Cold Polar Molecules and their Applications for Quantum Information

H.P. Büchler

Theoretische Physik III, Universität Stuttgart, Germany
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

Static electric field

- internal Hamilton

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

- finite averaged dipole moment

\[ D = |\langle g | d_i | g \rangle|^2 \leq d^2 \]

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

- integrating out the fast transverse motion of the molecules

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

Effective 2D potential

- integrating out the fast transverse motion of the molecules
- large distances \( |\mathbf{R}| > l_\perp \)

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

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

Hamiltonian

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

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

interaction strength:

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

Polar molecule: SrO

- dipole moment:

\[ \approx 4m \text{K} \quad (2.4 \text{ Debye} \sim e a_0) \]

\[ r_s \sim 121 \mu m / a \]

- interparticle distance:

\[ a \sim 100 - 300 \text{nm} \]

- stability:

\[ S_E / \hbar \gtrsim 130 \]

- transverse confining:

\[ a_\perp \sim 40 \text{nm} \]
Strong interactions

- leading order: only keep the interaction term
- describes purely classical problem
- minimization of energy: hexagonal lattice

\[ E_{\text{crystal}} = \sum_{i \neq j} V_D (R_i - R_j) = c N \frac{D}{a^3} \]

Lattice vibrations

- harmonic oscillations around equilibrium: phonon modes
- energy correction due to zero point fluctuations of the phonons
- lattice turns unstable to shear modes for weak transverse confining

\[ \gamma < \gamma_c \sim 3 \]

\[ E_{\text{phonon}} = \sum_{\lambda,k} \hbar \omega_{\lambda,k} / 2 = c \frac{1}{\sqrt{r_s}} \frac{D}{a^3} \]
Quantum Phase transition

Crystal phase
- triangular lattice structure
- phonon modes

Quantum melting
- indication of a first order transition
- Quantum Monte Carlo simulations

Kosterlitz-Thouless transition

Quantum melting (Kalida ’81)

Strongly interacting superfluid
- superfluid stiffness
- large depletion

instability at weak interactions
Microwave fields
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

\[ N = 0 \]
\[ N = 1 \] \( \sim 20\text{GHz} \)

Accessible via microwave
- anharmonic spectrum
- electric dipole transition
- microwave transition frequencies
- no spontaneous emission

\[ \Delta N = \pm 1 \quad \Delta m_z = -1, 0, 1 \]
**Microwave field**

- coupling the state $|1, 1\rangle$ and $|1, 1\rangle$

  : detuning
  : rabi frequency

- rotating wave approximation
- dressed states (rotating frame)

$$|\mp\rangle_i = \alpha |0, 0\rangle_i + \beta |1, 1\rangle_i$$

$$|\rangle_i = -\beta |0, 0\rangle_i + \alpha |1, 1\rangle_i$$
Interactions between atoms and molecules

- attractive van der Waals
  \[ V_{\text{vdw}}(r) = -\frac{C_6}{r^6} \]
- dipole-dipole interactions

- inelastic collisions
- three-body losses
- lifetime of trapped gases
- meta-stability of cold gases

- s-wave scattering:
  attractive/repulsive
- Feshbach resonances

- knowledge of elastic and inelastic scattering properties
- dilute gases
- “weak” interactions

Can we trick nature?

- “blue shield” for atoms
  (see Review by Weiner et al, RMP 1999)
Repulsive shield

- repulsive van der Waals interaction between polar molecules
- thermal activation
- quantum tunneling

- suppression of inelastic collisions
- large positive scattering length

$\tau_B \sim 10\text{nm}$

stable region

unstable region

repulsive barrier
Repulsive shield

Setup

- molecules prepared into the state: \( |+\rangle_i \)

- dipole moment along the z-axes
  \[
  d_z = \alpha^2 d_e + \beta^2 d_g
  \]
  \[
  V(r) = d_z^2 \frac{1 - 3 \cos^2 s \theta}{r^6}
  \]

- rotation dipole moment within the plane
  \( d_\perp = \alpha \beta d_c \)

\[
V(r) = -d_\perp^2 \frac{1 - 3 \cos^2 s \theta}{r^6}
\]

  time averaged

- cancelation of dipole-dipole interactions

- remaining van der Waals interaction: repulsive and tunable

rotating frame
Effective interaction

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

$$\sum_i H^{(i)}_0 + H_{\text{int}}^{\text{stat}} + H_{\text{int}}^{\text{ex}}$$

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

(iii) Adiabatically connected to the groundstate

$$|G\rangle = \Pi_i |+\rangle_i$$

Length scales:

$$r_B = (d^2 / B)^{1/3}$$

$$r_\Delta = (d^2 / \Delta)^{1/3}$$
Repulsive shield

Long distance behavior: \( r \gtrsim r_\Delta \gg r_B \)

- cancelation of dipole-dipole interaction

\[ d_\perp = d_z \]

- anisotropic van der Waals repulsion

\[
V_{\text{eff}}(r) = \frac{1}{r^6} \left[ C_6^{(0)} \left( 1 - 3 \cos^2 \theta \right)^2 + C_6^{(2)} 9 \sin^4 \theta \right]
\]

\[
C_6^{(0)} \approx C_6^{(2)} \approx \frac{d^4}{\Delta}
\]

- crossover for \( r_\Delta > r \gg r_B \)

\[
V_{\text{eff}}(r) = \frac{d_c^2 + d_g d_e \left[ 1 - 3 \cos^2 \theta \right]}{r^3}
\]

What are optimal parameters for highest possible shield?
Repulsive shield

Shorter distances \( r > r_B \)
- requires to take into account all internal states
- repulsive shield is limited by the first level crossing

Optimal parameters

\[
\frac{dE_{dc}}{B} = 1 \quad \text{: static electric field}
\]

\[
\Delta = 0.015B \quad \text{: detuning}
\]

\[
\frac{\Omega}{\Delta} \approx 0.926 \quad \text{: Rabi frequency}
\]

\[
E_{\text{shield}} \approx 0.02B \quad \text{: shield barrier}
\]

\[
\approx 4\text{mK} \quad \text{: Li Cs}
\]
Validity of Born-Oppenheimer approximation:

- transitions between different levels
- mass of molecules plays an important role

\[ \gamma = \frac{d^2 m}{\hbar^2 r_B} = \frac{m (d^4 B)^{1/3}}{\hbar^2} \]

- semi-classical analysis is valid for large values of \( \gamma \).
  - determine the classical motion during a collision \( r_c(t) \)
  - full numerical solution of the Schrödinger equation for the internal states with the time-dependent position \( r_c(t) \)
  - depletion at the turning point determines transition to different levels

- algebraic behavior (no Landau-Zener like exponential behavior)

\[ \sigma_{\text{int}} = \rho \left( \frac{E_{\text{int}}}{\Delta} \right)^\kappa r_0^2 \]
\[ \rho \approx 0.043 \]
\[ \kappa \approx 2.2 \]
Quantum tunneling:

- semi-classical probability (instanton techniques)
- Euclidean action of the instanton trajectory

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

\[ \frac{S_E}{\hbar} = 2 \int_C d\mathbf{r} \sqrt{m \left[ V_{\text{eff}}(\mathbf{r}) - E_{\text{kin}} \right]} = c \sqrt{\gamma} \]

numerical factor: \( c = 0.32 \)

Inelastic losses

- suppressed three-body losses, as it first requires two particles to approach on short distances
- dominant loss mechanism: diabatic transitions between different levels

\[ \frac{1}{\tau_{\text{ine}}} \approx 10 \frac{B n r_B^3}{\hbar} \left( \frac{T}{B} \right)^{\kappa + 1/2} \]

- parameters: Li Cs

\[ n \sim 10^{15} \text{ cm}^{-3} \]

\[ T < 100 \mu \text{K} \]

\[ \tau_{\text{ine}} > 1 \text{sec} \]
**Elastic collisions**

**Effective potential**

- low energy scattering dominated by the van der Waals part
- symmetric effective repulsion

\[ V_{\text{eff}} \sim \frac{C_6}{r^6} \quad C_6 = \frac{4C_6^{(0)} + 24C_6^{(2)}}{5} \]

- s-wave scattering length

\[ a_s \approx 0.68 \left( \frac{C_6 m}{\hbar^2} \right)^{1/4} \approx 66\text{nm} \]

- large ratio between elastic and inelastic cross section

\[ \frac{\sigma_{\text{el}}}{\sigma_{\text{ine}}} \sim 10^6 \quad \text{at} \quad 1 \text{ mK} \]

route towards evaporative cooling of polar molecules
Cristalline phases
Many-body Hamiltonian

\[ H = \sum_i \frac{p_i^2}{2m} + \sum_{i \neq j} V(\mathbf{r}_i - \mathbf{r}_j) + \ldots \]

- dimensionless parameter

\[ r_6 = \frac{E_{\text{int}}}{E_{\text{kin}}} = \frac{C_6 m}{\hbar^2} n^{4/3} \]

- closed packing for ellipsoid
- distorted FCC lattice

- realistic parameters for the lattice spacing
  \[ a \sim 100 - 300 \text{nm} \]

- three-body interactions cannot be neglected
Three-body interactions
Three-body interactions

Many-body interaction potential

- Hamiltonians in condensed matter are effective Hamiltonians after integrating out high energy excitations

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

Why is it interesting?

- novel tool for strongly correlated states

- Exotic phases
  - emergent symmetry
  - no spontaneous symmetry breaking: RVB, spin liquid, ...

- Topological phases
  - fractional quantum Hall states
  - (non)-abelian anyons
  - application in topological quantum computing

Do such phases exist in nature?
How often do they appear?
Circuit CQED and Molecular Quantum Memory
Molecular Quantum Memory

- superconducting transmission line cavities
- rotational excitation of polar molecule(s)

\[ N=1 \]
rotational excitations
\[ \mu \text{ large!} \]
\[ N=0 \]
\[ g \sim 2\pi \times 10 \text{ KHz } \sqrt{\# \text{molecules}} \]
\[ \sim 2\pi \times 1 \ldots 10 \text{MHz} \]
ensemble
AMO- solid state interface

- solid state quantum processor
- molecular quantum memory
(P. Rabl, D. DeMille, J. Doyle, M. Lukin, R. Schoelkopf and P. Zoller, PRL 2006)

Spin toolbox

- polar molecules with spin
- realization of Kitaev model
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