Hubbard Models with Molecules in Optical Lattices: Engineering three-body interactions

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Atomic and molecular gases

Bose-Einstein condensation
- Gross-Pitaevskii equation
- non-linear dynamics

Quantum degenerate dilute atomic/molecular gases of fermions and bosons

Rotating condensates
- vortices
- fractional quantum Hall

Molecules
- Feshbach resonances
- BCS-BEC crossover
- polar molecules

Optical lattices
- Hubbard models
- strong correlations
- exotic phases

control and tunability
Crystalline phases
- long range dipole-dipole interaction
- interaction energy exceeds kinetic energy

Three-body interaction
- tunable three-body interaction
- extended Hubbard models in the presence of optical lattices
Polar molecules

Why polar molecules?
- coupling to optical and microwave fields
  - trapping/cooling
  - internal states
- permanent dipole moment
  - strong dipole-dipole interaction
  - long-range interaction

Polar molecules in 2D
- stability for strong interactions
  - suppressed three-body recombination
  - absence of thermodynamic instabilities
  - tunable long range interaction in strength and shape
  - tool for exploring novel quantum phenomena

Quantum melting
- appearance of a crystalline phase
- quantum melting to a superfluid phase
Experimental status

- Polar molecules in the rotational and vibrational ground state
- Cooling and trapping techniques being development:
  
  - Cooling of polar molecules:
    D. De Mille, Yale
    J. Doyle, Harvard
    G. Rempe, Munich
    G. Meijer, Berlin

  - Photo association
    (all cold atom labs)

- Bosonic molecules with closed electronic shell, e.g., SrO, RbCs, LiCs
Polar molecule

Low energy description
- rigid rotor in an electric field

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

- \( N_i \): angular momentum
- \( d_i \): dipole operator

\[ N = 2 \quad BN_i(N_i + 1) \]

\[ N = 1 \quad \sim 20\text{GHz} \]

\( N = 0 \)

Accessible via microwave
- anharmonic spectrum
- electric dipole transition

\[ \Delta N = \pm 1 \quad \Delta m_z = -1, 0, 1 \]
- microwave transition frequencies
- no spontaneous emission
heteronuclear molecule with strong persistent dipole moment in electronic groundstate.

Sr\(^{2+}\)O\(^{2-}\) ... ionic binding

\(r_{eq} = 1.919 \, \text{Å} \) ... equilibrium distance
\(d = 8.900 \, \text{D} \) ... dipole-moment

\(\omega_{eq} = 19.586 \, \text{THz} \) ... vibrational const.

\(B_{eq} = 10.145 \, \text{GHz} \) ... rotational

\(I = 0 \) ... no nuclear momenta for \(^{88}\text{SrO}, \, ^{86}\text{SrO}\)
Interaction between polar molecules

Hamiltonian

\[ H^{(1,2)} = \sum_{i=1}^{2} \left[ \frac{p_i^2}{2m} + V_{\text{trap}}(r_i) + B N_i^2 - d_i E \right] + \frac{d_1 d_2 - 3(d_1 n)(d_2 n)}{r^3} \]

- kinetic energy
- trapping potential
- rigid rotor
- electric field
- interaction potential

Without external drive

- van der Waals attraction
  \[ V_{\text{vdW}}(r) = -\frac{C_6}{r^6} \]

Static electric field

- internal Hamilton
  \[ H_{\text{rot}}^{(i)} = B N_i^2 - d_i E \]

- finite averaged dipole moment
  \[ D = \left| \langle g|\hat{d}_i|g \rangle \right|^2 \leq d^2 \]
Dipole-dipole interaction

- anisotropic interaction
- long-range

\[ V(r) = D \left[ \frac{1}{r^3} - 3 \frac{z^2}{r^5} \right] \]

- Born-Oppenheimer
  valid for:
  \[ r > R_{\text{rot}} = (D/B)^{1/3} \]
  \[ r > (Ed/D)^{1/3} \]

Instability in the many-body system

- collaps of the system for increasing dipole interaction
- roton softening
- supersolids?
  (Goral et. al. ‘02, L. Santos et al. ‘03, Shlyapnikov ‘06)

Stability:

- strong interactions
- confining into 2D by an optical lattice
Stability via transverse confining

Effective interaction

- interaction potential with transverse trapping potential

\[ V(r) = D \left[ \frac{1}{r^3} - 3 \frac{z^2}{r^5} \right] + \frac{m\omega_z^2}{2} z^2 \]

- characteristic length scale

\[ l_\perp = \left( \frac{Dm}{\hbar^2 a_\perp} \right)^{1/5} a_\perp \]

- potential barrier: larger than kinetic energy

Tunneling rate:

- semi-classical rate (instanton techniques)

\[ \Gamma = A \exp \left( - \frac{S_E}{\hbar} \right) \]

- Euclidean action of the instanton trajectory

\[ S_E = \hbar \left( \frac{Dm}{\hbar^2 a_\perp} \right)^{2/5} C \]

numerical factor: \( C \approx 5.8 \)

kinetic energies

bound states

attempt frequency
Transverse trapping

- integrating out the fast transverse motion of the molecules

\[ V_{\text{eff}}(\mathbf{R}_i - \mathbf{R}_j) = \int dz_i dz_j V(\mathbf{r}_i - \mathbf{r}_j) |\psi(z_i)|^2 |\psi(z_j)|^2 \]

transverse wave function

\[ \psi(z) = \frac{1}{(\pi a_{\perp}^{1/4})} \exp \left( -\frac{z^2}{2a_{\perp}^2} \right) \]

Effective 2D potential

- large distances \( |\mathbf{R}| > l_{\perp} \)

\[ V_{\text{eff}}(\mathbf{R}) = \frac{D}{R^3} \]
Crystalline phase
Hamiltonian

- polar molecules confined into a two-dimensional plane
- dipole interaction

Effective Hamiltonian

\[ H_{\text{eff}} = \sum_i \frac{P_i^2}{2m} + \frac{D}{2} \sum_{i \neq j} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|^3} \]

interaction strength:
\[ r_s = \frac{E_{\text{int}}}{E_{\text{kin}}} = \frac{Dm}{\hbar^2 a} \]

Polar molecule: SrO

- dipole moment:
  \[ d \sim 9D \quad \text{(2.4 Debye \sim ea_0)} \]

- interparticle distance:
  \[ a \sim 300 - 500\text{nm} \]

- stability:
  \[ S_E/\hbar \gtrsim 130 \]

- transverse confining:
  \[ a_\perp \sim 40\text{nm} \]
Quantum Phase transition

Kosterlitz-Thouless transition

First order melting (Kalida '81)

Crystal phase
- triangular lattice structure
- phonon modes

Strongly interacting superfluid
- superfluid stiffness
- large depletion

\[
\frac{T a^3}{D} = \frac{\pi \hbar^2}{2ma^2}
\]

\[
T_m
\]

instability at weak interactions

Quantum melting
- indication of a first order transition
- Quantum Monte Carlo simulations
Three-body interactions
Single polar molecule

Static electric field
- along the z-axes
- splitting the degeneracy of the first excited states
- induces finite dipole moments

\[ d_g = \langle g | d_z | g \rangle \]
\[ d_e = \langle e, 1 | d_z | e, 1 \rangle \]

Mircowave field
- coupling the state \( |g\rangle \) and \( |e, 1\rangle \)
- anharmonic spectrum
- electric dipole transition
- microwave transition frequencies
- no spontaneous emission

\[ \Delta N = \pm 1 \quad \Delta m_z = -1, 0, 1 \]
Many-body Hamiltonian

\[ H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_i V_{\text{trap}}(\mathbf{r}_i) + \sum_i H^{(i)}_0 + H^{\text{stat}}_{\text{int}} + H^{\text{ex}}_{\text{int}} \]

- external potentials:
  - trapping potential
  - optical lattices

- dipole-Dipole interaction
  - restriction to the two internal states:
    \[ |g\rangle_i \quad |e, 1\rangle_i \]

Two-level System

- rotating wave approximation

\[ H^{(i)}_0 = \frac{1}{2} \begin{pmatrix} \Delta & \Omega \\ \Omega & -\Delta \end{pmatrix} = \hbar S_i \]

- two-level system in an effective magnetic field

- two 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

\[ E_\pm = \pm \sqrt{\Omega^2 + \Delta^2 / 2} \]
Dipole-dipole interaction

Microwave photon exchange

- \( D = |\langle e, 1|d|g\rangle|^2 \approx d^2/3 \)

\[
H_{\text{int}}^{\text{ex}} = -\frac{1}{2} \sum_{i \neq j} \frac{D}{2} \nu(r_i - r_j) \left[ S_i^+ S_j^- + S_j^+ S_i^- \right]
\]

\( \nu(r) = \frac{1 - \cos \theta}{r^3} \)

Induced dipole moments

- \( \eta_{d,g} = d_{e,g}/\sqrt{D} \)

\[
H_{\text{int}}^{\text{stat}} = \frac{1}{2} \sum_{i \neq j} D \nu(r_i - r_j) \left[ \eta_g P_i + \eta_e Q_i \right] \left[ \eta_g P_j + \eta_e Q_j \right]
\]

\( P_i = |g\rangle\langle g|_i \)

\( Q_i = |e, 1\rangle\langle e, 1|_i \)
Effective interaction

(i) diagonalizing the internal Hamiltonian for fixed interparticle distance \( \{ \mathbf{r}_i \} \).

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

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

(iii) Adiabatically connected to the groundstate

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

“weak” dipole interaction

\[
\frac{D}{\sqrt{\Delta^2 + \Omega^2}} = R_0^3 \ll a^3
\]
Born-Oppenheimer potential

First order perturbation

\[ E^{(1)}(\{r_i\}) = \langle G | H_{\text{ex}} + H_{\text{stat}} | G' \rangle \]

\[ |G'\rangle = \prod_i (\alpha |g_i\rangle + \beta |e, 1\rangle_1) \]

\[ E^{(1)}(\{r_i\}) = \frac{1}{2} \lambda_1 \sum_{i \neq j} D\nu (r_i - r_j) \]

dipole-dipole interaction:

\[ V_{\text{eff}}(r) = \lambda_1 \frac{1 - 3 \cos \theta}{r^3} \]

Dimensionless coupling parameter

\[ \lambda_1 = (\alpha^2 \eta_g + \beta^2 \eta_e)^2 - \alpha^2 \beta^2 \]

- tunable by the external electric field \( dE/B \) and the ratio \( \Omega/\Delta \).

- for a magic rabi frequency the dipole-dipole interaction vanishes

\[ \lambda_1 = 0 \]
Second order perturbation

\[ E^{(2)}(\{r_i\}) = \sum_{k \neq i \neq j} \frac{|M|^2}{\sqrt{\Delta^2 + \Omega^2}} D^2 \nu (r_i - r_k) \nu (r_j - r_k) \]

\[ + \sum_{i \neq j} \frac{|N|^2}{\sqrt{\Delta^2 + \Omega^2}} [D \nu (r_i - r_j)]^2 \]

Matrix elements

- \( M = \alpha \beta \left[ (\alpha^2 \eta_g + \beta^2 \eta_e) (\eta_e - \eta_g) + (\beta^2 - \alpha^2)/2 \right] \)

- \( N = \alpha^2 \beta^2 \left[ (\eta_e - \eta_g)^2 + 1 \right] \)

- special point

\[ \lambda_1 = 0 \]
\[ M = 0 \]
Effective Hamiltonian

Effective interaction

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

- two-body interaction

\[ V(r) = \lambda_1 D \nu(r) + \lambda_2 DR_0^3 [\nu(r)]^2 \]

- three-body interaction

\[ W(r_1, r_2, r_3) = \gamma_2 R_0^3 D [\nu(r_{12})\nu(r_{13}) + \nu(r_{12})\nu(r_{23}) + \nu(r_{13})\nu(r_{23})] \]

- validity is restricted to

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

interparticle distance

(i) transverse confining into 2D

(ii) vanishing dipole-dipole interaction
Bose-Hubbard model
Optical lattices

- AC Stark shift
- off-resonant laser
- periodic potentials

\[ V(x) = V_0 \sin^2 kx + \ldots \]

- 2D and 1D setups
- different lattice structures

- characteristic energies

\[ E_r = \frac{\hbar^2 k^2}{2m} \sim 10\text{kHz} \]

\[ \frac{V_0}{E_r} \sim 50 \]
Microscopic Hamiltonian

\[ H = \int d\mathbf{x} \psi^\dagger(\mathbf{x}) \left( -\frac{\hbar^2}{2m} \Delta + V_{\text{trap}}(\mathbf{x}) \right) \psi(\mathbf{x}) + H_{\text{int}} \]

- strong optical lattice \( V > E_r \)
- express the bosonic field operator in terms of Wannier functions
- restriction to lowest Bloch band
  Jaksch et al, PRL (1998)

\[ \psi(\mathbf{x}) = \sum_i w(\mathbf{x} - \mathbf{x}_i) b_i \]
Hubbard model

Extended Bose-Hubbard models

- hardcore bosons

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

- hopping energy
- two-body interaction
- three-body interaction

- interaction parameters for strong optical lattices

\[ U_{ij} = V(R_i - R_j) \]
\[ W_{ijk} = W(R_i, R_j, R_k) \]

Polar molecule: LiCs:

- dipole moment
  \[ d \approx 6 \text{Debye} \]
- hopping energy
  \[ J/E_r \approx 0 - 0.5 \]
- lattice spacing:
  \[ \lambda \approx 1000 \text{nm} \]
  \[ E_r \approx 1.4 \text{kHz} \]
- nearest neighbor interaction:
  \[ U/E_r \approx 30 \]
  \[ W/E_r \approx 30 \left( \frac{R_0}{a_L} \right)^3 \]
Supersolids on a triangular lattice

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

\[ U_{ij} \sim \frac{1}{|i - j|^3} \quad : \text{static electric field} \]

\[ U_{ij} \sim \frac{1}{|i - j|^6} \quad : \text{static electric field} + \text{microwave field} \]

Quantum Monte Carlo simulations

Wessel and Troyer, PRL (2005)
Melko et al., PRB, (2006)

- supersolid close to half filling and strong nearest neighbor interactions
  \[ n = 1/2 \]
  \[ U/J \gtrsim 10 \]
- stable under next-nearest neighbor interactions
One-dimensional model

Bosonization
- hard-core bosons
- instabilities for densities:
  \[ n = \frac{2}{3} \quad n = \frac{1}{2} \quad n = \frac{1}{3} \]
- 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)
  \[ \langle b_i^\dagger b_{i+1}^\dagger b_j b_{j+1} \rangle \]
**String nets**

**Honeycomb lattice**
- Interaction Hamiltonian
\[
H_{\text{int}} = W \sum_{\langle\langle ijk \rangle\rangle} n_i n_j n_k + H_{\text{n.n.n.}}
\]
- Integer filling within a single layer
- Split the layer into a double layer
- Maps to an effective spin system
- Each well splits into a double well
- \( \cos \theta = 1/3 \)
- \( \uparrow \rangle \) and \( \downarrow \rangle \)

**Spin-Hamiltonian**
\[
H_{\text{spin}} = W \sum_{\langle\langle ijk \rangle\rangle} PS_{\text{tot}} = \pm 3/2
\]
- Penalizes three successive spins
- Allowed configurations are characterized by string nets (Fidkowski, et al, 2006)

**Next-nearest neighbor interactions?**
Conclusion and Outlook

Polar molecular crystal
- reduced three-body collisions
- strong coupling to cavity QED
- ideal quantum storage devices

Lattice structure
- alternative to optical lattices
- tunable lattice parameters
- strong phonon coupling: polarons

Extended Hubbard models
- strong nearest neighbor interaction
- three-body interaction

Novel quantum matter
- supersolid phases
- string nets?