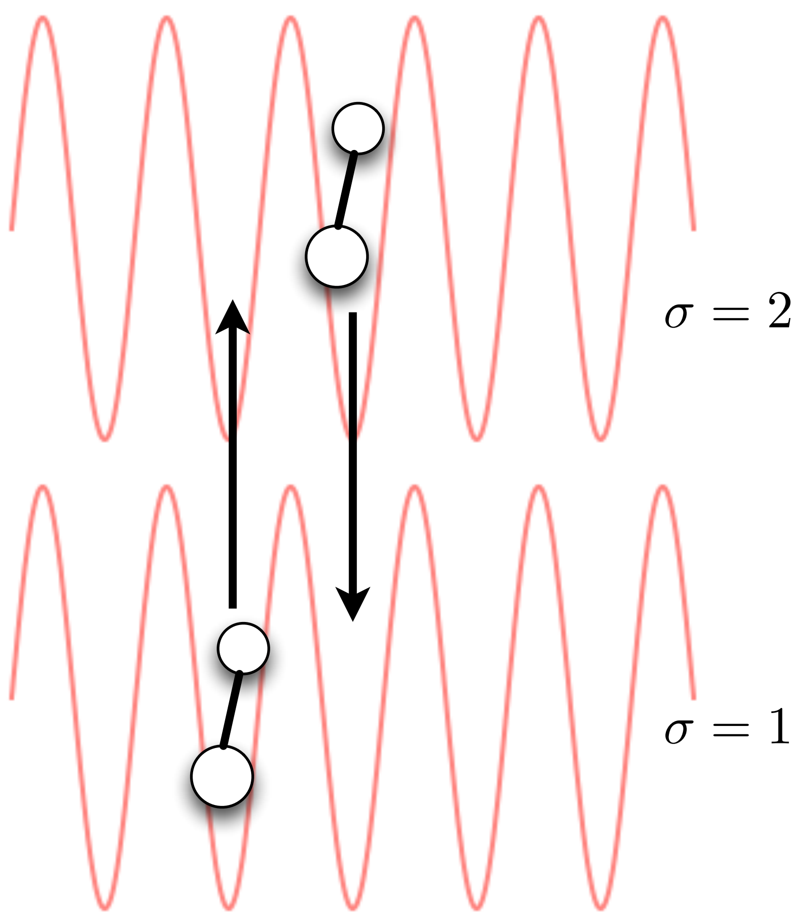


Quasi-1D, 2 internal states
r, distance
σ, internal state

Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma_2'\sigma_1'}$

Many-body case studies

	$^6Li^{133}Cs$	$^{23}Na^{40}K$	$^{87}Rb^{133}Cs$	$^{40}K^{87}Rb$	$^6Li^{23}Na$
E_{DC}= 1 kV/cm					
$U_{1,11}$ (kHz)	0.70	0.218	0.253	0.002	2×10^{-5}
$U_{1,22}/U_{1,11}$	0.084	0.085	0.108	0.082	0.08
$U_{1,12}/U_{1,11}$	0.28	0.29	0.32	0.28	0.28
$t_{1,1}/U_{1,11}$	0.33	2.36	0.58	93.74	5×10^{5}
$t_{1,2}/U_{1,22}$	1.76	12.37	2.25	508.9	3×10^{6}
$E_{1,1212}/U_{1,11}$	7.93	6.05	0.99	20.97	2×10^{3}
E_{DC}= 5 kV/cm					
$U_{1,11}$ (kHz)	8.97	2.48	0.970	0.049	5×10^{-4}
$U_{1,22}/U_{1,11}$	0.14	0.16	0.35	0.11	0.08
$U_{1,12}/U_{1,11}$	0.38	0.40	0.59	0.32	0.28
$t_{1,1}/U_{1,11}$	0.026	0.20	0.15	5.13	2×10^{3}
$t_{1,2}/U_{1,22}$	0.068	0.48	0.14	19.75	1.2×10^{5}
$E_{1,1212}/U_{1,11}$	0.519	0.43	0.18	1.05	114



Quasi-1D, 2 internal states
r, distance
σ, internal state

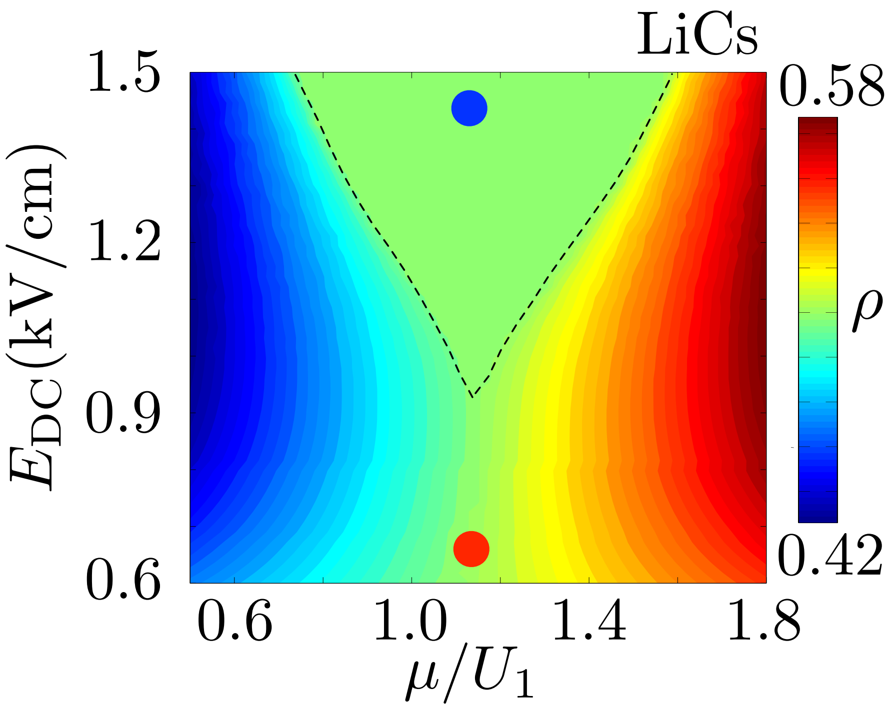
Tunneling
$t_{r,\sigma}$
Direct dipole-dipole interaction
$U_{r,\sigma\sigma'}$
Exchange dipole-dipole interaction
$E_{r,\sigma_1\sigma_2\sigma_2'\sigma_1'}$

Numerical Methods

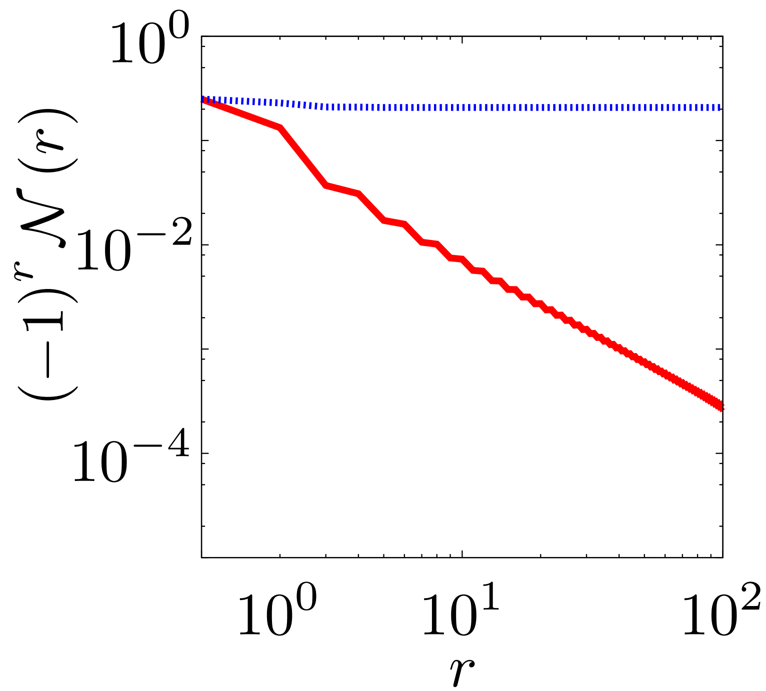
- Assume many-body state on infinite lattice has periodic structure
- Matrix product state ansatz for "unit cell"
- Recursive optimization of unit cell.
- Single convergence parameter; entanglement cutoff
- Straightforward extensions to long-range interactions
- Finite-system algorithms for excited states, time evolution

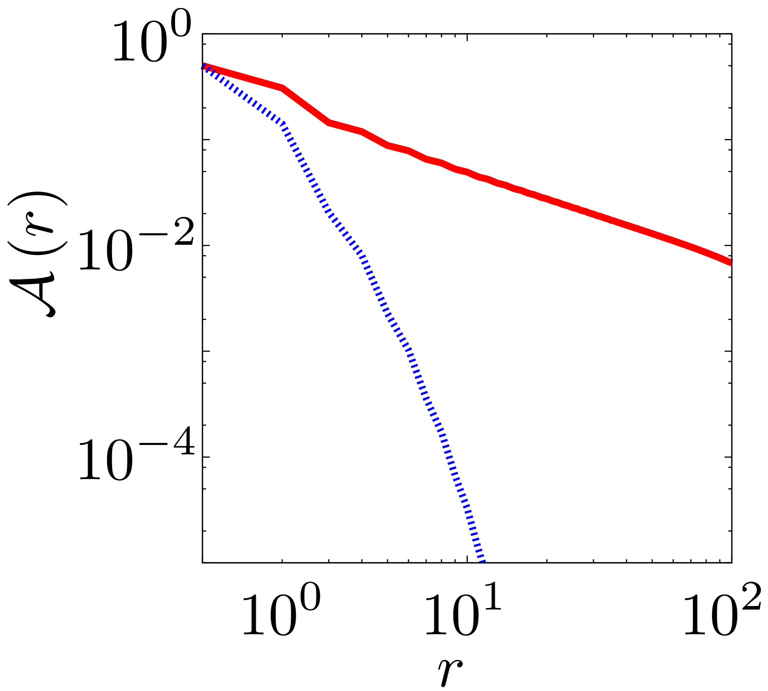
MLW and L.D.Carr NJP **14** 125015

Many-body case studies

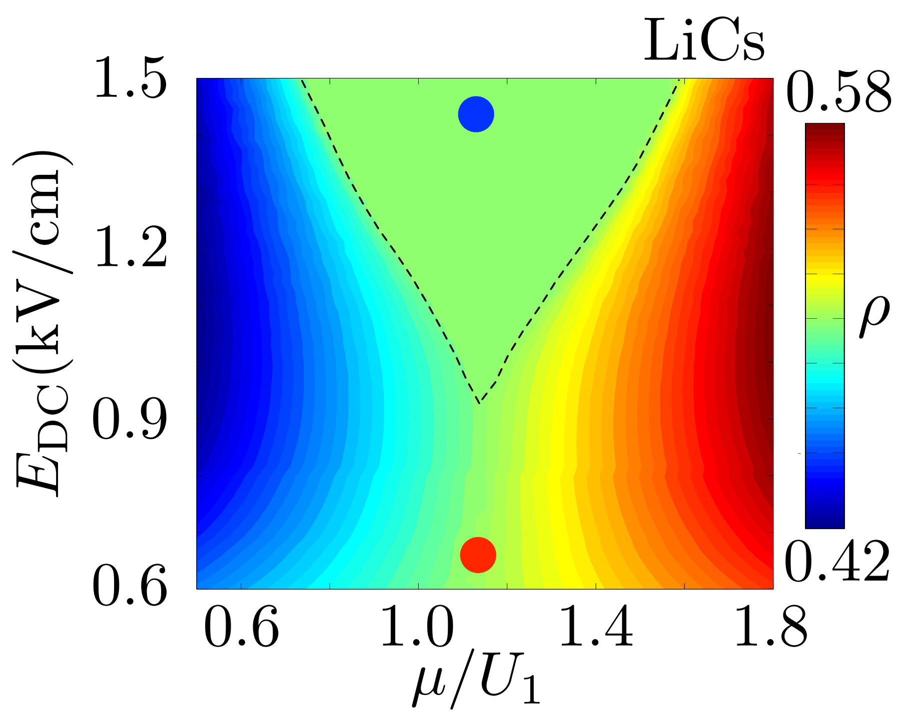


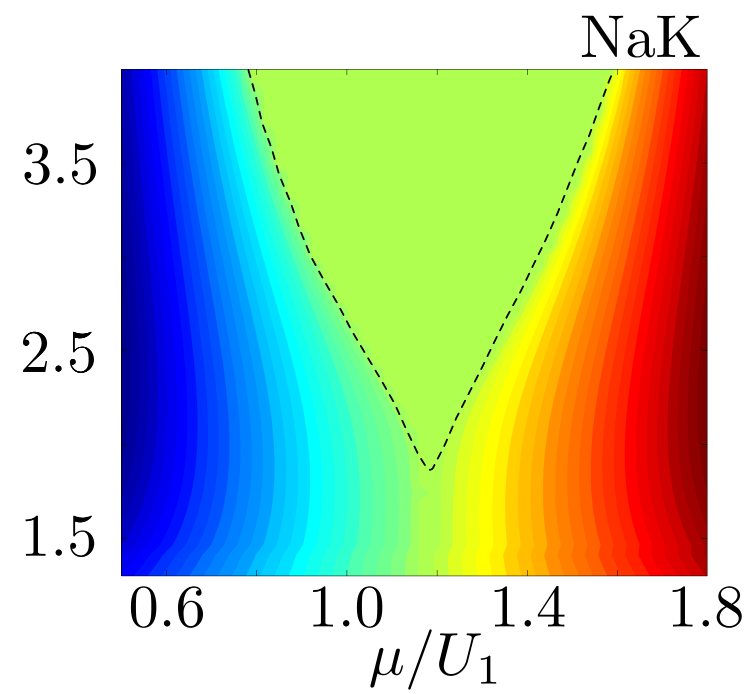
$$\mathcal{A}(r) = \langle \hat{a}_0^\dagger \hat{a}_r \rangle$$
$$\mathcal{N}(r) = \langle (\hat{n}_0 - \rho)(\hat{n}_r - \rho) \rangle$$



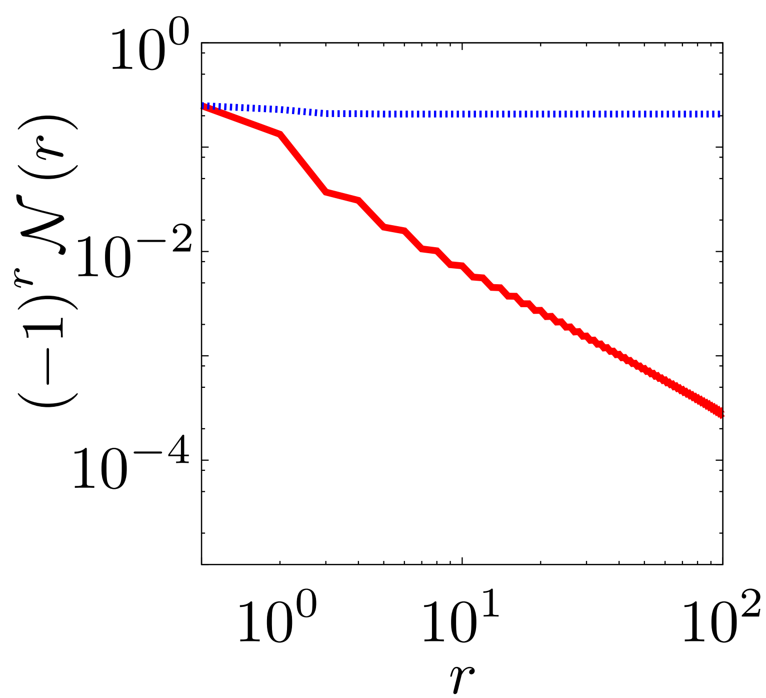


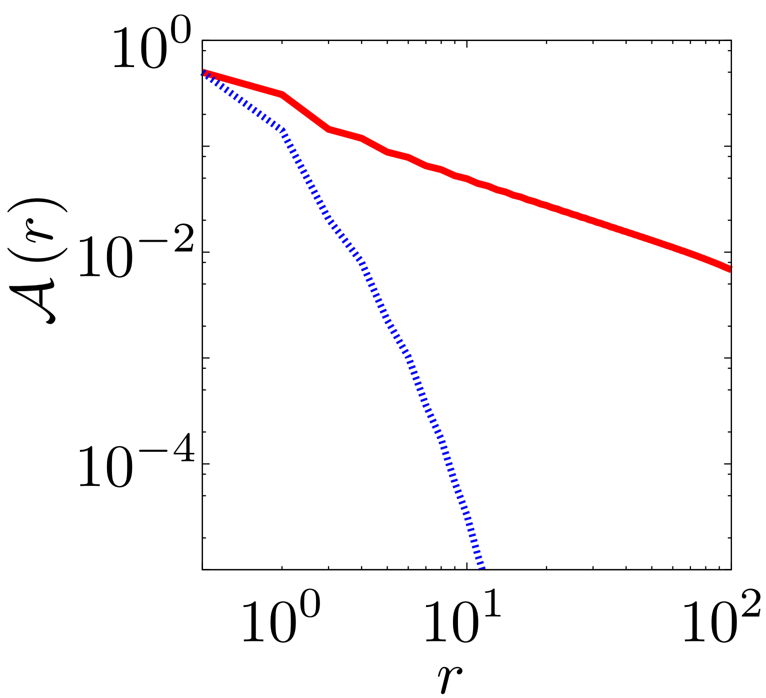
Many-body case studies



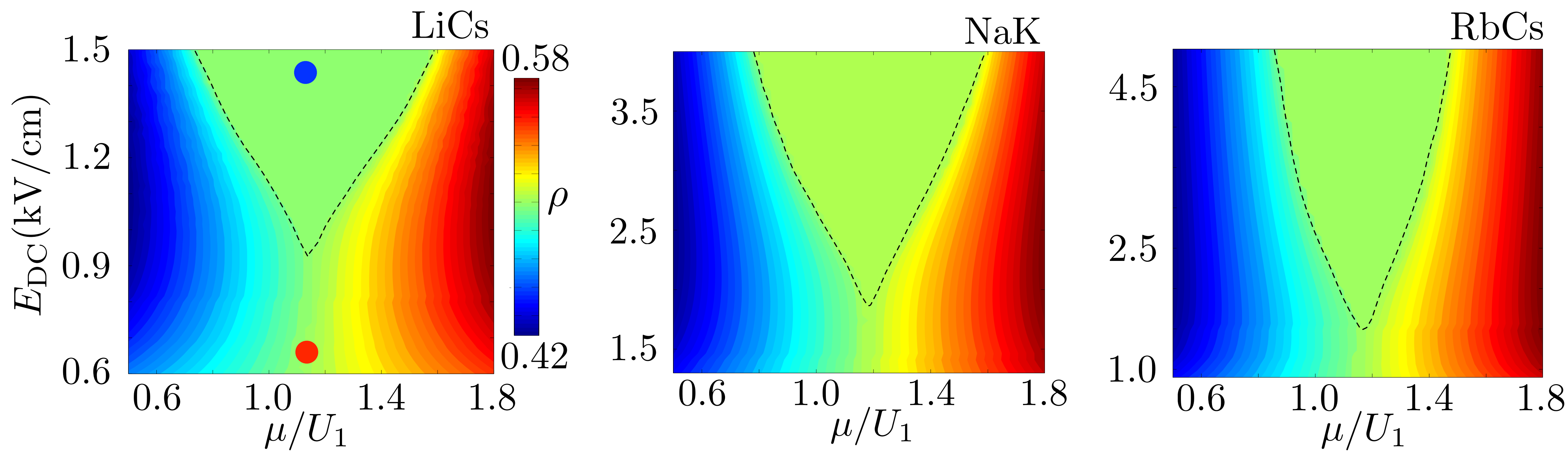


$$\mathcal{A}(r) = \langle \hat{a}_0^\dagger \hat{a}_r \rangle$$
$$\mathcal{N}(r) = \langle (\hat{n}_0 - \rho)(\hat{n}_r - \rho) \rangle$$

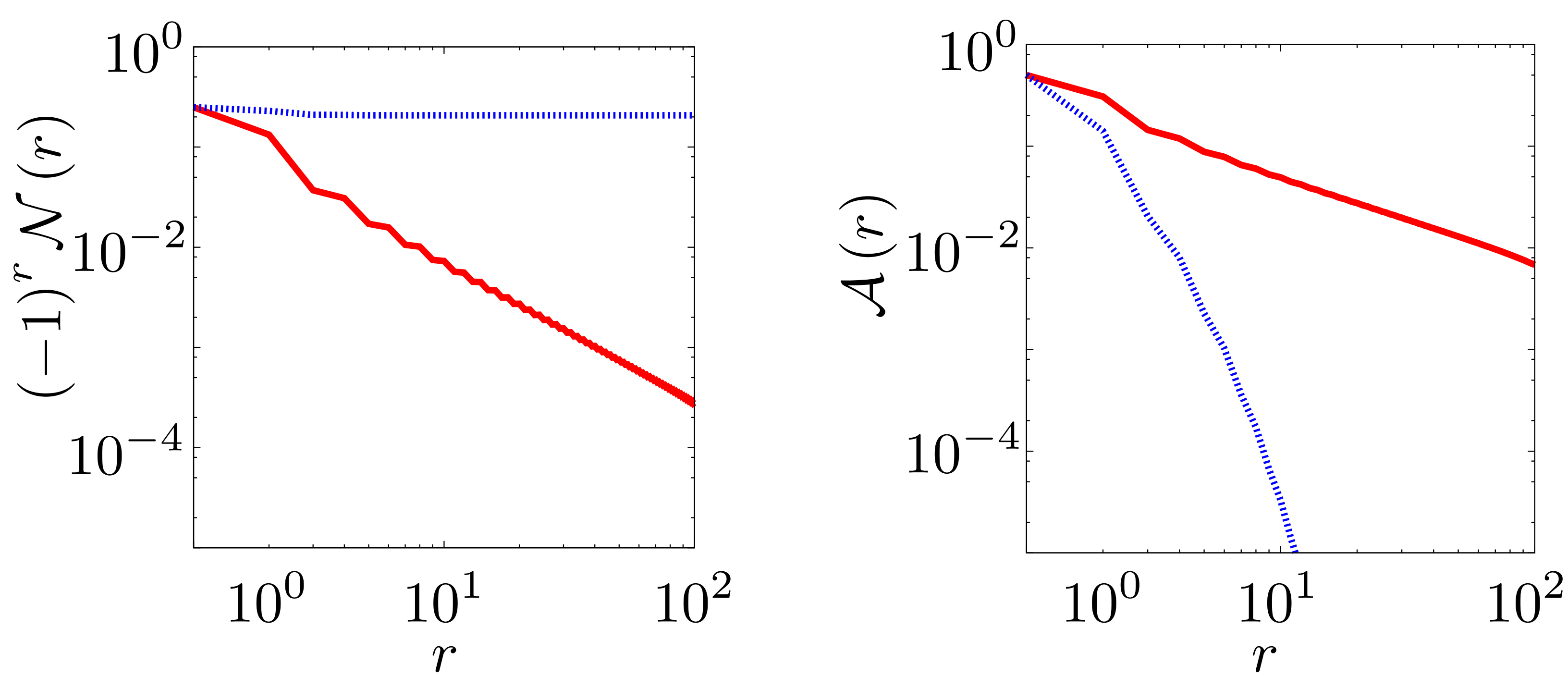




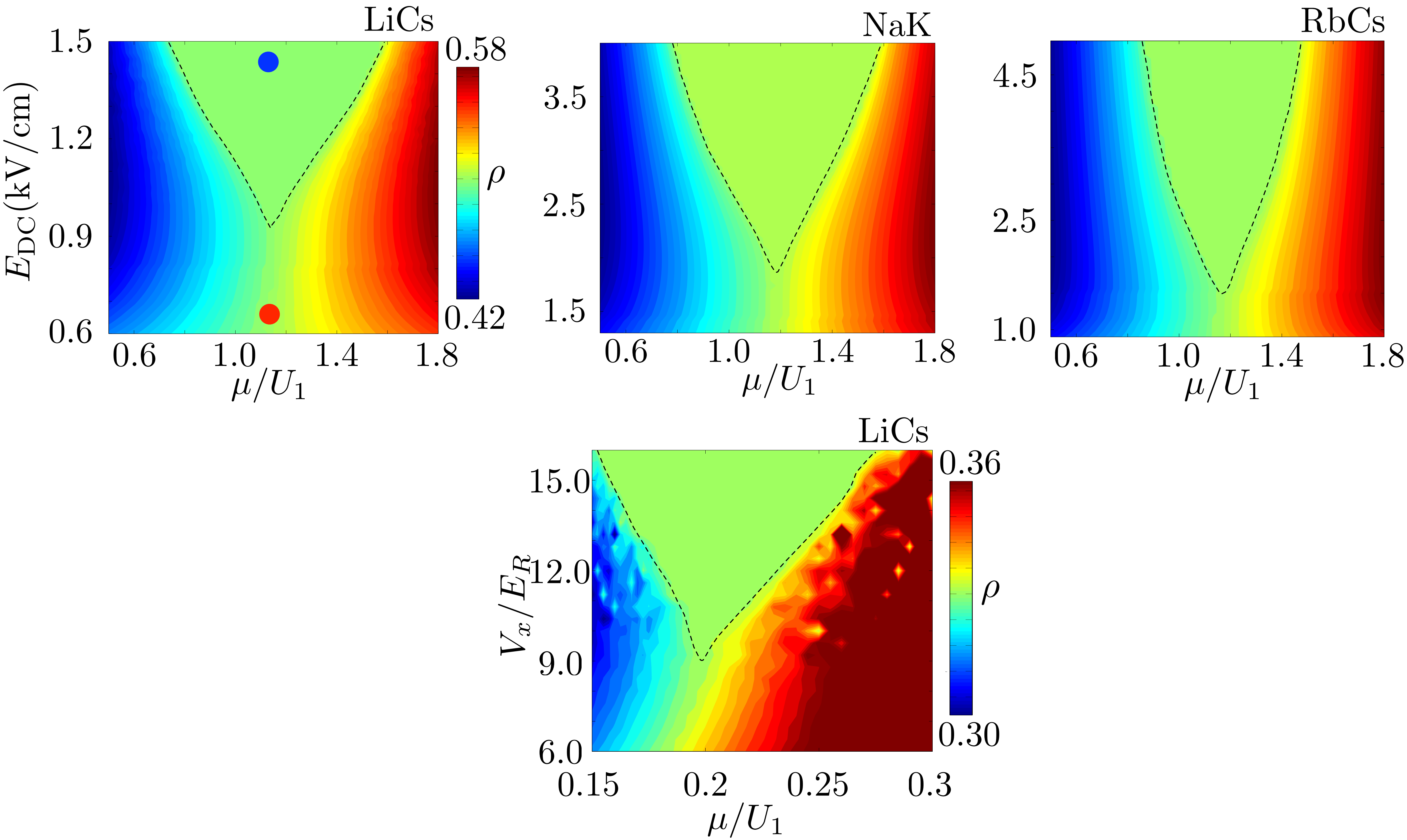
Many-body case studies



$$\mathcal{A}(r) = \langle \hat{a}_0^\dagger \hat{a}_r \rangle$$
$$\mathcal{N}(r) = \langle (\hat{n}_0 - \rho)(\hat{n}_r - \rho) \rangle$$



Many-body case studies



Summary

- Developed Molecular Hubbard Hamiltonian (MHH)
  - Treated $^1\Sigma$ case in detail, see also work of Gorshkov et al.
  - Different molecules access different regimes of MHH
- Wide array of experimental controls
  - Optical lattice intensity and polarization: tunneling and internal state character
  - Strength of DC field: ratio of direct and exchange dipolar interactions
  - AC field: number and timescale of internal states involved dynamically
  - B field: Coupling between hyperfine and rotation
  - Anisotropy in lattice confinement=> modified dipolar interactions
  - Species can also be considered an experimental control!
- New numerical many-body techniques
  - Able to handle long-range Hamiltonians, wide array of interactions
  - Used to explore phase diagrams of different molecules
  - Plan to open source code-contact us!

- MLW and L. D. Carr, New J. Phys. 11 055027 (2009)
- MLW and L. D. Carr Phys. Rev. A 82 013611 (2010)
- MLW, E. Bekaroglu, and L. D. Carr arxiv:1212.3042
- Confinement effects: MLW and L. D. Carr arxiv:1303.1230
- Algorithmic developments: MLW and L. D. Carr, New J. Phys. 14 125015 (2012)
- 4 posters in common room

Thank You!