Mixture of ultracold molecules as a crystal with tunable impurities

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Funding:

NSERC CRSNG
Canada Foundation for Innovation
Fondation canadienne pour l’innovation

British Columbia
The Best Place on Earth

Les Fiducies Killam Trusts

Peter Wall Institute for Advanced Studies

Canadian Centre for Research on Ultra-Cold Systems
Quantum Simulation

Design *simple controllable* systems with some of the same properties as complex quantum systems, such as solid-state crystals.
Quantum Simulation

Design simple controllable systems with some of the same properties as complex quantum systems, such as solid-state crystals.

This talk

I. Ultracold molecules on an optical lattice as a crystal with tunable exciton–impurity interactions

II. Ultracold molecules on an optical lattice as a crystal with tunable magnetic properties
Frenkel exciton

\[ \phi_n = |00\rangle_1 |00\rangle_2 \ldots |10\rangle_n |00\rangle_{n+1} \ldots |00\rangle_N \]

\[ \psi = \sum_n C_n \phi_n \]
Frenkel exciton

\[ \phi_n = |00\rangle_1|00\rangle_2 \ldots |10\rangle_n|00\rangle_{n+1} \ldots |00\rangle_N \]

\[ \psi_k = \sum_n \frac{e^{ik \cdot r_n}}{\sqrt{N}} \phi_n \]
Dispersion Curves

\[ E(k) = \text{in units of } 10^{-6} \text{ B} \]

\[ m_* < 0 \]
Negative effective mass => negative refraction of EM field
The graphs depict the energy $E(k)$ in kHz as a function of $k a$ for different orientations.

- **$E \perp x$**
  - $\gamma$ (solid line)
  - $\beta$ (dashed line)
  - $\alpha$ (dotted line)

- **$E \parallel x$**
  - $\gamma$ (solid line)
  - $\alpha$ (dotted line)
  - $\beta$ (solid line)
Impurities

Pure Exciton Hamiltonian:

\[ H = \left( \sum_n E_0 B_n^\dagger B_n + \sum_n J_{mn} B_m^\dagger B_n \right) \]
Impurities

One impurity:

\[ H = \sum_{n \neq 0} E_0 B_n^\dagger B_n + E_{imp} B_{n=0}^\dagger B_{n=0} + \sum_n J_{mn} B_m^\dagger B_n \]

Scatterer with the strength = difference in transition energies:

\[ H = \left( \sum_n E_0 B_n^\dagger B_n + \sum_n J_{mn} B_m^\dagger B_n \right) + (E_{imp} - E_0) B_{n=0}^\dagger B_{n=0} \]

Breaks translational symmetry \( \rightarrow \) Mixes states with different \( k \)

\[ H = \sum_k E(k) B^\dagger_k B(k) + \frac{V_0}{N} \sum_{k,q} B^\dagger_k (k) B(q) \]
Tunable impurities

\[ E_{\text{eg}} (\times 10^4 \text{ MHz}) \]

- CsF
- LiCs
- LiRb

\[ E \text{ (kV/cm)} \]
- 1.0
- 1.2
- 1.4
- 1.6
- 1.8
- 2.0

\[ E \text{ (mV/cm)} \]
- 10^2
- 10^4
- 10^6
- 10^8

\[ \sigma_{2D} \text{ (Å)} \]
- 10^2
- 10^4
- 10^6

\[ k = 10^{-8} \text{ Å}^{-1} \]
- 10^{-6} \text{ Å}^{-1}
- 10^{-5} \text{ Å}^{-1}
Exciton - impurity Hamiltonian matrix

\[
\langle \hat{H}_0 \rangle_{q,k} = E(k) \delta_{k,q},
\]

\[
\langle \hat{W} \rangle_{q,k} = \frac{2 \Delta J(a)}{N_{\text{mol}}} (\cos q \cdot a + \cos k \cdot a) \sum_{i_n=1}^{N_i} e^{i(q-k) \cdot i_n}
\]

Off-diagonal disorder

Diagonal disorder

\[
\langle \hat{V} \rangle_{q,k} = \frac{V_0}{N_{\text{mol}}} \sum_{i_n=1}^{N_i} e^{i(q-k) \cdot i_n}
\]
No diagonal disorder

Strong diagonal disorder

Diagonal disorder ~ off-diagonal disorder
\[ |\Psi(x)|^2 \left( \frac{1}{N_{\text{mol}}} \right) \]

- No diagonal disorder
- Diagonal disorder \sim off-diagonal disorder
- Large diagonal disorder
\[ |\Psi(x)|^2 \left( \frac{1}{N_{\text{mol}}} \right) \]

\[ f(t) \]

\[ C(k) \]

\[ k \alpha \]

\[ t (\mu s) \]
Applications

• Time-domain quantum simulation of localization of quantum particles:
  - timescale of Anderson localization
  - dynamics of exciton localization as a function of effective mass, exciton bandwidth, and exciton-impurity interaction strength
  - effect of disorder correlations on localization and delocalization

• Negative refraction of MW fields

• Controlled preparation of many-body entangled states of molecules

• Effects of dimensionality and finite size on energy transfer in crystals
Energy diagram of a $^2\Sigma$ diatomic molecule

How do electric fields affect spin relaxation?

- Induce couplings between the rotational levels ($N = 1$)
- Increase the energy gap between the rotational levels

Enhancement of spin relaxation

• First-order Stark effect

$^2\Sigma$ molecules

Energy diagram of a $^2\Sigma$ diatomic molecule
Spin exciton coupling constant

Magnetic field, Gauss

Coupling constant, kHz
Spin exciton bandwidth
Energy diagram of a $^2\Sigma$ diatomic molecule
$^2\Sigma$ molecules

Energy diagram of a $^2\Sigma$ diatomic molecule

$\Delta E$

$N = 0$

Spin-rotation interaction

$N = 1$

Interaction potential

$J$
Lattice of 1000 molecules

\( |\Psi|^2 \) vs. Position of the molecules
1000 molecules with 10 impurities
Applications

Crystal with tunable impurities:

• **Time-domain quantum simulation** of localization of quantum particles:
  
  timescale of Anderson localization
dynamics of exciton localization as a function of effective mass, exciton bandwidth, and exciton-impurity interaction strength
effect of disorder correlations on localization and delocalization

• Negative refraction of MW fields

• Controlled preparation of many-body entangled states of molecules

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Optical lattice of magnetic molecules:

• Crystal with tunable magnetic properties, tunable spin waves

• Preparation of many-body entangled states of spin up-down pairs

• ???