Cold Atoms and Molecules: Condensed Matter Physics & Quantum Information

- introduction / review
- topics in more detail: “quantum simulators”
  - dissipative Hubbard dynamics
  - engineering three-body Hubbard Hamiltonians

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Collaborations:
Harvard, Yale, Oxford

\[ \text{EU networks} \]
quantum optics

- trapped ions

- cavity QED: atom - photon interfaces

|Ψ⟩ ~ |01⟩ – |10⟩
probalistic generation of EPR state

quantum info

- quantum computing: logic network

- building a network

qubits quantum gates read out

atom 1 atom 2 fiber

channel
node

quantum repeater
quantum optics

• atoms in an optical lattices

polar molecule in electronic and vibrational ground state

• polar molecules

rotation

electric dipole moment

cond mat & quantum info

• “quantum simulators” for cond mat models

2- & 3-body interactions
ring exchange...

- Hubbard & spin models
- analog vs. digital quantum simulations

• measurement based quantum computing

• topological phases and qc (?)

(analog vs. digital quantum simulators)
This talk ...

- Dissipative dynamics of atoms in optical lattices
  - immersion in a superfluid as a “phonon bath”
  - ... as quantum optics problem
  - quantum reservoir engineering


- Hubbard, spin models (with polar molecules)
  - short review of ideas and models
  - three-body interactions

\[
H = -J \sum_{\langle ij \rangle} b_i^+ b_j + \frac{1}{2} \sum_{i \neq j} V_{ij} n_i n_j + \frac{1}{6!} \sum_{i \neq j \neq k} W_{ijk} n_i n_j n_k.
\]

hopping  
\textit{tunable} two-body interaction  
\textit{strong repulsive} off-site three-body interaction

H.P. Büchler, A. Micheli, PZ, preprint

compare: string net
Fidkowski et al., cond-mat/0610583
Dissipative dynamics of cold atoms in optical lattices

- quantum optics with cold atoms
Cold atoms in optical lattices:

1. Coherent Hubbard dynamics

- Loading bosonic or fermionic atoms into optical lattices
- Atomic Hubbard models with controllable parameters
  - bose / fermi in 1,2&3D
  - spin models
  - “AMO Hubbard toolbox”

\[ \hat{H} = - \sum_{\alpha \neq \beta} J_{\alpha\beta} \hat{a}_{\alpha}^\dagger \hat{a}_{\beta} + \frac{1}{2} U \sum_{\alpha} \hat{a}_{\alpha}^\dagger \hat{a}_{\alpha}^\dagger \hat{a}_{\alpha} \hat{a}_{\alpha} \]

“(analog) quantum simulators”

optical lattice as array of microtraps

band structure (1D)

onsite interaction
tunneling

nonresonant laser

AC Stark shift

atomic Hubbard models:
kinetic energy: hopping
interaction: onsite repulsion

Jaksch et al. PRL 1998
AMO Hubbard toolbox

- time dependence
- 1D, 2D & 3D

- various lattice configurations

- create effective magnetic fields

\[ J_{\alpha\beta} \rightarrow J_{\alpha\beta} e^{i e \int_{\alpha} A \cdot d\vec{l}} \]

- spin-dependent lattices

\[ J_{\uparrow\uparrow} \neq J_{\downarrow\downarrow} \]

- laser induced hoppings

D. Jaksch & PZ, Annals of Physics 2005
Why? … condensed matter physics & quantum information

- condensed matter systems
  - strongly correlated systems
  - time dependence, e.g. quantum phase transitions
  - ...
  - exotic quantum phases(?)

- quantum information
  - new quantum computing scenarios, e.g. one way quantum computing

  analog & digital quantum simulators

- experiments [Bloch et al. 2001, Esslinger, Porto, Grimm & Denschlag …]
2. Dissipative Hubbard dynamics

- **BEC as a “phonon reservoir”**
  - quantum reservoir engineering

- **master equation:**
  \[
  \frac{d}{dt} \hat{\rho} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \mathcal{L} \hat{\rho}
  \]

- **coherent Hubbard dynamics**

  \[
  H = \ldots
  \]

  ✓ two band Hubbard model (1D)
  ✓ + Raman coupling

- **dissipative dynamics**

  \[
  \mathcal{L} \rho = \sum_k \frac{\Gamma_k}{2} \left( 2c_k \hat{\rho} c_k^\dagger - c_k^\dagger c_k \hat{\rho} - \hat{\rho} c_k^\dagger c_k \right)
  \]

  ✓ validity (as in quantum optics)
  ✓ interband transitions
  ✓ RWA + Born + Markov

- **1D model**

- **quantum jump operator**

- **does not see the optical lattice**

- **competing dynamics**

A. Griessner et al. PRL 2006; NJP 2007
2. Dissipative Hubbard dynamics

- BEC as a “phonon reservoir”
  - quantum reservoir engineering

- master equation:
  \[
  \frac{d}{dt} \hat{\rho} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \mathcal{L} \hat{\rho}
  \]

as opposed to ...

- Caldeira-Leggett
  - linear system-bath couplings, ohmic / superohmic
  - quantum phase transitions in Josephson Junction arrays
- polarons
- phonon mediated interactions
Why (controlled dissipation)?

- why? engineering reservoirs for ...
  - dissipative quantum phase transitions / crossover
  - ...
  - applications: cooling etc.

- Anderson (1987): ground state = resonating valence bond state

High-Tc superconductors

Minimal model: two-dimensional one-band Hubbard model

\[
\hat{H} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_i
\]

\[
\frac{d}{dt} \hat{\rho} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \mathcal{L} \hat{\rho}
\]

Competing dynamics

Binding energy 4% of width of Bloch band

(Units of hopping t)
“think quantum optics”

- driven two-level atom + spontaneous emission
- trapped atom in a BEC reservoir
- laser assisted atom + BEC collision
- reservoir: vacuum modes of the radiation field (T=0)
- reservoir: Bogoliubov excitations of the BEC (@ temperature T)
- optical pumping, laser cooling, ...
  - purification of electronic, and motional states
    \[ \rho_a \otimes |\text{vac}\rangle \langle \text{vac}| \rightarrow |\psi_a\rangle \langle \psi_a| \otimes \rho' \]
Models ...

- **Model A: Dark state cooling in a Bloch band** ("dark state laser cooling")
  - single atom
  - N non-interacting atoms + adiabiatic turn on off interactions

- **Model B: Master equations N interacting atoms**

\[
\frac{d}{dt} \hat{\rho} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \mathcal{L} \hat{\rho}
\]

Hubbardology

Hubbard dynamics (superfluid / Mott)

quantum reservoir engineering

coupling to a local current drives system into N-body dark state

\[
|\psi_{\text{BEC}}\rangle = \frac{1}{\sqrt{N!}} \left( \sum_i a_i^\dagger \right)^N |\text{vac}\rangle
\]

competing dynamics
Subrecoil ("dark state") laser cooling

Raman subrecoil cooling (Kasevich and Chu)  (see also: VSCPT Cohen et al.)

step 1: excitation & filtering

step 2: diffusion

- "dark state" laser cooling: accumulate atoms near $q \approx 0$
Levy statistics approach (Cohen-Tannoudji et al.)

- excitation profile and trapping region

Excitation profile:

\[ R(q) \sim |q|^{\lambda} \]

\( \lambda = 2 \) square pulse

\( \lambda = 4 \) Blackman pulse

- time evolution

Trapping times

\[ P(\tau) \sim \tau^{-(1+1/\lambda)} \]

\[ \langle \tau \rangle \rightarrow \infty \quad (\lambda > 1) \]

\[ T(N) = \sum_{i=1}^{N} \tau_i \sim N^\lambda \]

Return times

\[ \hat{T}(N) = \sum_{i=1}^{N} \hat{\tau}_i \sim N \langle \tau \rangle \]

generalized central limit theorem
iff $\lambda > 1$, then all atoms for $\Theta = T(N) + \hat{T}(N) \to \infty$ in cooling region

\[ R(q) \sim |q|^\lambda \]

\[ \frac{1}{2} k_B T = \frac{\delta q^2}{2m} \sim \Theta^{-2/\lambda} \]

\[ n_0(\Theta) \sim \Theta^{1/\lambda} \]
Raman cooling within a Bloch band: qualitative

- step 1: (coherent) quasimomentum selective excitation

\[ \Omega \ll |J^1| \]

Note: relevant energy scale given by \(|J^1|\)

Laser: square pulse sequence

\[ P(q) = \frac{\Omega^2}{(\delta^2_{q+\delta q} + \Omega^2)} \sin^2 \left( \sqrt{\delta^2_{q+\delta q} + \Omega^2} \frac{\tau}{2} \right) \]

- requirements: \( \Omega \ll 8|J^1| \)

Note: relevant energy scale given by \(|J^1|\)
Raman cooling within a Bloch band: qualitative

- step 1: (coherent) quasimomentum selective excitation

- step 2: (dissipative) decay to ground band
Model: 1. Coherent dynamics

- 1D lattice

\[ \hat{H}_0 = \sum_{q, \alpha} \varepsilon_q^\alpha (\hat{A}_q^\alpha)^\dagger \hat{A}_q^\alpha + (\omega - \delta) \sum_q (\hat{A}_q^1)^\dagger \hat{A}_q^1 + \frac{\Omega}{2} \sum_q [(\hat{A}_q^1)^\dagger \hat{A}_q^0 - \delta_q + \text{h.c.}] \]

\[ \varepsilon_q^\alpha = -2J^\alpha \cos(qd) \]

- Hamiltonian

\[ \hat{H}_I = \frac{1}{2M} \sum_{q_1, q_2, q_3, \alpha} U^{\alpha\beta} \left( \hat{A}_{q_1}^\beta \right)^\dagger \left( \hat{A}_{q_2}^\alpha \right)^\dagger \hat{A}_{q_3}^\alpha \hat{A}_{q_1+q_2-q_3}^\beta \]

validity: \( J^\alpha, U^{\alpha,\beta'}, \Omega \ll \omega, \omega \ll \omega_\perp \)
Model: 2. “Spontaneous Emission”

- BEC reservoir

\[ \hat{H}_{\text{BEC}} = E_0 + \sum_{\mathbf{k} \neq 0} \varepsilon(\mathbf{k}) \hat{b}^\dagger \mathbf{k} \hat{b}_\mathbf{k} \]

- interaction: interband 0 - 1

\[ \hat{H}_{\text{int}} = g_{ab} \int \hat{\psi}^\dagger_a(\mathbf{r}) \hat{\psi}_a(\mathbf{r}) \hat{\psi}_b(\mathbf{r}) \hat{\psi}^\dagger_b(\mathbf{r}) \, d^3\mathbf{r} \]

\[ \approx g_{ab} \sum_{\mathbf{k}} S(\mathbf{k}, \omega)^{1/2} \langle w_1 | e^{i \mathbf{k} \cdot \mathbf{r}} | w_0 \rangle \hat{b}_\mathbf{k} |1\rangle \langle 0 | + \text{h.c.} \]

“spontaneous emission”

\[ \varepsilon_k = [c^2(\hbar k)^2 + (\hbar k)^4/(2m_b)^2]^{1/2} \]

\[ \hat{\psi}_b = \sqrt{\rho_0 + \delta \hat{\psi}_b} \]

\[ \delta \hat{\psi}_b = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \left( u_k \hat{b}_\mathbf{k} e^{i \mathbf{k} \cdot \mathbf{r}} + v_k \hat{b}^\dagger_\mathbf{k} e^{-i \mathbf{k} \cdot \mathbf{r}} \right) \]

Bogoliubov

\[ \approx 1 \]

\[ S(\mathbf{k}) = (u_k + v_k)^2 = \frac{|\mathbf{k}|^2}{2m_b E_k} \]

spectrum of Bogoliubov excitations
“Spontaneous Emission”

- interband transitions spontaneous emission rate
  - typical numbers
    \[ \Gamma = 2\pi \times 1.1 \text{ KHz} \]
    weak coupling
  - tunability
    \[ \Gamma \sim \rho_0 a_s^2 \sqrt{\omega} \]

- spectrum of Bogoliubov excitations

- scattering length: magnetic or optical Feshbach resonance
- density

- scattering length
- density

- weak coupling

- trap frequency

- typical numbers
  - scattering length
  - density

- weak coupling

- trap frequency
• interaction: intraband ...

\[ \varepsilon_{q\approx 0}^0 = \varepsilon_{q'}^0 + c|k| \]

\[ q = q' + k \]

forbidden if \[ J^0 < \frac{\sqrt{\mu \omega R m a/(2m_b)}}{\pi} \]

✓ no heating / cooling due to intraband transitions
✓ we ignore intraband processes in the following
✓ Rem.: validity of master equation ...

We can cool to temperatures lower than the BEC
Master equation

- In analogy with spontaneous emission \((k_B T \ll \hbar \omega\), i.e. \(T = 0\))

\[
\mathcal{L} \hat{\rho} = \sum_k \frac{\Gamma_k}{2} \left( 2c_k \hat{c}_k^\dagger - c_k^\dagger c_k \hat{\rho} - \hat{\rho} c_k^\dagger c_k \right)
\]

1D momentum along lattice axis

\(|k| \leq k_{\text{max}} = \sqrt{2m_b \omega}\)

- Spontaneous emission rate \(\Gamma = \sum_k \Gamma_k\)

\[
\frac{d\Gamma}{dk} = \frac{L}{2\pi} \Gamma_k = \frac{g_{ab}^2 \rho_b m_a a_0^2 k^2}{4\pi} e^{-a_0^2 k^2 / 2}
\]

\[
\Gamma = \frac{g_{ab}^2 \rho_b m_b}{2\pi a_0} \left[ \sqrt{\frac{m_b}{m_a}} e^{-\frac{m_b}{m_a}} - \sqrt{\frac{\pi}{2}} \text{erf} \left( \sqrt{\frac{m_b}{m_a}} \right) \right]
\]

1. \(k_{\text{max}} \gg \pi / d\), no superradiance
2. \(k_{\text{max}} < \pi / d\), superradiance
Results: single atoms

- Ground state $q=0$ momentum peak $4J^0 \ll k_B T \ll \omega$.
- Quantum trajectory simulation of the master equation

Laser: square pulse sequence

![Graph showing temperature relation](image)

Temperature: $k_B T = 2J^0(\Delta q)^2$

Dark state occupation: $n^0(q=0)$

- Typical temperatures $k_B T / 4J^0 \sim 2 \times 10^{-3}$ in $t_f J^0 \sim 50$
- Analysis in terms of Levy flights
Many (non-interacting) bosons

- Assume: we can switch off interaction between bosons $a_{aa} \rightarrow 0$ with Feshbach resonance; independent bosons
- Ground state cooling: $q = 0$ peak in momentum distribution
- Numerical analysis: Quantum Boltzmann master equation

\[
\dot{w}_m = \sum_{k,q} \Gamma_k \left[ m^0_{q-k} (1 \pm m^1_{q}) w_{m'} - m^1_{q} (1 \pm m^0_{q-k}) w_m \right]
\]

occupation of momentum state $q$ in Bloch band

QBME is a rate equation for $w_m \equiv \langle m | \rho | m \rangle$, i.e. classical configurations $w_m$ of atoms occupying momentum states $m = \{m^0_q\}_q, \{m^1_q\}_q$ in the two Bloch bands.

Temperature:

Dark state occupation: $n^0(|qd|<0.06)$

- Bosonic enhancement of cooling
Many fermions

- Many spin-polarized (non-interacting) fermions
- Ground state: filled Fermi sea

Typical temperatures $k_B T / 4J^0 \sim 10^{-2}$ in $t_f J^0 \sim 500$

- Slowing down due to Pauli blocking
Strongly correlated systems, and many body dark states (?)

- above scheme works well for (essentially) non-interacting systems
- strongly correlated systems
  - cooling $N$ atoms with $U=0$ (tune scattering length $a=0$)
  - turn $U$ on adiabatically to obtain a strongly correlated state

A. Griessner et al. PRL 2006; NJP 2007

- many-body dark states ?
Atoms & Ions
• cold atoms in optical lattices
• trapped ions / Wigner crystals
• CQED
• atomic ensembles

Polar Molecules
• ... in electronic & vibrational ground state
• what’s new? ... electric dipole moment
  – couple rotation to DC / AC microwave fields
  – strong dipole-dipole / long range couplings
• ... in addition what we do with cold atoms

Questions:
• motivation? ... coming experiments
• new physics?
Polar molecules

Background material:
Preparation of polar molecules in ground state

- Techniques are being developed for ...
  - trapping and cooling
  - generation: photoassociation & buffergas cooling

exp: all cold atom labs
exp: Demille, Doyle, Mejer, Rempe, Ye …

Mott insulator: atoms to molecules

photoassociation: 100% efficient 😊

heteronuclear molecule with strong persistent dipole moment in electronic groundstate.

\[ \text{Sr}^{2+}\text{O}^{2–} \quad \text{... ionic binding} \]

**Sr2+O2−** ... ionic binding

\[ \text{Sr}^{2+} \quad \text{O}^{2–} \]

**X \, 1\Sigma^+** ... electronic groundstate:

S=0 ... closed shell \((..9\sigma^2 \, 10\sigma^2 \, 4\pi^4)\)

\[ r_{eq} = 1.919 \, \text{Å} \quad \text{... equilibirum distance} \]

\[ d = 8.900 \, \text{D} \quad \text{... dipole-moment} \]

\[ \omega_{eq} = 19.586 \, \text{THz} \quad \text{... vibrational const.} \]

\[ B_{eq} = 10.145 \, \text{GHz} \quad \text{... rotational} \]

l=0 ... no nuclear momenta for \(^{88}\text{SrO}, \, ^{86}\text{SrO}\)

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l=0 ... no nuclear momenta for \(^{88}\text{SrO}, \, ^{86}\text{SrO}\)
CaF - rotational, fine and hyperfine structure

\[ X \ ^2\Sigma_{1/2} \ldots \ el. \ groundstate: \]

- \( S = \frac{1}{2} \) ... from open (Ca-)shell
- \( I = \frac{1}{2} \) ... nuclear momentum (of F)
- \( r_{eq} = 1.951 \ \text{Å} \) ... eq. distance
- \( \mu_0 = 3.077 \ \text{D} \) ... dipole-moment

\[ \text{el.spin..} \ S \]

\[ \text{N.. orb.ang.mom.} \]

\[ \text{F–} \]

\[ \text{Ca}^{2+} \]

\[ \text{e–} \]

\[ \text{strong coupling} \]

\[ \text{electric dipole moment} \]

- talks to optical radiation: electronic excitations
  (like an alkali atom)

- talks to microwave radiation: rotational excitations
  (alkali atom: hyperfine / magnetic)

\[ \text{weak couplings :-(} \]
Single polar molecule I: Rotational spectroscopy

1) Rigid Rotor:

\[ H = B N^2 \]

\( \chi^1 \Sigma_g^+ \)  closed shell molecules  
(SrO, CsRb, …)

\( \text{Sr}^{2+} - \text{O}^{2-} \)

- anharmonic spectrum  \( E_N = B N(N+1) \)
- electric dipole transitions  \( d \sim 3-10 \text{ Debye} \)
  - microwave transition frequencies
- no spontaneous emission  \( \Gamma < 0.1 \text{ mHz} \)
  - excited states are "useable"
- encode qubit

\( \text{charge qubit} \)

\( 2B \sim 20 \text{GHz} \)

\( 4B \sim 40 \text{GHz} \)
2) Spin Rotation Coupling

\[ H = B N^2 + \gamma N \cdot S \]

- for \( e^- \) providing spin degree of freedom
  - encode qubit in rot. ground states
- strong spin-rotational mixing in \( N>0 \)
  - Raman transitions
- for nuclear degree of freedom
  - magnetic trapping, clock states, ...

\( \frac{1}{2} \Sigma_g^+ \) molecules with an unpaired electron spin (CaF, CaCl, ...)
Two polar molecules: dipole – dipole interaction

- dipole moment gives rise to interaction of two 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
- strong! (temperature requirements)
Adiabatic potentials for two (unpolarized) polar molecules

- Rotor

\[ V_{dd}(R) \]

\[ R_B = \left( \frac{\mu^2}{3B} \right)^{1/3} \]

\[ V_{\text{eff}}(R) = -\frac{C_6}{R^6} \]

\[ C_6 = \frac{\mu^4}{6B} \]

\( \sim 30-60 \text{ nm} \)
Effective Spin-Spin Interactions: qualitative picture

- effective spin-spin coupling: microwave drive + dipole-dipole

Integrating out high energy excitations gives an effective low energy Hamiltonian, we can engineer spin-Hamiltonian

\[ H = g \sum_{i \neq j} \sigma^{(i)}_\alpha A^{\alpha\beta}(\vec{x}_i, \vec{x}_j) \sigma^{(j)}_\beta \]
Overview:

Condensed matter and quantum information with cold polar molecules
Condensed matter aspects

- Spin toolbox with cold molecules in optical lattices

\[ H_{\text{spin}} = J_\perp \sum_{x-\text{lks}} \sigma_x^i \sigma_x^j + J_\perp \sum_{y-\text{lks}} \sigma_y^i \sigma_y^j + J_z \sum_{z-\text{lks}} \sigma_z^i \sigma_z^j \]

Kitaev model

A. Micheli, G. Brennen, PZ, Nature Physics 2006

- Extended Hubbard models in 1D and 2D in optical lattices

\[ H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{1}{2} \sum_{i \neq j} U_{ij} n_i n_j + \frac{1}{6!} \sum_{i \neq j \neq k} W_{ijk} n_i n_j n_k. \]

hopping \hspace{1cm} \textit{tunable} two-body interaction \hspace{1cm} \textit{strong repulsive} off-site three-body interaction

compare: string net

Fidkowski et al., cond-mat/0610583

H.P. Büchler, A. Micheli, PZ, preprint
Self-assembled “dipolar crystals” with cold polar molecules

**dipolar crystal:**
- induced & aligned dipoles

**Quantum melting**
- appearance of a crystalline phase
- quantum melting to a superfluid phase

• Self-assembled “dipolar crystals” with cold polar molecules

**dipolar crystal:**

induced & aligned dipoles

\[
\frac{d^2_{\text{ind}}}{R^3}
\]

E-field


**applications:**

atoms in dipolar lattices: Hubbard models + phonons

\[\psi_{1,2}\]

G. Pupillo, M. Ortner et al., work in progress

quantum information:
- memory
- ion-trap type quantum computing

\[\sim 100 \text{ nm}\]
Quantum information

- AMO - solid state interfaces: hybrid quantum processors
  - solid state quantum processor
  - molecular quantum memory

- Remark: trapping and cooling / read out of molecules close to / via strip line

P.Rabl, D. DeMille, J. Doyle, M. Lukin, R. Schoelkopf and PZ, PRL 2006
Three-body interactions & extended Hubbard models

- how to ...
  - generate strong three-body interactions while switching off two-body terms

- extended Hubbard models in 1D and 2D
  - with tunable two body interactions & repulsive three-body
  - phases: example 1D hard core bosons with repulsive three-body terms

H.P. Büchler, A. Micheli, PZ, preprint
Dynamics with n-body interactions

• Hamiltonians of condensed matter physics are effective Hamiltonians, obtained by integrating out the high energy excitations

\[ H = \sum_i \left( \frac{p_i^2}{2m} + V_T(r_i) \right) + V_{\text{eff}}(\{r_i\}) \]

effective interaction

\[ V_{\text{eff}}(\{r_i\}) = \frac{1}{2} \sum_{i \neq j} V(r_i - r_j) + \frac{1}{6} \sum_{i \neq j \neq k} W(r_i, r_j, r_k) + \ldots \]

two particle interaction

three particle interaction
effective interaction

• Hamiltonians with three-body interactions
  - ground states with exotic phases & excitations (topological, spin liquids etc.)
  - difficult to find examples in nature (Fractional Quantum Hall Effect, ... AMO?)

We start in the continuum and add the optical lattice later
Dynamics with n-body interactions

- Hamiltonians of condensed matter physics are effective Hamiltonians, obtained by integrating out the high energy excitations

\[
H = \sum_i \left( \frac{p_i^2}{2m} + V_T(r_i) \right) + V_{\text{eff}}(\{r_i\})
\]

**effective interaction**

\[
V_{\text{eff}}(\{r_i\}) = \frac{1}{2} \sum_{i \neq j} V(r_i - r_j) + \frac{1}{6} \sum_{i \neq j \neq k} W(r_i, r_j, r_k) + \ldots
\]

**two particle interaction**

**three particle interaction**

**strong & repulsive**

- Cold gases of atoms and molecules
  - we know the high energy degrees of freedom & manipulate by external fields
  - Q.: switch off two-body, while generating strong repulsive three-body (?)

... with polar molecules dressed by external fields
(without introducing decoherence)
Hubbard models with three-body interactions

- Rem.: Typical Hubbard models with polar molecules involve strong dipole-dipole (two-body) offsite interactions

- Extended Hubbard models in 1D and 2D

\[ H = -J \sum_{\langle ij \rangle} b_i^{\dagger} b_j + \frac{1}{2} \sum_{i \neq j} U_{ij} n_i n_j + \frac{1}{6!} \sum_{i \neq j \neq k} W_{ijk} n_i n_j n_k. \]

- strong three-body interaction
  \[ W/J \sim 0...30 \]
  \[ J \sim 0.1 E_r \]

- tunable two-body interaction
  \[ U/J \sim -300 ... 300 \]
Hubbard models with three-body interactions

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- Extended Hubbard models in 1D and 2D

\[ H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{1}{2} \sum_{i \neq j} U_{ij} n_i n_j + \frac{1}{6!} \sum_{i \neq j \neq k} W_{ijk} n_i n_j n_k \]

hopping energy  two-body interaction  three-body interaction

+ small next-nearest neighbor interactions

- Rem.: effective higher-order interactions are also obtained from a Hubbard models in J/U-perturbation theory ...

  - example: tJ-model
  - however, these effective interactions are necessarily small
How to calculate effective n-body interactions ... basic idea

- **Step 1:** “dressed” single polar molecule
  
  We dress molecules prepared in the ground state by adiabatically switching on AC / DC electric fields.

- **Step 2:** interaction between molecules
  
  For fixed positions of the molecules we adiabatically switch on dipole-dipole interactions.

We identify the interaction energy

\[ V_{\text{eff}} \left( \{ \mathbf{r}_i \} \right) = \frac{1}{2} \sum_{i \neq j} V (\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{6} \sum_{i \neq j \neq k} W(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \ldots \]

... with the interaction potential in the spirit of a Born-Oppenheimer approximation.

Our goal is now (i) to choose a molecular setup and (ii) calculate the BO potential.
Step 1: Single molecule as an effective spin-1/2

- Single molecule as a “spin-1/2 in an effective magnetic field”

Two-level System

- in rotating frame / RWA

\[ H_0^{(i)} = \frac{1}{2} \begin{pmatrix} \Delta & \Omega \\ \Omega & -\Delta \end{pmatrix} = \hbar S_i \]

- dressed eigenstates

\[ |+\rangle_i = \alpha |g\rangle_i + \beta |e, 1\rangle_i \]
\[ |-\rangle_i = -\beta |g\rangle_i + \alpha |e, 1\rangle_i \]

and energies

\[ E_\pm = \pm \sqrt{\Omega^2 + \Delta^2 / 2} \]

- adiabatically turning on AC field

\[ |g\rangle_i \rightarrow |+\rangle_i \quad (\text{for } \Delta > 0) \]

rotation spectrum:

microwave field + static electric field

- induced static dipole moments due to the static electric field
Details ...

• rotational spectrum in AC & DC field
• DC field

- induced static dipole moments due to the static electric field
Convenient mapping: (fixed) molecules to (fixed) spin-1/2

- **Single molecule**
  
  ![Single molecule diagram]

  \[ H^{(i)}_{\text{rot}} = B N_i^2 - d_i E(t) \]

- **Spin-1/2 in magnetic field**
  
  ![Spin-1/2 in magnetic field diagram]

  \[ H^{(i)}_0 = \hbar S_i \]

- **Interacting (fixed) molecules**
  
  ![Interacting molecules diagram]

  \[ V_{\text{d-d}}(r_{ij}) \]

- **Interacting (fixed) spins**
  
  ![Interacting spins diagram]

  \[ \text{spin-spin} \]

Our goal is to calculate the energy for fixed \( \{r_i\} \), i.e. the Born-Oppenheimer potential \( V_{\text{eff}}(\{r_i\}) \). This is conveniently done in the spin-picture.
Step 2: Interactions

- Ensemble of (static) molecules as interacting spins in magnetic field

Dipole-dipole interaction
- in rotating frame / RWA

\[ H = \sum_i \hbar S_i + \sum_{i \neq j} D \left[ (\cdots)(S_i^x S_j^x + S_i^y S_j^y) - (\cdots)S_i^z S_j^z + (\cdots)S_i^z S_j^z \right] \]

XXZ- model in a magnetic field

- Paramagnetic phase \( \hbar >> D/a^3 \) or \( D/(a^3|\hbar|) = (R_0/a)^3 << 1 \)
  weakly interacting regime:
  interaction potential in perturbation theory

- Provided \( |r_i - r_j| > R_0 \) we can calculate the interaction energy perturbatively
Interaction energy (= Born Oppenheimer potential)

Interaction energy

(i) diagonalizing the internal Hamiltonian for fixed interparticle distance \( \{ r_i \} \).

\[
\sum_i H_0^{(i)} + H_{\text{int}}^{\text{stat}} + H_{\text{int}}^{\text{ex}}
\]

(ii) The eigenenergies \( E(\{ r_i \}) \) describe the Born-Oppenheimer potential a given state manifold.

(iii) Perturbation theory to calculate the interaction energy

\[
\Pi_i |+\rangle_i \rightarrow |G\rangle
\]

\[
E^{(1)}(\{ r_i \}) = \ldots \quad \text{valid for:}
\]

\[
E^{(2)}(\{ r_i \}) = \ldots \quad |r_i - r_j| > R_0
\]

\[
\frac{D}{\sqrt{\Delta^2 + \Omega^2}} = R_0^3 < a^3
\]

"weak" dipole interaction for ...

Condon point

\( \Delta/\omega \)

\( \Omega \)

\( |e;e\rangle \)

\( |g;e\rangle_+ \)

\( |g;e\rangle_- \)

\( |g;g\rangle \)
Extended Hubbard model

- Hamiltonian:

\[ H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{1}{2} \sum_{i \neq j} U_{ij} n_i n_j + \frac{1}{6!} \sum_{i \neq j \neq k} W_{ijk} n_i n_j n_k. \]

- two-body interaction

\[ U_{ij} = U_0 \frac{a^3}{|R_i - R_j|^3} + U_1 \frac{a^6}{|R_i - R_j|^6}. \]

\[ U_0 = \lambda_1 D/a^3 \quad \text{repulsive} \]

\[ \text{tunable} \]

- three-body interaction

\[ W_{ijk} = W_0 \left[ \frac{a^6}{|R_i - R_j|^3 |R_i - R_k|^3} + \text{perm} \right]. \]

\[ \text{repulsive} \]

- hard core onsite condition ... \( a_0 \ll R_0 \ll \lambda/2 \)
1D hard core Boson with three-body

\[ H = -J \sum_i \left[ b_i^{\dagger} b_{i+1} + b_{i+1}^{\dagger} b_i \right] + W \sum_i n_{i-1} n_i n_{i+1} \]

**Bosonization**
- hard-core bosons
- instabilities for densities:
  \( n = 2/3 \quad n = 1/2 \quad n = 1/3 \)
- quantum Monte Carlo simulations (in progress)

**Critical phase**
- algebraic correlations
- compressible
- repulsive fermions

**Solid phases**
- excitation gap
- incompressible
- density-density correlations

\[ \langle \Delta n_i \Delta n_j \rangle \]
- hopping correlations (1D VBS)

\[ \langle b_i^{\dagger} b_{i+1}^{\dagger} b_j b_{j+1} \rangle \]