Exploring Quantum Matter with Ultracold Atoms

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Course Outline



- Introduction to UCG
- Interactions (Scattering, Feshbach, ...)
- Introduction to Optical Lattices
- Detection Techniques
- Many-Body Physics in Optical Lattices
 - Bose Hubbard Model
 - Fermi Hubbard Model
- Controlling Few Body Physics
 - Repulsively Bound Pairs, Correlated Atom Tunneling
 - Superexchange Interactions
 - Creating & Probing Entangled Atom States
 - Minimal Versions of Topologically Ordered States (RVB, d-Wave,...)
- Non-Equilibrium Dynamics
- Outlook
 - Polar Molecules, Rydberg Atoms

The Challenge of Quantum Many Body Systems

- Understand and Design Quantum Materials one of the biggest challenge of Quantum Physics in the 21st Century
- Technological Relevance

High-Tc Superconductivity (Power Delivery)

Magnetism (Storage, Spintronics...)

Novel Quantum Sensors (Precision Detectors)

Quantum Computing



Many cases: lack of basic understanding of underlying processes Difficulty to separate effects: probe impurities, complex interplay, masking of effects... Many cases: even simple models "not solvable" Need to synthesize new material to analyze effect of parameter change

Strongly Correlated Electronic Systems



Underlying many solid state & material science problems: Magnets, High-Tc Superconductors, Spintronics

Roadrunner – Los Alamos



State of the art: < 40 spins (2⁴⁰x 2⁴⁰) (what does it take to simulate 300 spins ?)

each doubling allows for one more spin 1/2 only

2³⁰⁰ estimated number of protons in the universe

Introduction

• Controlling Single Quantum Systems



Single Atoms and Ions



Photons



Quantum Dots

• New challenges ahead: control, engineer and understand complex quantum system

quantum computers, quantum simulators, novel (states of) quantum matter, advanced materials, multi-particle entanglement





R. P. Feynman's Vision

A Quantum Simulator to study the quantum behaviour of another system.

R.P. Feyman, Int. J. Theo. Phys. (1982) R.P. Feynman, Found. Phys (1986)

From a Classical Gas to a Bose-Einstein-Condensate



Why is it Difficult to Reach BEC?



JNIVERSITÄT

The Path to Bose-Einstein Condensation







Magnetic Traps for Neutral Atoms



Energy of an atom in an external magnetic field

$$E = -\vec{\mu} \cdot \vec{B}$$

Force on an atom in an inhomogeneous field

$$\vec{F} = -\mu \cdot \nabla B$$







Evaporative Cooling



With the help of RFtransitions between neighbouring magnetic sublevels, the hottest atoms can be selectively removed from the trap.





Elastic collisions rethermalize the atoms resulting in a cooler and denser atomic distribution.



Phase space density
is increased



- I. Magneto Optical Trap (MOT) (10⁹ atoms)
- 2. Compressed MOT to increase density of atom cloud
- 3. Optical molasses mooling
- 4. Optical pumping to spin polarize atoms
- 5. Magnetic trapping
- 6. Evaporative cooling
- 7. Bose-Einstein condensation (10^{5} - 10^{6} atoms) around temperatures of 1μ K and densitied of 10^{14} cm⁻³



From a Bose Gas without Interactions to a Strongly Correlated Bose System















Our Starting Point – Ultracold Quantum Gases

Parameters: Densities: 10¹⁵ cm⁻³ Temperatures: Nano Kelvin Atom Numbers 10⁶

Ground States at T=0



Bose-Einstein Condensates e.g. ⁸⁷Rb Degenerate Fermi Gases e.g. ⁴⁰K

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From Artificial Quantum Matter to Real Materials



New tunable model systems for many body systems!

Atomic Interactions

Scattering Theory

Schrödinger Equation of Scattering Problem

$$\hat{H}_0 + \hat{U}(\mathbf{r}) | \boldsymbol{\psi}_k \rangle = E | \boldsymbol{\psi}_k \rangle$$



Wave function in far-field (outside region of scattering potential)

$$\Psi_k^+ = e^{i\mathbf{k}\mathbf{r}} + f(\mathbf{k}, \mathbf{k}')\frac{e^{ikr}}{r}$$



Scattering Cross Section

Differential Scattering Cross Section

 $\frac{d\sigma}{d\Omega} = \frac{\text{Rate of particles scattered into solid angle } d\Omega}{\text{incident particle flux}}$

Particle flux

$$\mathbf{j} = \frac{\hbar}{m} \operatorname{Im} \left\{ \Psi^* \nabla \Psi \right\}$$

we obtain

$$\left(\frac{d\sigma}{d\Omega} = |f(\theta)|^2\right)$$

total scattering cross section

$$\sigma = \int rac{d\sigma}{d\Omega} d\Omega$$



Partial Wave Expansion

For spherically symmetric scattering potential we can write (partial wave decomposition)

$$\psi_k = \sum_{l=0} A_l P_l(\cos\theta) R_l(r)$$

For every angular momentum I, we obtain radial wave equation

$$\left(\frac{\hbar^2}{2m}\left\{-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{l(l+1)}{r^2}\right\} + U(r)\right)R_l(r) = ER_l(r)$$

For free particle motion (U=0), this corresponds to the differential equation of the spherical Bessel functions.

$$R_l(r) \propto \cos \delta_l j_l(kr) + \sin \delta_l n_l(kr)$$

This yields in the far field limit:

$$R_l(r) \underset{r \to \infty}{\propto} \frac{1}{kr} \sin(kr + \delta_l - l\frac{\pi}{2})$$



Scattering Phase Shift & Scattering Amplitude

We can relate the scattering phase shift δ_l to the scattering amplitude, via:

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1)e^{i\delta_l} \sin \delta_l P_l(\cos \theta)$$

scattering cross section

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

unitarity limit for partial wave cross sections

$$\sigma_l \leq \frac{4\pi}{k^2}(2l+1)$$



s-Wave Scattering

Far field radial wave function

$$R_0(r) \propto_{r \to \infty} \frac{1}{kr} \sin(kr + \delta_0)$$

For $r_0 < r < 1/k$ we can approximate the above to

$$R_0 \approx 1 + \frac{\delta_0}{kr} = 1 - \frac{a}{r}$$

Scattering Length

$$a = -\frac{\delta_0}{k} \qquad \tan \delta_0 \simeq -ka$$

Scattering amplitude (including effective range)

$$f(k) = \frac{1}{k \cot \delta_0(k) - ik} \to -\frac{a}{1 - ar_e k^2/2 + ika}$$



Scattering from Attractive Square Well Potential





Scattering Wave Functions





Scattering Length (Box Potential)



Resonances for:
$$\kappa_0 r_0 = (n+1/2)\pi$$



Weakly Bound "Halo" States

Very extended "*Halo states*" are formed close to a Feshbach Resonance for a>0. These correspond to weakly bound states that enter the potential well.

Binding energy of Halo state

$$E_b = -\frac{\hbar^2}{2ma^2}$$

Wave function of Halo state





Some s-wave Scattering Spheres





Multiple scattering spheres become between different momentum components become visible!

Images shown after time of flight period.



Scattering of Bosons



from. Ch. Buggle (thesis UoA 2005)



Pseudopotential

For ultracold collisions, scattering between particles is characterized by a single parameter - the scattering length.

We can replace the molecular scattering potential with alternative potential that gives same scattering length!

e.g. Pseudopotential

$$U(\mathbf{r})(\cdots) = \frac{4\pi\hbar^2}{2m_r k \cot \delta_0} \delta(\mathbf{r}) \frac{\partial}{\partial r} r \cdots = \frac{4\pi\hbar^2 a}{2m_r} \delta(\mathbf{r}) \frac{\partial}{\partial r} r \cdots$$

For regular functions at the origin, this latter derivative may be omitted:

$$U(\mathbf{r})(\cdots) = \frac{4\pi\hbar^2 a}{2m_r} \delta(\mathbf{r})\cdots$$



Identical Particle Scattering

For scattering of identical particles, the scattering wave-function has to obey the right symmetry under particle exchange!

$$\boldsymbol{\psi}_{k}(\mathbf{r}) = \frac{1}{\sqrt{2}} \left[e^{ikz} \pm e^{-ikz} + (f_{k}(\boldsymbol{\theta}) \pm f_{k}(\boldsymbol{\theta} + \boldsymbol{\pi})) \frac{e^{ikr}}{r} \right]$$

+ for Bosons, - for Fermions

Leads to constructive or destructive interference in partial wave amplitudes!

Identical Boson: s,d,f... wave scattering (even partial waves) Identical Fermions: p,g,h... wave scattering (odd partial waves)

$$\sigma = \int |f(\theta) \pm f(\theta \pm \pi)|^2 d\Omega = \frac{8\pi}{k^2} \sum_{l=e,o} (2l+1)^2 \sin^2 \delta_l$$

s-wave scattering

distinguishable particles $\sigma = 4\pi a^2$ indistinguishable particles $\sigma = 8\pi a^2$

Consequence: no s-wave scattering for identical fermions!



Feshbach Resonance



Potential curves of open and closed scattering channels.

Scattering length and binding energy of weakly bound state across Feshbach resonance.



Feshbach Resonances - Experiment







S. Cornish et al. PRL



Converting Atoms Pairs into Bound Molecules





Creating a MBEC out of a Fermi Gas



Molecular Bose-Einstein Condensates



S. Jochim et al., Science, 2003 (Innsbruck)

M. Greiner, C. Regal and D. Jin Nature, 2003 (JILA)





M. W. Zwierlein et al., Phys. Rev. Lett, 2003 (MIT)

see also Ch. Salomon (ENS) and J. Thomas (Duke)

Atoms in Periodic Potentials

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Optical Lattice Potential – Perfect Artificial Crystals



Periodic intensity pattern creates 1D,2D or 3D light crystals for atoms (Here shown for small polystyrol particles).

1D, 2D & 3D Lattices



2D Lattices Array of one-dimensional quantum systems

3D Lattices Array of quantum dots

...and in Higher Dimensions



Tunnel Coupling Tunable!

...and in Higher Dimensions



Tuning the Dimensionality

$$H\phi_q^{(n)}(x) = E_q^{(n)}\phi_q^{(n)}(x)$$
 with $H = \frac{1}{2m}\hat{p}^2 + V(x)$

Solved by Bloch waves (periodic functions in lattice period)

$$\phi_q^{(n)}(x) = e^{iqx} \cdot u_q^{(n)}(x)$$

q = Crystal Momentum or Quasi-Momentum *n* = Band index

Plugging this into Schrödinger Equation, gives:

$$\left[H_B u_q^{(n)}(x) = E_q^{(n)} u_q^{(n)}(x) \quad \text{with} \quad H_B = \frac{1}{2m} (\hat{p} + q)^2 + V_{lat}(x) \right]$$

Single Particle in a Periodic Potential - Band Structure (2)

Use Fourier expansion

$$V(x) = \sum_{r} V_r e^{i2rkx} \quad \text{and} \quad u_q^{(n)}(x) = \sum_{l} c_l^{(n,q)} e^{i2lkx}$$

yields for the potential energy term

$$V(x)u_{q}^{(n)}(x) = \sum_{l} \sum_{r} V_{r} e^{i2(r+l)kx} c_{l}^{(n,q)}$$

and the kinetic energy term

$$\frac{(\hat{p}+q)^2}{2m}u_q^{(n)}(x) = \sum_l \frac{(2\hbar kl+q)^2}{2m}c_l^{(n,q)}e^{i2lkx}.$$

In the experiment standing wave interference pattern gives

$$V(x) = V_{lat} \sin^2(kx) = -\frac{1}{4} \left(e^{2ikx} + e^{-2ikx} \right) + \text{c.c.}$$

Single Particle in a Periodic Potential - Band Structure (3)

Use Fourier expansion

$$\sum_{l} H_{l,l'} \cdot c_l^{(n,q)} = E_q^{(n)} c_l^{(n,q)} \quad \text{with} \quad H_{l,l'} = \begin{cases} (2l+q/\hbar k)^2 E_r & \text{if } l = l' \\ -1/4 \cdot V_0 & \text{if } |l-l'| = 1 \\ 0 & \text{else} \end{cases}$$

$$\begin{pmatrix} (q/\hbar k)^{2} E_{r} & -\frac{1}{4} V_{0} & 0 & 0 & \dots \\ -\frac{1}{4} V_{0} & (2+q/\hbar k)^{2} E_{r} & -\frac{1}{4} V_{0} & 0 & \\ 0 & -\frac{1}{4} V_{0} & (4+q/\hbar k)^{2} E_{r} & -\frac{1}{4} V_{0} & \\ & & -\frac{1}{4} V_{0} & \ddots & \\ & & & & \end{pmatrix} \begin{pmatrix} c_{0}^{(n,q)} \\ c_{1}^{(n,q)} \\ c_{2}^{(n,q)} \\ \vdots \end{pmatrix} = E_{q}^{(n)} \begin{pmatrix} c_{0}^{(n,q)} \\ c_{1}^{(n,q)} \\ c_{2}^{(n,q)} \\ \vdots \end{pmatrix}$$

Diagonalization gives us Eigenvalues and Eigenvectors!

Bandstructure - Blochwaves



Wannier Functions

An alternative basis set to the Bloch waves can be constructed through localized wavefunctions: Wannier Functions!



Dispersion Relation in a Square Lattice

$$E(q) = -2J\cos(qa)$$



Measuring Momentum Distributions

Time of flight interference pattern



Momentum Distributions – 1D

Momentum distribution can be obtained by Fourier transformation of the macroscopic wave function.

$$\Psi(x) = \sum_{i} A(x_j) \cdot w(x - x_j) \cdot e^{i\phi(x_j)}$$



Preparing Arbitrary Phase Differences Between Neighbouring Lattice Sites



lattice potential + potential gradient

Phase difference between neighboring lattice sites

$$\Delta \phi_j = (V'\lambda/2)\,\Delta t$$

(cp. Bloch-Oscillations)



 $\Delta \phi = 0$



 $\Delta \phi = \pi$

But: dephasing if gradient is left on for long times !

Mapping the Population of the Energy Bands onto the Brillouin Zones



Experimental Results







3D

Populating Higher Energy Bands



From a Conductor to a Band Insulator



Fermi Surfaces become directly visible!

M. Köhl et al. Physical Review Letters (2005)