Quantum Simulationand Computationwith Ultra-cold Atoms and Molecules

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Part I: Overview and fundamental concepts

Thirst for computational capacity

In 1943: "I think there is a world market for maybe five computers"

--Thomas Watson, Chairman of IBM



Colossus, weight: 1 ton, power: 8.5kw, 5 kOPS (operations per second)

In 2010's: The computing power in a mobile phone is larger than the total computing power used in Apollo Program!





Apple A12, power: <5W, 5 trillion OPS

The world's data volume roughly grow 40% per year

Challenges in the computational capacity

Classical computational bottleneck

The world's total computing power is insufficient to search a target in 2^{80} database within a year

A technological limit

The Moore's law that predicts the transistor density doubles every 18 months has come to an end



0.2 nm (atomic scale) 븆 ???



Tunneling induced leakage
The "0/1" logic in the transistors will fail

Challenges in the computational capacity

Much more hardly accessible for classical computers to simulate a quantum system

A quantum system of 300 two-level particles:
 ☑ Described by a 2³⁰⁰ dimensional Hilbert space → Larger than total number of atoms in the known Universe!



Natural solution: quantum simulator Consisting of superposition quantum states engineered to simulate a quantum system





Quantum parallelism

Quantum Parallelism

 Bits
 Qubits

 0 or 1
 V. S.
 0 + 1

 00, 01, 10 or 11
 00 + 01 + 10 + 11

 000, 001, 010.....
 000 + 001 + 010 +

Evaluating function f(x) for many different x simultaneously

$$U\frac{1}{\sqrt{2^{N}}}\sum_{i=0}^{2^{N}-1}|i\rangle|0\rangle = \frac{1}{\sqrt{2^{N}}}\sum_{i=0}^{2^{N}-1}|i\rangle|f(i)\rangle$$
 Exponentially speedup!

Quantum computation

Shor Algorithm (1994):

- E.g. factor a 300-digit number with
- Classical THz computer: 150,000 years
- Quantum THz computer: 1 second!

- Code-breaking can be done in minutes, not in millennia
- Public key encryption, based on factoring, will be vulnerable!









Code-breaking

Weather forecast

Financial analysis

Drug design

Quantum circuit computation model



Single-qubit SU(2) gates + two-qubit controlled-NOT gates Universal quantum computation [Lloyd, PRL 75, 346 (1995)]



> Universal QC resource: multi-particle entanglement

Cluster state $|\Phi\rangle_C$:

$$\sigma_x^{(a)} \bigotimes_{a' \in ngbh(a)} \sigma_z^{(a')} |\Phi\rangle_C = \pm |\Phi\rangle_C$$



 Quantum gate is implemented by measuring particles in a certain order and in a certain basis

Raussendorf and Briegel, PRL 86, 5188 (2001)

Scalability: fault tolerable qubits



Inevitable noise

qubit error
during quantum computation

- Error-correction code
 - Shor, PRA 52, R2493 (1995) 9qubits
 - Steane, PRL 77, 793 (1996) 7qubits
 - Laflamme et al., PRL 77, 198 (1996) 5qubits

☑ Challenge: traditional error-correction codes require error rate < 2×10⁻⁵ !

Quantum simulation

Achieving a programmable universal quantum computer (even a prototype) is a long-term process, maybe need 20-30 years or more
 Fortunately, scalable quantum simulator is achievable in the near future!



A quantum simulator

- Manipulating Hamiltonian of a controllable quantum system to mimic the evolution of another complex quantum system
 Do not need high precise quantum logical actor and
- Do not need high precise quantum logical gates and entanglement of so many qubits

To solve various complex problems in condensed matter physics:

- High-temperature superconducting
- (fractional) Quantum Hall effect

Candidates for quantum computation and simulation



"Quantum engineering" of Hamiltonians



Optical lattices:
✓ To mimic crystal structures
✓ To entangle many atoms

✓ To synthesize artificial gauge potentials by Raman technique

Ultra-cold atoms: a novel system

"Quantum engineering" of Hamiltonians



✓ Tunable atom-atom interaction strength by Feshbach resonance



✓ To study ultra-cold chemical dynamics



✓ To simulate electron correlation in lattices

Why do we need ultra-cold atoms?

From classical statistics to quantum statistics

Atomic ensemble at room temperature T Maxwell-Boltzmann statistics

$$\overline{n_i}(\varepsilon_i) = \frac{g_i}{e^{(\varepsilon_i - \mu)/k_B T}}$$

 g_i : degeneracy ε_i : energy of the state μ : chemical potential k_B : Boltzmann constant T: temperature



Maxwell-Boltzmann Molecular Speed Distribution for Noble Gases

Why do we cool atoms to ultralow temperature

From classical statistics to quantum statistics

> Atomic ensemble at near zero temperature

Bose-Einstein statistics

$$\overline{n_i}(\varepsilon_i) = \frac{g_i}{e^{(\varepsilon_i - \mu)/k_B T} - 1}$$

Bose Einstein Condensate (BEC):

all atoms collect to the ground state

Fermi-Dirac statistics

$$\overline{n_i}(\varepsilon_i) = \frac{g_i}{e^{(\varepsilon_i - \mu)/k_B T} + 1}$$

Fermi degeneracy:

- One atom per state due to Pauli exclusion principle
- Atoms fill from the lowest energy level, up to the Fermi energy E_F

Why do we cool atoms to ultralow temperature

Significant quantum effect

de Broglie wavelength of particles $\lambda = \frac{h}{\sqrt{3mk_BT}}$, k_B is Boltzmann constant





Atoms condensed to a narrow momentum space

First achievement of BEC, Cornell, Wieman and Ketterle (1995), Nobel Prize in Physics 2001

How to cool atoms?

Optical radiation pressure



Johannes Kepler (1571-1630)

"Let us create vessels and sails adjusted to the heavenly ether, and there will be plenty of people unafraid of the empty wastes"



- Momentum of a photon $p = \hbar k$
- Solar Sail Demonstrator ('Sunjammer') by NASA: using the pressure of sunlight itself to provide propellant-free transport

Light pressure for atoms





The atom decay back to ground state via spontaneous emission

- Directions of emitted photon is random and isotropic
 - Average emitting momentum is 0

• Total effect: the atom obtain momentum $\hbar k \Rightarrow$ the atom have a scattering force $F_{\text{scatt}} = -\sigma I/c$

Acceleration can be 10,000g



Hänsch and Shawlow, Opt. Commun. 13, 68 (1975)

Doppler cooling

Doppler effect

For stationary observer:

ω	ω



- ► If we set $\omega + \Delta \omega = \omega_0$ (ω_0 is the transition frequency of the atoms), atoms will only absorb the photons oppositely running to its movement direction \Rightarrow slow down
- Using 3D Doppler cooling to slow down atoms moving in all directions



Magneto-optical trap (MOT)

When atoms are slowed down, the oppositely running laser's frequency will not be resonant with atom's transition \Rightarrow atoms will not absorb opposite photons any further. How to continue cooling?

Using Zeeman effect to tune atom's transition frequency $\Delta \omega_B = \pm \frac{\mu_B}{\hbar} B$ With magnetic field gradient, $M_{\rm F}$ $M_{
m F}$ atom's transition frequency 2p 0 F = 1varies with positions: Transitions $\omega_0 + \Delta \omega_Z$ ($\Delta \omega_Z = \frac{\mu_B}{\hbar} \frac{dB}{dz} Z$) \Rightarrow The atoms with velocity in a $\mathbf{F} = \mathbf{0}$ specific range can always No Magnetic Field **Magnetic Field** find the resonant frequency!

 $\omega - kv$

 $\omega + kv$

at certain place!

Limit of Doppler cooling



• The average total force of atoms:

$$F = F_{\text{scatt}}(\omega - \omega_0 - kv) + F_{\text{scatt}}(\omega - \omega_0 + kv) \approx -2\frac{\partial F}{\partial \omega}kv$$

- Statistical fluctuation of spontaneous emission directions \blacklozenge Fluctuation of force ΔF
- When $v \to 0$, $\Delta F \sim F \Rightarrow$ laser heating!

Doppler limit (around 100uk): $T_D = \frac{\hbar \Gamma}{2k_B}$, Γ is the spontaneous emission rate

Optical molasses

Sub-Doppler cooling with polarization gradient potential Two counter propagating orthogonal linearly polarized fields



Spatially varying polarization:

$$E(z,t) = E \cdot e^{i(\omega t + kz)} \left(\hat{\mathbf{e}}_{x} + e^{i(-2kz + \phi)} \hat{\mathbf{e}}_{y}\right)$$

Optical molasses



Sisyphus cooling



For an moving atom:

Step 1: "climbing" in potential, loss kinetic energy Step 2: absorbing σ^- photon at the top of potential (smallest detune, high transition probability), excited to upper state and decay \Rightarrow

 If decay to |1/2> (p=1/3), nothing would happen, repeat step 1

• If decay to $|-1/2\rangle$ (p=2/3), different potential Step 3: climb a hill and loss kinetic energy again



Sisyphus' punishment

Cooling atoms with laser

MOT + Optical molasses:

Chu, Tannoudji and Phillips, method to cool and trap atoms with laser light Noble Prize in Physics 1997



Limit of Sisyphus cooling:

Recoil momentum of photons in transition

$$T_R = rac{\hbar^2 k^2}{k_B M}$$
 M is the mass of an atom

For ⁸⁷Rb atom, $T_R \sim 1 \mu k$

Further cooling by evaporative cooling



Evaporative cooling in daily life





In view of physicist: thermal equilibrium is re-established through collisions

To cool atoms: Ramp down optical potential, hotter atoms will escape from trap

Optical potential induced by light-atom interaction

Optical trap for evaporative cooling



Optical potential induced by light-atom interaction

Red and blue detuned trap

 $U(r) \propto \frac{I}{\Lambda} I(r)$

- Red detuning ($\Delta < 0$): a trap is formed at the position of maximal intensity
- Blue detuning ($\Delta > 0$): a trap is formed at the position of minimal intensity



Grimm et al., Adv. At. Mol. Opt. Phys. 42, 95 (2000)

Optical traps

Gaussian beam to form a 3D optical trap



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 v/2·w o
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Atoms are trapped near the waist



Gradient of intensity in z-direction is small

Decrease the intensity of light, evaporative cooling to around 100 nk = achieving BEC

Cross beams to trap atoms at the waist

Typical route for cooling atoms



Evaporative cooling of Fermi atoms

Physical problem: identical Fermions cannot stay close enough to undergo effective collisions due to Pauli blocking

Evaporative cooling cannot happen!

Solutions:

> Sympathetically cooling by another coolant (Boson)





Observation of degenerate Fermi gas by sympathetically cooling Truscott *et al.*, Science 291, 2570 (2001)]



Typical detection methods

Time of flight (TOF) g $r = v \cdot \Delta t$ Imaging beam CCD

TOF images reflect the momentum distribution of the atoms \Rightarrow derive information of temperature and coherence

Via in-situ imaging with a highresolution microscope
Real-space density distribution of the atoms

In-situ imaging

Part II: Quantum computation and simulation with atomic spin entanglement in optical lattices

Dai et al., Nature Physics 12, 783 (2016) Dai et al., Nature Physics 13,1915 (2017)

Topological quantum computing

Protect quantum bits/gates at the physical level

- Kitaev, Ann. Phys. 303, 2 (2003); Ann. Phys. 321, 2 (2006)
- Raussendorf et al., Ann. Phys. 321, 2242 (2003)
- Nayak et al., RMP 80, 1083 (2008)
- ➡ Relax the error threshold rate from 10⁻⁵ to 10⁻²



☑ No naturally occurring system is likely to have a Hamiltonian of the Kitaev model
☑ Purpose-engineered systems of optical lattices or Josephson junction arrays
--Anthony J. Leggett

Scalability: atoms in optical lattice



Atom-atom entanglement in optical lattices (87Rb)

- Generate large number atom-atom entanglement
- ✓ Demonstrate the braiding Anyons required by topological quantum computation
Optical lattices



Scalability: atoms in optical lattice





Optical lattice: an array of well coherently controlled cold atoms

in-situ imaging: only one atom trapped in a lattice



Spin exchange interaction: generate spin-spin entanglement

Multi-atom entanglement!



Vaucher et al., NJP 10, 023005 (2008)

Preparing one atom per site

Bose-Hubbard model (BMH)



J: nearest-neighbor tunneling U_0 : onsite interaction

Theory: Jaksch et al., PRL 81, 3108 (1998)



 U_0

 $U_0 \gg J$ Mott insulator phase

Through the phase transition, one atom per site can be prepared

Phase transition from SF to MI



Fist observation of quantum phase transition from a superfluid to a Mott insulator Greiner *et al.*, Nature 415, 39 (2002)

Experimental setup







Prepare a 2D quantum gas with in-situ imaging



> ⁸⁷Rb: $|F = 1, m_F = -1$ BEC 2×10⁵ atoms

- Load into a pancake lattice N_{2D}~15000, T_{2D}=23(3) nK
- SF to MI transition by ramping up lattice depth

Objective: NA=0.48, resolution 2 µm

Optical super-lattice



Isolated double wells: $V(x) = V_s \cos^2(2kx + \phi_x) + V_l \cos^2(kx)$

Theory: Duan et al., PRL 91, 090402 (2003) Experiment: Trotzky et al., Science 319, 295 (2008)

Spin super-exchange: generating spin entanglement

BHM (two-site, spin dependent)

$$\widehat{H} = \sum_{\sigma=\uparrow,\downarrow} \left[-J(\widehat{a}_{\sigma L}^{+} \widehat{a}_{\sigma R} + \widehat{a}_{\sigma R}^{+} \widehat{a}_{\sigma L}) \right] + U[\widehat{n}_{\uparrow L} \widehat{n}_{\downarrow L} + \widehat{n}_{\uparrow R} \widehat{n}_{\downarrow R}]$$

Interaction dominated $(U \gg J)$, in low-energy state subspace $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$



Single atom tunneling is suppressed

$$\widehat{H}_{eff} = J_{ex} \begin{pmatrix} -1 & -1 & 0 & 0 \\ -1 & -1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix} = -2J_{ex}\widehat{S}_L \cdot \widehat{S}_R + C$$
$$J_{ex} = 2J^2/U, \, \widehat{S}_j = \left(\widehat{S}_j^x, \widehat{S}_j^y, \widehat{S}_j^z\right), \, \widehat{S}^k = \frac{1}{2}\sigma_k$$

Spin super-exchange: generating spin entanglement



- Initial state: $|\uparrow\downarrow\rangle = \frac{1}{\sqrt{2}}(|t_0\rangle + |s_0\rangle)$, degenerate with $|\downarrow\uparrow\rangle = \frac{1}{\sqrt{2}}(|t_0\rangle |s_0\rangle)$
- Spins will oscillate between two configurations with a period of $1/J_{ex}$
- Stop the oscillation by increasing the barrier to create spin entanglement

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle+i|\downarrow\uparrow\rangle)$$

Theory: Duan et al., PRL 91, 090402 (2003)

Spin-dependent superlattices



 ∇B

Right well is higher

Spin-dependent superlattices



Spin super-exchange: generating spin entanglement



• Switch off effective magnetic gradient, $|\!\uparrow\downarrow\rangle$ and $|\!\downarrow\uparrow\rangle$ degenerate

• Decrease $V_i \rightarrow$ spin oscillation



• Increase $V_i \rightarrow$ Freeze entangled state

How to detect entanglement?

Entanglement detection

Entangled state: $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\uparrow\downarrow\rangle)$ Spin-dependent collisional loss: identify $|\downarrow\downarrow\rangle$ from 4 orthogonal states $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle$, $|\uparrow\uparrow\rangle$, $|\uparrow\uparrow\rangle$,



Entanglement detection

Probabilities in different basis



$$F \ge (P_{\uparrow,\downarrow} + P_{\downarrow,\uparrow} - 2\sqrt{P_{\uparrow,\uparrow} P_{\downarrow,\downarrow}} + P_{+,+} + P_{-,-} - P_{+,-} - P_{-,+})$$
$$\ge (P_{\uparrow,\downarrow} + P_{\downarrow,\uparrow} - P_{\uparrow,\uparrow} - P_{\downarrow,\downarrow} + P_{+,+} + P_{-,-} - P_{+,-} - P_{-,+})$$
$$= 0.79 \pm 0.06$$

Spin correlation curve and entanglement



Violation of CHSH type Bell's inequality $S = 2.21 \pm 0.08$

Dai et al., Nature Physics 12, 783 (2016)

Kitaev model: Toric code

Manipulating the interaction and entanglement of atomic spins in optical lattices
mimic a unit Hamiltonian of the Toric code model and demonstrate fractional Anyonic statistics

Hamiltonian:

$$H_0 = -\sum_s A_s - \sum_p B_p$$

 $A_s = \prod_{j \in \text{star}(s)} \sigma_j^x$
 $B_p = \prod \sigma_j^z$

Four-body interaction

• Abelian Anyons: *e*, *m* excitations

 $j \in \text{boundary}(p)$



Kitaev, Annals of Physics 303, 2 (2003)

Toric code -- Braiding



Toric code -- Braiding



Questions

Can we build a many-body quantum system which is described by the Toric-code Hamiltonian?

Requirements:

- Create the four-body interaction
- > Demonstrate the topological phase

Previous efforts:

Theory: Han et al., PRL 98,150404 (2007) Experiments: Lu et al., PRL102, 030502 (2009). photons Pachos et al., NJP 11, 083010 (2009). photons Barreiro et al., Nature 470, 486 (2011). ions Song et al., PRL 121, 030502 (2018). superconductors

No background Hamiltonian
There is no energy gap to protect the qubit!

2D-optical superlattice

BHM $\widehat{H} = \sum_{\sigma=\uparrow,\downarrow} \left[-J(\widehat{a}_{\sigma L}^{+} \widehat{a}_{\sigma R} + \widehat{a}_{\sigma R}^{+} \widehat{a}_{\sigma L}) \right] + U[\widehat{n}_{\uparrow L} \widehat{n}_{\downarrow L} + \widehat{n}_{\uparrow R} \widehat{n}_{\downarrow R}]$



Super-exchange dominated : $H_{ex} = -2J_{ex}S_L \cdot S_R$

> In isolated plaquettes one can suppress super-exchange by 2D effective magnetic gradients

Ring-exchange dominated : $H_{\Box} = -J_{\Box}\hat{\sigma}_{1}^{x}\hat{\sigma}_{2}^{x}\hat{\sigma}_{3}^{x}\hat{\sigma}_{4}^{x}, J_{\Box} = 40 J^{4}/U^{3}$



isolated plaquettes

Paredes & Bloch, PRA77, 23603 (2008)

Suppress super-exchange



Low-energy state subspace: $\{|\uparrow\downarrow\uparrow\downarrow\rangle, |\downarrow\uparrow\downarrow\uparrow\rangle, |\uparrow\uparrow\downarrow\downarrow\rangle, |\uparrow\uparrow\downarrow\downarrow\rangle, |\uparrow\downarrow\downarrow\uparrow\rangle, |\downarrow\uparrow\uparrow\downarrow\rangle\}$

Super-exchange is suppressed: Non-degeneration due to effective magnetic gradients

 $\frac{dB_x}{dx}$

Minimum Toric code Hamiltonian



Site-resolved addressing: state initialization

Due to the 2D effective magnetic gradients, the atoms on sites 2 and 4 have the same Zeeman shift

Flip atoms on sites 2 and 4 to prepare an anti-ferromagnetic order



Ring exchange driven oscillation



Observation of ring exchange driven oscillation

Count the populations of different states



Topological phase of Abelian anyons, $\theta = \pi / 2$



Observation of anyonic fractional statistics



Dai et al, Nature Physics 13, 1195 (2017)

Outlook: towards large entangled state

Seneration of multi-atom entanglement: remove defects, connect the atom pairs Challenge: cool the atoms in optical lattices?



MI samples, staggered immersed in SF reservoirs [arXiv 1901. 01146]
 Entropy of MI taken away by the SF, 60-fold reduction; 10,000 sites, 0.8% defects



Motivated by the theoretical schemes: Griessner et al, PRL (2006) Ho and Zhou, PNAS (2009)

Outlook: towards large entangled state

> Two gubits entangling gates with superexchange after cooling: 99.3% > Lifetime of entanglement: ~700ms





Fidelity = 99.3(1)% (in preparation)

Outlook: towards large entangled state

> High-resolution imaging system



Numerical aperture: NA=0.8; Resolution: 690 nm

- Large entangled state; e.g. 100 (10x10) particles, how to identify? Simulating spin dynamics.
- > Challenge theoreticians at an unprecedented level

Outlook: simulating topological materials

> Couple the plaquettes: a many-body strongly correlated topological system



Reviews on topological matters with ultracold atoms:

- Goldman, Budish & Zoller, Nat. Phys. (2016)
- Zohar et al. Rep. Prog. Phys. (2016)

> Extend to fermionic systems; non-Abelian ...

• Theory: Zhang et al, PNAS (2007)



Part III: Quantum simulation of Gauge potential with neutral atoms

Zhang et al., PRL 109, 115301 (2012) Ji et al., Nature Physics 10, 314 (2014) Wu et al., Science 354, 83 (2016) Sun et al., PRL 121, 250403 (2018)

Spin-orbit coupling (SOC)

Electrons moving in an electric field:

- Electron experiences a magnetic field proportional to its velocity and
- Couples to its spin by the magnetic dipole interaction





Gauge potential coupling to electrons' spin

$$H = \frac{1}{2m} \left(\mathbf{k} - \frac{q}{c} \mathbf{A(s)} \right)^2 + V + q\varphi(\mathbf{s})$$

s: spin of an electron A(s): vector potential $\varphi(s)$: scalar potential

Novel quantum system

SOC leads to numerous interesting quantum phenomena in electron systems

- Quantum Hall effect
- Spin-Hall effect
- Topological insulator
- Majorana Fermions
- Weyl Fermions

...



However, uncontrollable in natural materials!

Synthesize Gauge potential with neutral atoms

Mimicking spin-orbit coupling with BEC: coupling inner states with momentum Theory: Liu et al., PRL 102, 046402 (2009)

Experiment: Spielman's group, Nature 471, 83 (2011)



Dipole trap ₿ O BEC $\omega_{L} + \Delta \omega_{L}$ $\omega_{\rm L}$ Raman π Raman σ $H = \frac{1}{2m} \left(k_x - \frac{1}{2} k_0 \sigma_z \right)^2 + \frac{\delta}{2} \sigma_z + \frac{\Omega}{2} \sigma_x$ V. S. $H = \frac{1}{2m} \left(\mathbf{k} - \frac{q}{c} \mathbf{A}(\mathbf{s}) \right)^2 + V + q\varphi(\mathbf{s})$

Raman process:

 $|-1\rangle \rightarrow |0\rangle$: obtaining momentum $-k_0$ $|0\rangle \rightarrow |-1\rangle$: obtaining momentum k_0

Synthesize Gauge potential with neutral atoms

$$H = \frac{1}{2m} \left(k_x - \frac{1}{2} k_0 \sigma_z \right)^2 + \frac{\delta}{2} \sigma_z + \frac{\Omega}{2} \sigma_x$$

Coupling strength (Raman Rabi frequency) $\Omega = \frac{\Omega_1 \Omega_2}{\Delta}$ $\Omega_1 = \frac{\varepsilon_1 E_1}{\hbar}$, ε is transition dipole moment



For $\Omega \ll 4E_r$ (recoiling energy $E_r = \frac{\hbar^2 k_0^2}{2m}$), the eigenstates of *H* are: $|L\rangle = |-1\rangle + \alpha |0\rangle, |R\rangle = |0\rangle + \alpha |-1\rangle$

 $lpha \ll 1$ is determined by coupling strength Ω and two-photon detuning δ




Theoretical phase diagram involving SO-coupling

- Wang et al., PRL 105, 160403 (2010)
- Ho and Zhang, PRL 107, 150403 (2011)



Spielman's group, Nature 471, 83 (2011)



However, to characterize the second order phase transition quantitatively
☑ The static way is not valid since the ground state only occupies single momentum minimum in both two phases
☑ Method: measurements based on dynamical process

Realization of 1D SO coupling



Pure condensate: $\sim 2 \times 10^5$ ⁸⁷Rb atoms Trapping frequency: {50,50,80}Hz



Raman coupling

b

Excite the collective dipole oscillation



Collective dipole & spin state oscillations

> Dipole oscillation frequency shift away from trap frequency (measured with $\Omega = 3.3Er$)



> Spin-state oscillation is highly correlated with momentum oscillation (measured with $\Omega = 4.8Er$)





Spin polarizability χ : how easy or hard a system could be spin polarized

Evaluating infinite χ at phase transition point from the experimental data

 $\frac{A_{\sigma}}{A_{k}/k_{r}} = \frac{E_{r}\chi}{1 + E_{r}\chi} \quad \begin{array}{l} A_{\sigma}: \text{ amplitude of spin oscillation} \\ A_{k}: \text{ amplitude of momentum oscillation} \\ \end{array}$ When the left value approaching to 1, $\chi \to \infty$

Li et al., EPL 99, 56008 (2012)



Zhang et al., PRL 109, 115301 (2012)

Phase diagram at finite temperature

Yet phase diagram at $T \neq 0$ is unknown



Magnetization and phase transition

Discriminating stripe phase and magnetized phase by magnetization M: $M = \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}}$



Magnetization and phase transition



Finite-temperature phase diagram of SOC Bose gas

Ji et al., Nature Physics 10, 314 (2014)



Though theoretical result was not clear yet at that time!

From 1D to 2D spin-orbit coupling

- However, mimicking 1D spin-orbit coupling is like a toy, 1D SOC does not have the real topological properties.
- 2D or higher dimensional SOC play central role in most of topological quantum matters, such as...



From 1D to 2D spin-orbit coupling



Superposition of two 1D SOC

From 1D to 2D spin-orbit coupling

 Some proposals: PRL 108, 235301 (2013) PRL 111, 125301 (2013) PRA 85, 043605 (2012), etc.

Experiment:
 2D SOC with Fermion (⁴⁰K)
 Nature Physics 12, 540 (2016)



Major challenge:

- Large heating rate
- Phase coherence between atom-laser couplings
- Fast switch on/off the magnetic fields

Optical lattice + running wave scheme



The phase of the lasers go through the loop: Lattice light $w_1 : \varphi_L = k_0 L$

Raman light $w_2 : \varphi_L + \delta \varphi_L = (k_0 + \frac{\delta \omega}{c})L, \delta \omega = w_2 - w_1$ \checkmark Less lasers and stable energy levels, low heating rate

✓ Robust phase relation

2D Lattice



Optical lattice potential:

$$V_{Latt}(x,y) = V_{0x}\cos^2(k_0x + \frac{\varphi_{1x} - \varphi_{1z} - \varphi_L}{2}) + V_{0z}\cos^2(k_0z + \frac{\varphi_{1z} - \varphi_{1x} - \varphi_L}{2})$$

x

Raman coupling lattices

Lattice laser and Raman laser form Raman coupling lattices **>** spin-flip tunneling Standing wave Running wave ₿ Raman coupling strength: $M_x = M_0 \cos k_0 x e^{ik_0 z}$ $= M_0 \cos k_0 x \cos k_0 z$ $E_{1x}, \omega_1, \pi \qquad E_{1x}, \omega_1, \pi \\ E_{2z}, \omega_2, \sigma$ $+iM_0\cos k_0x\sin k_0z$ In tight binding condition: $M_x = M_0 \cos k_0 x \sin k_0 z$ tunneling: *M* = 1 on site: ZM = 0x M_{x} E_{2x}, ω_2, π *E*_{1z}, ω₁, σ # $M_z = M_0 \cos k_0 z \sin k_0 x$ Ζ x M_{ν}

2D spin-orbit coupling

Total coupling potential:

 $|g_{\uparrow}\rangle \rightarrow |g_{\downarrow}\rangle : M_{\chi} + M_{z}e^{-i\delta\varphi_{L}} = M_{\chi} + M_{z}\cos\delta\varphi_{L} - iM_{z}\sin\delta\varphi_{L}$ $|g_{\downarrow}\rangle \rightarrow |g_{\uparrow}\rangle : M_{\chi} + M_{z}e^{i\delta\varphi_{L}} = M_{\chi} + M_{z}\cos\delta\varphi_{L} + iM_{z}\sin\delta\varphi_{L}$

Coupling term in effective Hamiltonian:

 $\begin{bmatrix} \cdots & M_x + M_z \cos \delta \varphi_L - iM_z \sin \delta \varphi_L \\ M_x + M_z \cos \delta \varphi_L + iM_z \sin \delta \varphi_L & \cdots \end{bmatrix}$ $= (M_x + M_z \cos \delta \varphi_L)\sigma_x + iM_z \sin \delta \varphi_L \sigma_v$

Effective Hamiltonian: $H = \frac{p^2}{2m} + V_{latt} + \mathcal{M}_x \sigma_x + \mathcal{M}_y \sigma_y + m_z \sigma_z$ $\mathcal{M}_x = M_x + M_z \cos \delta \varphi_L$ $\mathcal{M}_y = M_z \sin \delta \varphi_L$

Liu et al., PRL 112, 086401 (2014)

2D spin-orbit coupling

$$H = \frac{p^2}{2m} + V_{\text{latt}} + \mathcal{M}_x \sigma_x + \mathcal{M}_y \sigma_y + m_z \sigma_z$$

$$\mathcal{M}_{\chi} = M_{\chi} + M_{Z} \cos \delta \varphi_{L}$$
$$\mathcal{M}_{\chi} = M_{Z} \sin \delta \varphi_{L}$$

If initial state is prepared in the spin up state $|\uparrow\rangle$, when SOC involved:

> 1D SOC: $\delta \varphi_L = \pi \Rightarrow (M_x - M_z)\sigma_x$ spin state: $|\uparrow\rangle + \varepsilon(|k_x + k_z\rangle + |-k_x - k_z\rangle)|\downarrow\rangle$

 $\delta \varphi_L = 2\pi \Rightarrow (M_x + M_z)\sigma_x$ spin state: $|\uparrow\rangle + \varepsilon(|-k_x + k_z\rangle + |k_x - k_z\rangle)|\downarrow\rangle$

> Optimal 2D SOC:

$$\delta\varphi_L = \frac{\pi}{2} \Rightarrow M_x \sigma_x + M_z \sigma_y$$





Experimental setup



- 2D Lattice and Raman Laser Wavelength: 767nm
- Bias field: ~50 Gauss, 2-level system, $\delta w=2\pi \times 35MH$ Wu et al., Science 354, 83 (2016)

Adjust length of the loop

$$H = \frac{p^2}{2m} + V_{\text{latt}}(x, z) + m_z \sigma_z + (M_x - M_y \cos \delta \varphi_L) \sigma_x + M_y \sin \delta \varphi_L \sigma_y$$

Probe: TOF + Stern Gelach

- BEC of ⁸⁷Rb
- Adiabatically ramp up the lattice and Raman coupling
- Lattice depth: $V_0 = 4.16E_r$, Raman coupling: $M_0 = 1.32E_r$ Lifetime ~ 300ms



Topological feature



Topological feature



Detect spin populations at 4 symmetric momenta M, X_1, X_2 and Γ , multiply signs

$$\Theta = \prod_{j=1}^{4} \operatorname{sgn}[P(\Lambda_j)] = \frac{+1}{-1} \operatorname{Trivial}_{\text{Topological}}$$

Chern number	
$\mathrm{Ch}_{1} = -\frac{\Theta}{4} \sum_{j=1}^{4} \mathrm{sgn} \left[P(\Lambda_{j}) \right]$)]

Liu et al., PRL 111, 120402 (2013)

Observation of topological feature



Some drawbacks



> Unstable optical setup: imperfect interference cause low SNR



> Running wave + standing wave: asymmetric Raman coupling



Two running waves alone x and y directions play as lattice laser and Raman laser E_{xz}, E_{xy} : y, z components of polarization of x-running wave E_{yx}, E_{yz} : x, z components of polarization of y-running wave



> Two 1D Raman coupling strength: $M_x = M_0 \cos k_0 x \sin k_0 y$ $M_y = M_0 \cos k_0 y \sin k_0 x$

> Relative phase can be adjusted by the phase between polarization components

Experimental setup



- Symmetric lattice and Raman lasers
- Adjustable phase between polarizations, avoiding path instability

Two symmetric Raman coupling with different polarizations





Long lifetime



Sun et al., PRL 121, 250403 (2018)

Outlook

Observing Weyl points with 3D SOC (experiment in progress)



Weyl semimetal: a new kind topological phase of matter

Low energy consumption electronic transmissions
 Topological quantum computing

••••

Feature: Dirac point is separated into two Weyl points

Outlook

Observing Weyl points with 3D SOC (experiment in progress)



 With 3d-SOC, the Dirac point can be separated to two Weyl points with opposite chiral number

- The dispersion of Weyl points are linear in all 3 dimensions
- The regions containing only two Weyl points have not yet been observed in condensed matter materials

Part IV: Quantum simulation with ultra cold molecules Bose-Fermi Mixture

Rui et al., Nature Physics 13, 699 (2017) Yang et al., Science 363, 261 (2019)

Ultra-cold chemistry

V. S.

Conventional reactions/collisions

- Hard-sphere classical collision
- Average of many partial waves
- Average of many rovibrational states



🗵 Very hard to study quantum effects!

Ultracold reactions/collisions

- de Broglie wave quantum collision
- Single partial wave, pure s- or p- wave
- Reactants in a single quantum state

Quantum mechanics dominated

- ✓ resonances and tunneling
- 🗹 quantum interference
- 🗹 quantum statistics



Understand how quantum mechanics affects chemical reactions!

Scattering of atoms



Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\Psi(r) = E\Psi(r)$$

Partial wave expansion, if V is isotropic $\Psi(r) = r^{-1} \sum_{L} \Psi_l(r) P_l(\cos \Theta)$ P_l is Legendre function

Asymptotic solution

$$\Psi(r) \sim \Psi_0(r) + f(\Theta) \frac{e^{ikr}}{r}, r \to \infty$$

 $f(\Theta)$ is scattering probability amplitude to be solved

Orbital angular momentum l = 0, 1, 2... \Rightarrow s, p, d... partial wave

Scattering of atoms



For each partial wave

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_l(r)\right]\Psi_l(r) = E\Psi_l(r)$$

Asymptotic solution $\Psi_l(r) \sim \sin(kr - \pi l/2 + \delta_l), r \to \infty$ $f(\Theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) (e^{2i\delta_l} - 1) P_l(\cos \Theta)$

In low energy scattering, only s wave is important: phase shift $\delta_0 \ll 1$ is proportional to k S-wave scattering length $a = -\delta_0/k$

The interaction can be replaced by a simplified Fermi contact pseudopotential

$$V_{\text{pseudo}}(r) = \frac{2\pi\hbar^2}{\mu}a\delta(r)\frac{\partial}{\partial r}r$$
 $a > 0$: repulsive
 $a < 0$: attractive

Controls the interaction by adjusting scattering length
Atomic Feshbach resonances

Scattering involving different internal states



Feshbach resonances:

- Channel 1: Potential for two atoms in an internal state $|\Psi_1\rangle$ (set the internal energy of $|\Psi_1\rangle$ to be 0)
- Atoms cannot form bound state in this channel since the energy of bound state is always less than kinetic energy E
- Channel 2: Potential for two atoms in internal state $|\Psi_2\rangle$ with higher internal energy
- In channel 2, there exist a bound state with energy close to the collisional energy in channel 1
- If there is coupling between $|\Psi_1\rangle$ and $|\Psi_2\rangle$, two atoms scattering in channel 1 can temporary form a bound state in channel 2



The energy of bound state in channel 2 can be tuned by magnetic field to coincide with collisional energy in channel 1

Scattering length will be greatly enhanced $a(B) = a_{bg} \left(1 - \frac{\Delta}{B - B_0} \right)$



 a_{bg} : background scattering length Δ : width of resonance B_0 : position of the resonance

Ultra-cold Feshbach molecular

For large positive values of scattering length a, Feshbach molecular state exists, with binding energy $E_b = \hbar^2/(2\mu a^2)$, μ is the reduced mass



Chin, et al., RMP 82, 1225 (2010)

Forming Feshbach molecule





Magnetic field is ramped across the resonance \Rightarrow adiabatically convert interacting atom pairs into one molecule

Or radio frequency field drives the transition from scattering state to molecular state

Study ultra-cold chemistry with Feshbach molecules

Ultracold chemistry weakly bound molecules

Exothermic reactions with weakly bound molecules

Stwalley, Contemp. Phys. 19, 65 (1978); Can. J. chem. 82, 709 (2004)
✓ Novel reaction: Single reaction channel dominant
✓ Weakly bound molecules do not exist at high temperatures

☑ Ultracold chemistry with Feshbach molecules!

Reqiurement: weakly bound reactant and product molecules coexist

Overlapping

Feshbach resonances

D'Incao et al., PRL 103, 083202 (2009)

- Released energy small and tunable
- Reaction products can be trapped and observed
- State-to-state reaction dynamics



Ultra-cold exothermic reaction with Feshbach molecules

 $A_2 + B \rightarrow AB + A$ (A, B are different internal states of Cs atom)



Lompe et al., PRL105, 103201 (2010)





Only overall loss rate of molecule reactant is measured State-to-state reaction dynamics remains challenging!

Na-Kultra-cold Bose-Fermi mixture

• Detect the atom and molecule products

Our goal:

- Demonstrate the selectivity of the reaction
- Study the state-to-state reaction dynamics

Overlapping Feshbach		B ₀	ΔB
resonance of ²³ Na ⁴⁰ K dimers	2211 14 4	96.5	0.5
(⁴⁰ K: Fermion, ²³ Na: Boson) ²³ Na 1,1 $\rangle \rightarrow A$ Mimicking reactions with ⁴⁰ K 9/2, -5/2 $\rangle \rightarrow B$ internal states of atoms: ⁴⁰ K 9/2, -3/2 $\rangle \rightarrow C$	²³ Na 1,1>+ ⁴⁰ K 9/2,-5/2>	106.9	1.8
		138	30
	²³ Na 1,1>+ ⁴⁰ K 9/2,-3/2>	116.9	0.5
		129.5	4.6
$\mathbf{K}[\mathbf{y}/\mathbf{z}, -\mathbf{y}/\mathbf{z}] \rightarrow \mathbf{C}$		175	20

Reaction: $AB + C \rightarrow AC + B$

Park et al., PRA 85, 051602 (2012)

Na-Kultracold Bose-Fermi mixture

Experimental setup



Initial state: ~3×10⁵ ²³Na, ~1.6×10⁵ ⁴⁰K @ 500-600 nK

Form Feshbach molecules

Preparing AB from A and C: $AB + C \rightarrow AC + (B)$ Reaction product to be identified

If preparing AB from A and B: 🗵 Low conversion efficiency 🗭 residual B

Radio frequency association @ B~130 G, RF Rabi frequency ~ 20 kHz



Klempt et al., PRA 78,061602 (2008)

Ulmanis et al., NJP 17, 055009 (2015)

Characterizing Feshbach resonances

Measuring binding energy of the Feshbach molecules: Dissociation to internal state ${}^{40}K|9/2,-7/2>$



Characterizing Feshbach resonances

Binding energies of two Feshbach molecules



Overlapping Feshbach resonances

Binding energy and released energy in a reaction



Observation of atom product B

Prepare the reactants and observe the products



Observation of atom product B

Prepare the reactants and observe the products



- ✓ B and AB signals are clearly separated in rf spectrum
- ✓ B atom appears in the desired magnetic window

Strong evidence but not smoking gun

Breaking AB molecule due to unknown mechanism can also produce B atom
 Observe AC molecule product!

Observation of molecule product



• But in small AC binding energy region, since its narrow magnetic field window, creation of AB molecule from A+C is suppressed: coexist two resonances, the creation efficiency of AB is $F_{\rm bf} \propto (1 - a_{\rm AC}/a_{\rm AB})^2$, $a_{\rm AC(B)}$ are scattering length

Chin et al., PRA 71,012713 (2005)

Observation of molecule product

Solution:

- Association AB from $A + |9/2, -7/2\rangle$
- Two π pulses to prepare C

Atomic peak of C

- Dissociation AC into $A + |9/2, -1/2\rangle$
- $|9/2, -1/2\rangle$ initially unoccupied



Observation of the molecule product: smoking gun!

 $|-3/2\rangle \rightarrow |-1/2\rangle$ Dissociation freq. (kHz)

100

150

300

100

200

5

0

0

State-to-state reaction dynamics

Reaction dynamics

$$\dot{N}_{AB} = -\gamma_{AB}N_{AB},$$

$$\dot{N}_{B} = \beta_{r}\bar{n}_{C}N_{AB},$$

Solution

$$N_{B}(t) = N_{AB}(0)e^{-\gamma_{AB}t},$$

$$N_{B}(t) = \frac{\beta_{r}\bar{n}_{C}N_{AB}(0)}{\gamma_{AB}}(1 - e^{-\gamma_{AB}t}) + N_{B}(0)$$

Reaction rate coefficient

$$\beta_{r} = \frac{\Delta N_{B}\gamma_{AB}}{\alpha N_{C}N_{AB}(0)}$$

with $DN_{B} = N_{B}(\infty) - N_{B}(0)$ and $\partial = \left(\frac{m_{K}\overline{w}_{K}^{2}}{4\rho k_{B}T_{K}}\right)^{3/2}$



 $N_{(.)}$: number of atom or molecule \overline{n}_C : average density of C atom γ_{AB} : decay rate of AB molecule $\overline{\omega}_K$: average trap frequencies of K atom

✓ Obtain the reaction rate coefficient in the exothermic regime

Rui et al., Nature Physics 13, 699 (2017)

Physical chemistry

Manipulation of ultra-cold molecules



New frontier of physical chemistry!

> Physical chemistry: study the molecule collisions at the quantum level

- > Major problems:
 - Potential energy surface (PES): solve the multi-electron Schrödinger equation for fixed nuclei configuration
 - Collision or reaction dynamics: simulate the dynamics of the nuclei under the PES

Physical chemistry

However, solving multi-electron Schrödinger equation to obtain PES is extremely difficult!

a few nuclei + many electrons + coulombic interaction

$$H = \sum_{\alpha} \frac{p_{\alpha}^2}{2m_n} + \sum_{i} \frac{p_i^2}{2m_e} + \sum_{\alpha,\beta} \frac{Z_{\alpha}Z_{\beta}}{|R_{\alpha} - R_{\beta}|} + \sum_{i,j} \frac{e^2}{|r_i - r_j|} - \sum_{\alpha,i} \frac{Z_{\alpha}e}{|R_{\alpha} - r_i|}$$







H atom

• Exactly solvable

 H_2 molecule

- Born-Oppenheimer potential
- Two-nuclei problem

 $H+H_2$ collision

Potential energy surface

.

Three-nuclei dynamics

Molecule collisions

Conventional way: obtaining information of PES by experiments



Molecule beam scattering: state-to-state collision dynamics
D. Herschbach and Y. T. Lee, Nobel Prize in Chemistry (1986)
Prepare the collision particles in a vibrational and rotational state

> Detecting the collision products resolving the vibrational and rotational state, angular distribution

Quantum phenomenon is difficult to observe in molecule collisions (conventional collisions @ a few hundred Kelvin)

- Average of many partial waves
- Average of many internal states
- Short de Broglie wave length

Cold collisions

Cold collisions @ a few Kelvin or sub Kelvin

- ✓ Suppression of high partial waves
- ✓ Initial states easily prepared
- ✓ Long de Broglie wave length

Scattering resonance is remarkable quantum phenomenon

- Collision energy coincides with a bound state (Feshbach or shape resonances)
- Extremely sensitive to the details of PES = Direct probe of PES!



Yuan Tseh Lee, Molecular Beam studies of elementary chemical process (Nobel Lecture), Angew. Chem. 26, 939 (1987)

Cold collisions

Collisional resonances with cold molecule beams

Atom-molecule reaction

• $F/Cl+H_2/HD/D_2$ reaction Skodje et al., PRL 85, 1206 (2000) Qiu, et al., Science 311, 1440 (2006) Dong et al., Science 327, 1501 (2010) Wang et al., Science 342, 1499 (2013) Yang et al., Science 347, 60 (2015) • He+H₂ ionization Henson, et al., Science 338, 234 (2012) Lavert-Ofir, et al., Nat. Chem. 6, 332 (2014) Klein et al., Nat. Phys. 13, 35 (2017)

Atom-molecule inelastic collision

• He+NO/CO

Vogels et al., Science 350, 787 (2015) Bergeat et al., Nat. Chem. 7, 349 (2015)

Molecule-molecule inelastic collision

• O₂+H₂

Chefdeville et al., Science 341, 1094 (2013)

• HD+D₂

Perreault et al., Science 358, 356 (2017)

• NO+H₂

Vogels et al., Nat. Chem. 10, 435 (2018)

These questions can be effectively solved with numerical calculations

Ultra-cold collision

Collision at nearly absolutely zero temperatures

🗹 Single partial wave	🗹 Long de Broglie wavelength
🗹 Single quantum state	🗹 Highly quantum mechanical

Scattering resonance is a rule rather than an exception $@ \sim 0 K$

Collisions involving light particles (Rb+OH, N+NH, Mg+NH, O_2+O_2 ...)

- Computation possible
- Many predictions
- Lack of experimental demonstrations



Ultra-cold collision

Collisions involving alkali-metal (heavy molecules) diatomic molecules



Mayle et al., PRA 85 062712 (2012)

Computation extremely difficult

- Heavy molecules
- Deep potential energy surface
- Many closed channels
- Highly resonant
- Many nuclear spin and electron spin degrees of freedom

Ultra-cold collision

Collisions involving alkali-metal (heavy molecules) diatomic molecules

Created alkali-metal diatomic molecules

- RbK, JILA (2008)
- RbCs, Innsbruck, Durham
- NaRb, HongKong
- LiNa, MIT
- NaK, MIT, MPQ



Possible atom-molecule collisions

Na + LiNa	Rb + NaRb
K+LiK	Cs + NaCs
Rb + LiRb	Rb + KRb
Cs + LiCs	Cs + KCs
K + NaK	Cs + RbCs

We are interested in the collision between NaK molecules and K atoms

Ultra-cold molecule

²³Na⁴⁰K+⁴⁰K ultra-cold collision

- Deep PES ~ 1900 cm⁻¹
- Statistical model estimates ~ 1 resonance per G

	-	-			$(\text{units of } E_{\text{vdW}}^{-1})$
K + NaK	1851	6297	1.22	0.150	0.18



"For s-wave resonances... measurements of two-body loss versus field for molecules in their first excited state would supply a reasonable observable"

Mayle, et al., PRA 85 062712 (2012)



Transfer Feshbach molecule to rovibrational state

Feshbach molecules are weakly bound molecules, but not conventional molecules in rovibrational state **>**

Transformed to rovibrational state with Stimulated Raman adiabatic passage (STIRAP)



$$\tan \Theta = \frac{\Omega_P(t)}{\Omega_S(t)}$$



Stimulated Raman adiabatic passage

Transfer Nak Feshbach state to rovibrational state



Park et al., PRL 114, 250302 (2015)

Hyperfine levels

Energy levels of ground state NaK



4 hyperfine levels of the rovibrational ground sate are selected

hyperfine ground state



Observation of enhanced loss

At fixed magnetic field ~100G, close to atomic Feshbach resonance





- 20 spin states combinations:
 ⁴⁰K in |9/2,-9/2>...|9/2,-1/2> and 4 hyperfine levels of NaK molecule
- Measure molecule loss
- Extract loss rate coefficient

Observation of enhanced loss



Sweep the magnetic field



 Residual magnetic field induced by eddy current
 Compensate the residual magnetic field by programing the current of the magnetic coil

Loss features



nethod	collision channel	$B_0(G)$	$\Delta B(G)$
	0,0,-3/2,-2> 9/2,-3/2>	101.4	0.6
Ι	0,0,-3/2,-2> 9/2,-7/2>	101.1*	0.2
	0,0,-1/2,-3> 9/2,-7/2>	101.0	0.2
	$ 0,0,-3/2,-2\rangle$ $ 9/2,-5/2\rangle$	68.0	1.6
		74.2	3.5
		83.2	2.0
II	$ 0,0,-3/2,-2\rangle$ $ 9/2,-7/2\rangle$	54.5	0.6
		59.1	3.7
		101.0*	0.6
		106.7	1.7
	$ 0,0,-3/2,-2\rangle$ $ 9/2,-9/2\rangle$	48.1	2.6
		89.8	2.9

- 8 new loss features are observed in the range 43-120 G, in total 11 atom-molecule Feshbach resonances in ²³Na⁴⁰K+⁴⁰K ultra-cold collisions
- Probe the K-Na-K PES (49 electrons +3 nuclei) with exceptional resolution

Yang et al., Science 363, 261 (2019)

Outlook

Many open questions in ultracold Chemistry:

- Density of resonant states
- The role of nuclear spins in the collisions
- Detect the collision product

....

Association of triatomic molecule



Part V: Towards Fermi-Hubbard model Fermi-Fermi/Bose Mixture

Yao et al., PRL 117 145301 (2016) Yao et al., Nature Physics 15, 570-576 (2019)

Fermi-Hubbard model

Advanced quantum materials: driving force of the modern technology

- High T_c superconductor
- Carbon nanotube

.....

• Giant magnetoresistance



Key problem: understanding the electron correlation in lattices The most important model: Fermi-Hubbard model (P. W. Anderson)

$$\widehat{H} = \left\{-\sum_{\langle n,m \rangle} (\widehat{c}_{n,\sigma}^{\dagger} \widehat{c}_{n,\sigma} + h.c.) + \left[U\sum_{n} \widehat{n}_{n,\uparrow} \widehat{n}_{n,\downarrow}\right]$$
Funneling between lattice sites On-site interaction

Quantum simulation of Fermi-Hubbard model



> High temperature superconductor may exist in this region (d-wave superconductivity)

> Many other interesting quantum phenomenon:

Quantum magnetism, pseudo-gap physics, doping and pairing.....

With two-species mixture of Li and K atoms Fermi-Fermi (Bose) mixture

To explore particle doping system

Bose and Fermi double superfluid with strong coupling heteronuclear particles

In real materials:

- ✓ ⁴He (Boson) superfluidity was achieved in 1938
- ✓ ³He (Fermion) superfluidity was achieved in 1972
- ☑ Uncontrollable strong interactions between the two isotopes makes mixture unstable
 - ➡ Double superfluidity of ⁴He and ³He has not been observed

With ultra-cold atoms (⁶Li, Fermion, ⁴¹K, Boson):

- Conclusive evidence of the double superfluidity: co-existence of vortex lattices in two isotopes
- ✓ Density deformation caused by strong coupling between two species

Yao et al., PRL 117 145301 (2016)



To explore d-wave superfluidity

Difficulties for d-wave Feshbach resonances:

⊠ Narrow resonances width (~mG) → hard to manipulate

 \boxtimes Short lifetime (~ms) \Rightarrow far less than the many-body equilibrium time

⊠ High temperature (~100µk) → quite short De Broglie wavelength, dominated by classical physics



Outlook



Loading mixtures in optical lattices, to find novel cooling method for lower entropy system



Developing high-efficient numerical methods to benchmark experiments



Developing single-site addressing techniques for the two species



Open question: How to detect d-wave superfluid?

Summary

Quantum computation will both call on and enable algorithms for increasingly sophisticated quantum gadgetry. Within 100 years it will become the central method of chemistry and materials science.



Physics in 100 years, Frank Wilczek, Physics Today 69, 32 (2016) Thank you for your attention!