Ultracold quantum scattering - Part I: Single-channel multi-partial-wave elastic collisions

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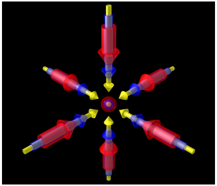
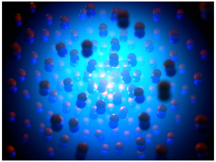
What is ultracold matter?

Cold (< 1K) and ultracold (< 1mK) gases



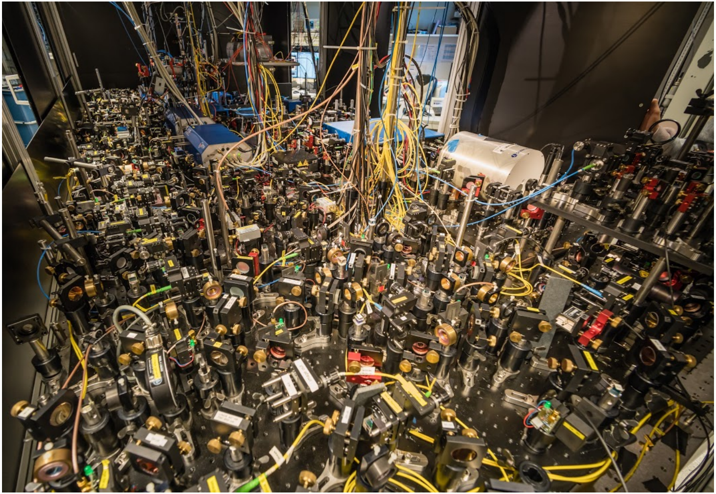
In magnetic, electric, optical traps



Fully controllable quantum objects

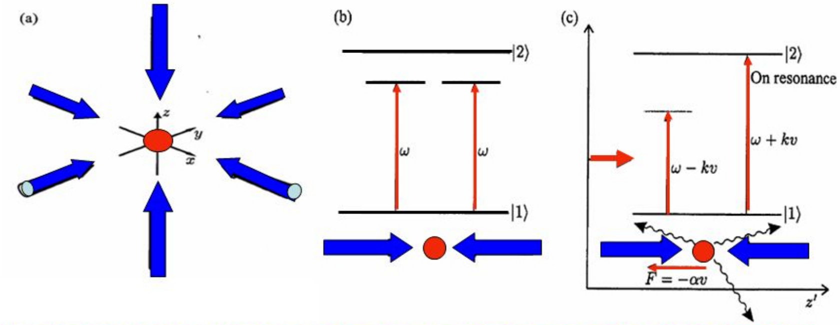
Experiments with ultracold atoms

Typical lab of quantum atomic opticians



Lab of Immanuel Bloch

Laser Doppler cooling

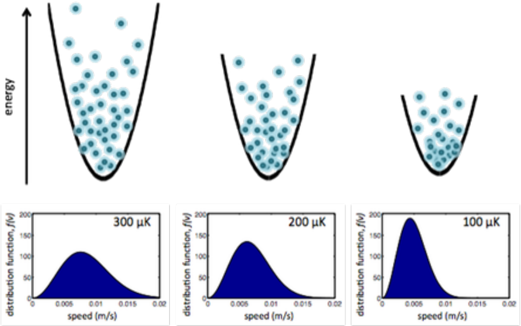


W. D. Phillips, Rev. Mod. Phys. 70, 721 (1998)

Slowing by the directional **momentum transfer** with red-detuned **photons** in a magneto-optical trap

Nobel 1997

Evaporative cooling

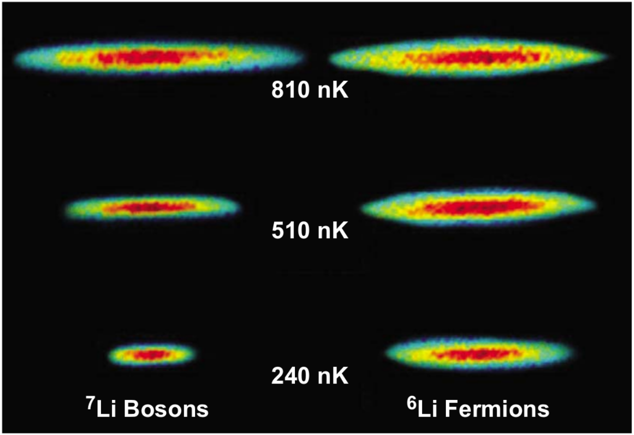


E. A. Cornell, C. E. Wieman, Rev. Mod. Phys. 74, 875 (2002)

Cooling by **removing** the warmest molecules slowly deceasing the trap depth with instantaneous **thermalization**

Nobel 1997

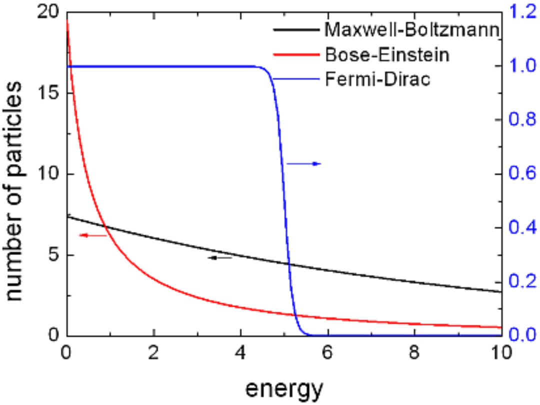
Cooling ^{6}Li and ^{7}Li



$\sim 10^6$ atoms, $n \approx 10^{13} - 10^{15}\text{cm}^{-1}$

Science 291, 2570 (2001)

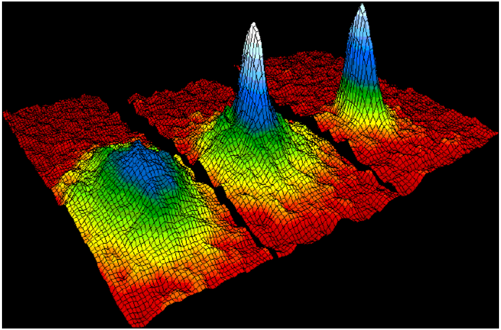
Bose-Einstein and Fermi-Dirac statistics



$$n_{\text{B-E}}(\epsilon) = \frac{1}{\exp[(\epsilon - \mu)/k_B T] - 1}$$

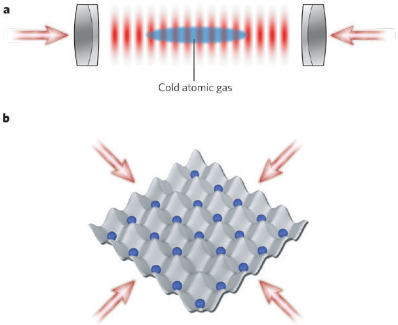
$$n_{\text{F-D}}(\epsilon) = \frac{1}{\exp[(\epsilon - \mu)/k_B T] + 1}$$

Bose-Einstein Condensation



Science 269, 198 (1995)

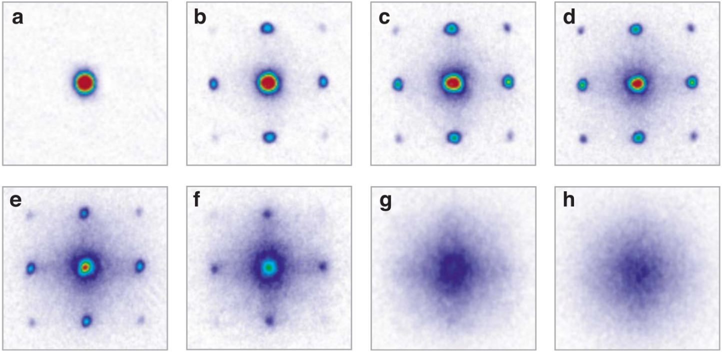
New **quantum** state of matter
Nobel 2001



Nature 415, 39 (2002)

Periodic systems of atoms in **"crystals"** of light
Nobel expected

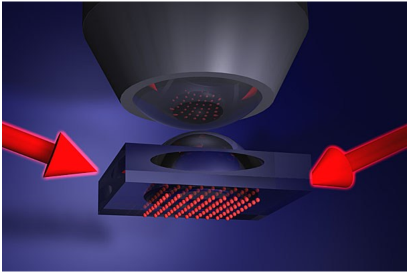
Quantum phases transitions

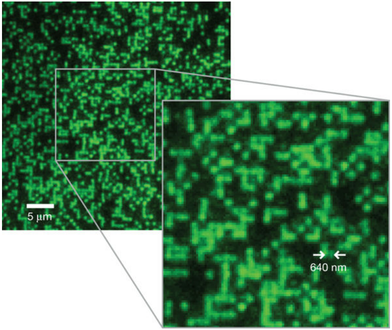


Nature 415, 39 (2002)

Quantum gas microscopy

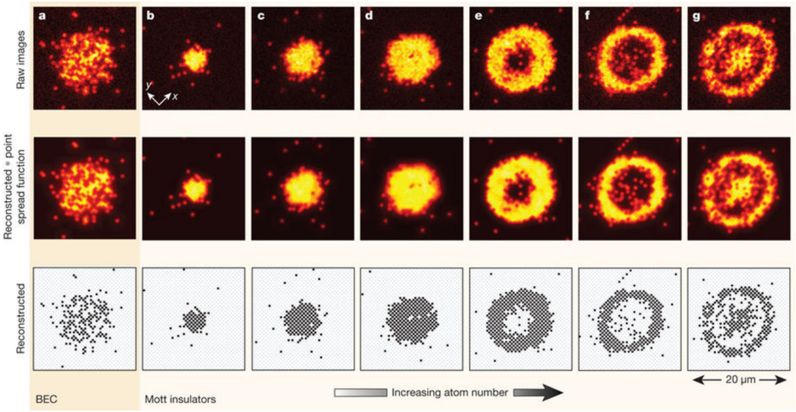
Quantum gas microscopy





Nature 462, 74 (2009) / Nature 467, 68 (2010)

Quantum gas microscopy

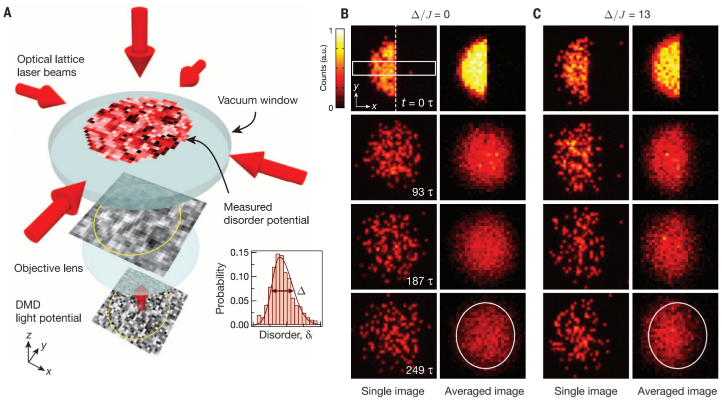


Nature 462, 74 (2009) / Nature 467, 68 (2010)

Quantum simulations

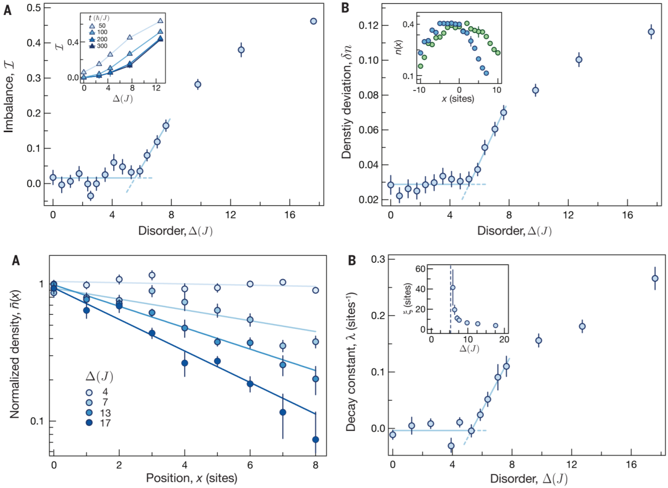
Many-body localization

$$\hat{H} = -J\sum_{\langle i,j\rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + \sum_i (\delta_i + V_i)\hat{n}_i$$



Science 352, 1547 (2016)

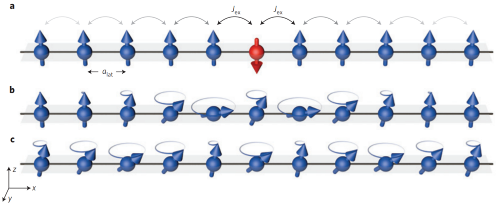
Many-body localization

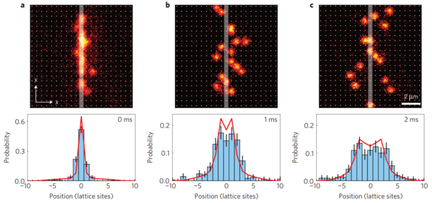


Science 352, 1547 (2016)

Quantum dynamics of a mobile spin impurity

$$\hat{H} = -J_{\mathrm{ex}} \sum_i \left[\frac{1}{2} \left(\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+ \right) + \Delta \hat{S}_i^z \hat{S}_{i+1}^z \right]$$

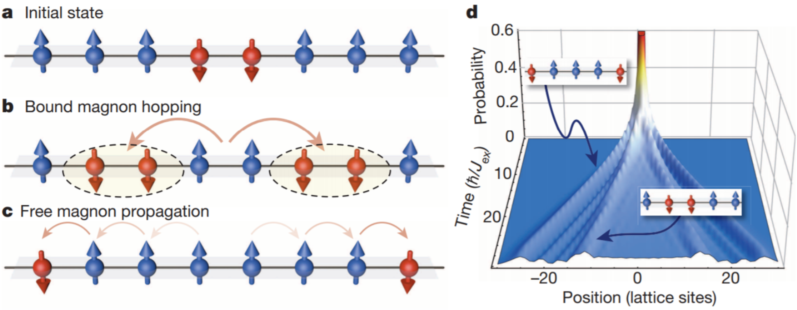




Nature Physics 9, 235 (2013)

Magnon bound states and their dynamics

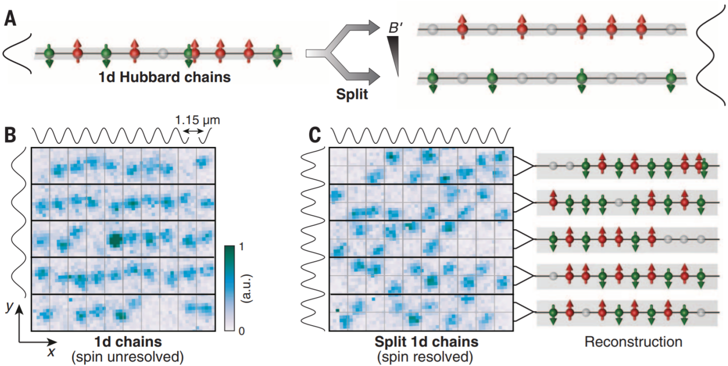
$$\hat{H} = -J_{\text{ex}} \sum_i \left[\frac{1}{2} \left(\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+ \right) + \Delta \hat{S}_i^z \hat{S}_{i+1}^z \right]$$



Nature 502, 76 (2013)

Spin- and density-resolved Fermi-Hubbard chains

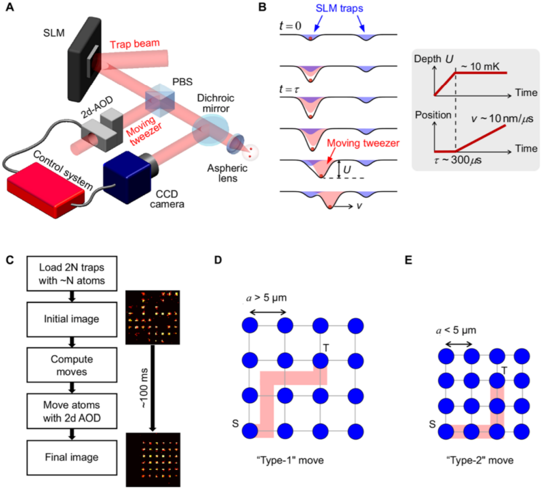
$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma}) + U \sum_{i=1}^{N} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



Science 353, 1257 (2016) / Science 354, 1024 (2016)

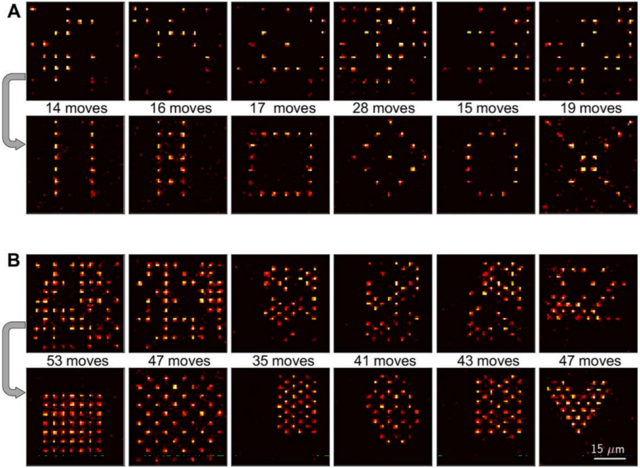
Atom-by-atom assemblers

Atom-by-atom assembler of defect-free atomic arrays



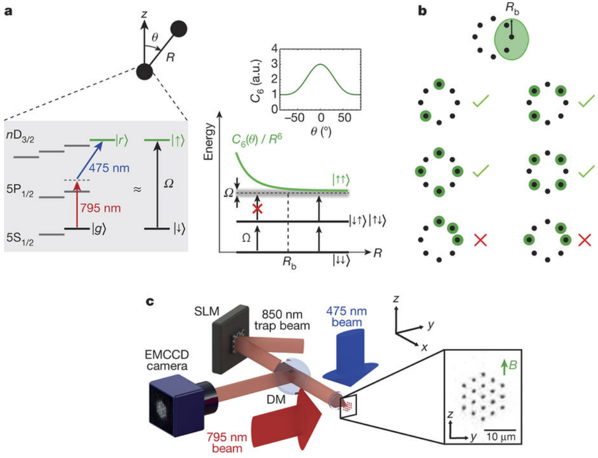
Science 354, 1021 (2016) / Science 354, 1024 (2016).

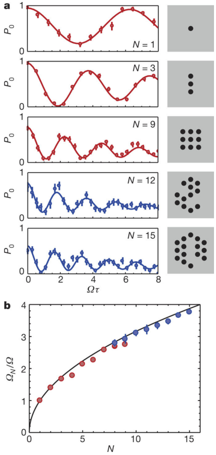
Atom-by-atom assembler of defect-free atomic arrays



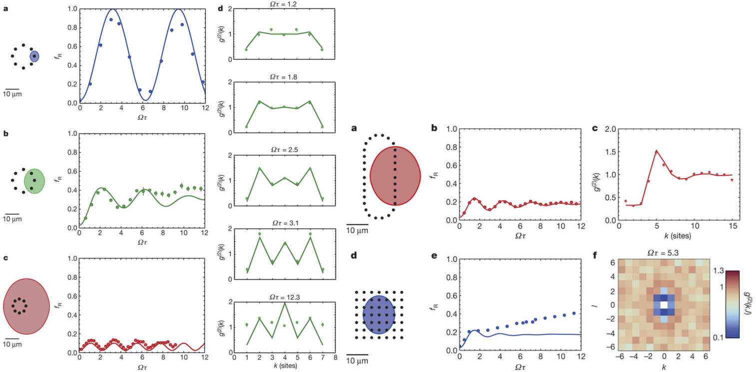
Science 354, 1021 (2016)

Rydberg atoms arrays for realizing quantum Ising models





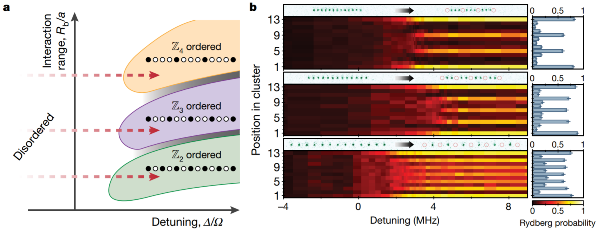
Nature 534, 667 (2016)

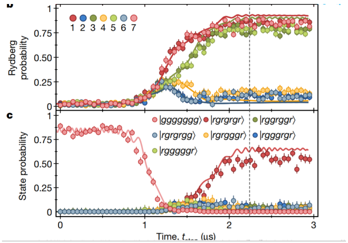


Nature 534, 667 (2016)

Many-atom quantum simulator

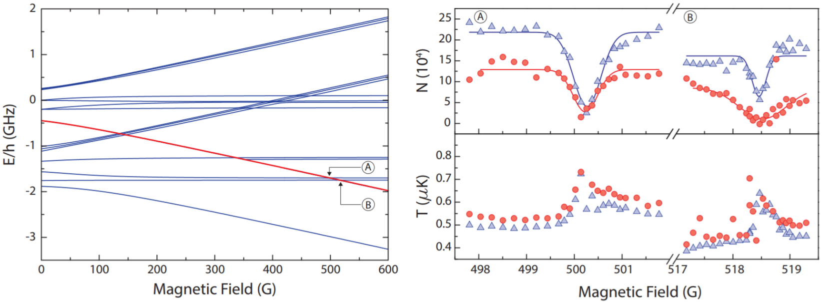
$$\frac{\mathcal{H}}{\hbar} = \sum_i \frac{\Omega_i}{2}\sigma_x^i - \sum_i \Delta_i n_i + \sum_{i<j} V_{ij} n_i n_j$$

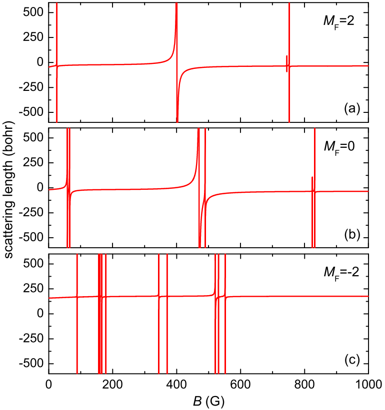


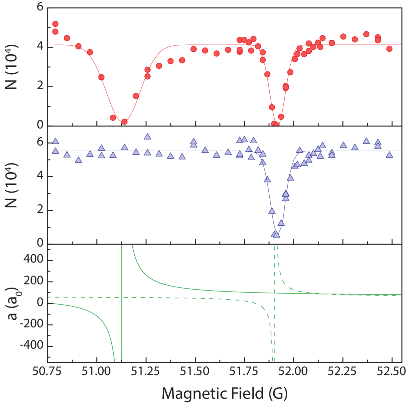


Nature 551, 579 (2017)

$^{41}K+^{41}K$

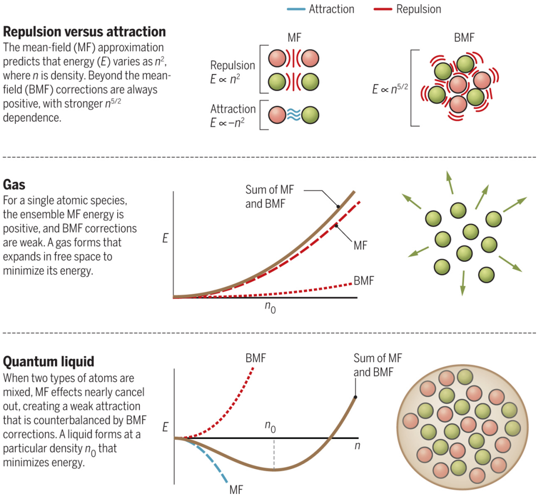






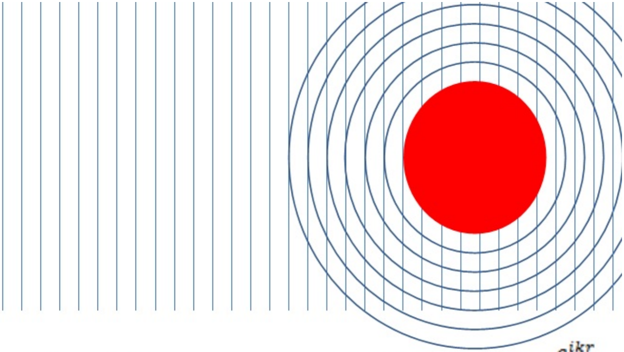
Phys. Rev. A in press (2018)

Quantum liquid droplets



Science 359, 301 (2018)

Quantum scattering theory



$\psi(z) = e^{ikz}$

$\psi(z,\theta) = e^{ikz} + f(\theta)\dfrac{e^{ikr}}{r}$

Quantum scattering - general formalism

The Schrödinger equation for the relative nuclear motion of two colliding species

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + \mathbf{V}(R,\tau) + \mathbf{H}_{\mathrm{mon}}(\tau)\right)\mathbf{\Psi}(R,\tau) = E\mathbf{\Psi}(R,\tau)\,, \qquad (1)$$

where

$\hbar^2/(2\mu)\nabla^2$ - the kinetic energy operator

μ - the reduced mass

$\tau = (\tau_A, \tau_B)$ - all coordinates (internal degrees of freedom) except the intermolecular distance R

$\mathbf{V}(R,\tau)$ - the interatomic or intermolecular interaction potential

$\mathbf{H}_{\mathrm{mon}}(\tau) = \mathbf{H}_A(\tau_A) + \mathbf{H}_B(\tau_B)$ - the Hamiltonian describing the internal degrees of freedom of the monomers A and B

$\mathbf{\Psi}(R,\tau)$ - the total wave function with the energy E.

Quantum scattering - general formalism

The total wave function can be decomposed into the basis set of N channel functions $\{\Theta_i(\tau)\}_{i=1}^{N}$

$$\mathbf{\Psi}(R,\tau) = \sum_i \Phi_i(R)\Theta_i(\tau)/R\,. \quad (2)$$

Channel functions can be or can contain spherical harmonics $Y_l^m(\theta,\phi)$ which are eigenstates of the orbital angular momentum operator for end-over-end motion of the two colliding particles around one another. Channels with different values of l are referred to as different partial waves (l-waves).

Quantum scattering - general formalism

Substituting $\mathbf{\Psi}(R,\tau)$ into the Schrödinger equation (1) gives a set of coupled equations

$$\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial R^2}+\mathbf{W}(R)\right)\mathbf{\Phi}(R)=E\mathbf{\Phi}(R)\,, \tag{3}$$

where $\mathbf{\Phi}(R)$ is a matrix of N linearly independent radial solutions and $\mathbf{W}(R)$ is a matrix describing the effective interaction, with elements given by $\mathbf{W}_{ij}(R)=\langle\Theta_i(\tau)|\mathbf{V}(R,\tau)+\mathbf{H}_{\mathrm{mon}}(\tau)|\Theta_j(\tau)\rangle$.

The long-range scattering boundary conditions on $\mathbf{\Phi}(R)$ in terms of Bessel functions

$$\mathbf{\Phi}(R)\overset{R\to\infty}{\longrightarrow}\left[\mathbf{J}(R)+\mathbf{N}(R)\mathbf{K}\right]\mathbf{A}\,, \tag{4}$$

where $\mathbf{J}(R)$ and $\mathbf{N}(R)$ are diagonal matrices with proper spherical Bessel functions and $\mathbf{A}$ is the normalization constant. $\mathbf{K}$ is the reactance matrix, which gives the $\mathbf{S}$ scattering matrix

$$\mathbf{S}=(\mathbf{1}-i\mathbf{K})^{-1}(\mathbf{1}+i\mathbf{K})\,. \tag{5}$$

The scattering length a_n, partial elastic cross section $\sigma^n_{\rm el}$, and partial inelastic cross section $\sigma^n_{\rm in}$ for channel n can be directly calculated from the **S** matrix

$$\begin{aligned} a_n =& \frac{1}{ik_n}\frac{1-S_{nn}}{1+S_{nn}} \,, \\ \sigma^n_{\rm el} =& \frac{\pi}{k_n^2}\left|1-S_{nn}\right|^2 \,, \\ \sigma^n_{\rm in} =& \frac{\pi}{k_n^2}\left(1-|S_{nn}|\right)^2 \,, \end{aligned} \tag{6}$$

where $k_n = \sqrt{2\mu(E-E^\infty_n)/\hbar^2}$ is the channel wave vector and E^∞_n denotes the threshold energy.

Single-channel multi-partial-wave scattering

for $V(R,\theta,\phi) = V(R)$, no internal structure

$$\boldsymbol{\Psi}(R,\theta,\phi) = \sum_{lm} \Phi_{lm}(R) Y_l^m(\theta,\phi)/R = \sum_l \Phi_l(R) P_l(\cos\theta)/R\,, \tag{7}$$

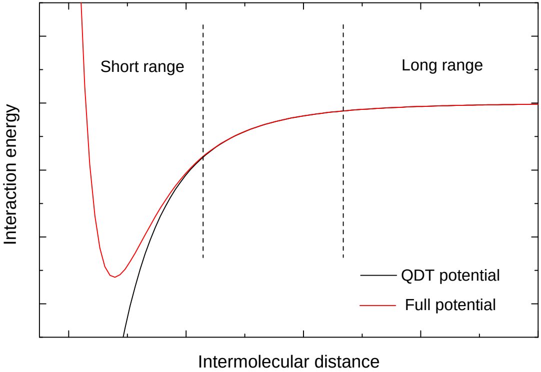
$$\hat{H}\boldsymbol{\Psi}(R,\theta,\phi) = E\boldsymbol{\Psi}(R,\theta,\phi) \tag{8}$$

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(R)\right]\boldsymbol{\Psi}(R,\theta,\phi) = E\boldsymbol{\Psi}(R,\theta,\phi) \tag{9}$$

$$\nabla^2 = \frac{1}{R^2}\left(\frac{\partial}{\partial R}R^2\frac{\partial}{\partial R} + \hat{L}^2\right) \qquad \hat{L}^2 P_l(\cos\theta) = l(l+1)P_l(\cos\theta) \tag{10}$$

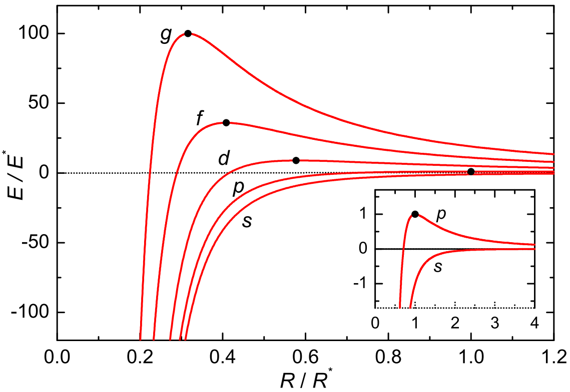
$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2} + \frac{\hbar^2 l(l+1)}{2\mu R^2} + V(R)\right]\Phi_l(R) = E\Phi_l(R) \tag{11}$$

Interaction potential - isotropic case



$$V_{\mathrm{tot}}(R) \xrightarrow{R\to\infty} \frac{\hbar^2 l(l+1)}{2\mu R^2} - \frac{C_6}{R^6}, \qquad k = \sqrt{2\mu E/\hbar^2}$$

Centrifugal barrier



$$R_6 = \left(\frac{2\mu C_6}{\hbar^2}\right)^{1/4}, \qquad E_6 = \frac{\hbar^2}{2\mu R_6^2}$$

Long-range boundary conditions

$$\Phi_l(R) \underset{R\to\infty}{\longrightarrow} kR[A_l j_l(kR) + B_l n_l(kR)] = kRA_l[j_l(kR) + K_l n_l(kR)]\,, \quad (12)$$

Spherical Bessel functions of the first and sec ond kind:

$$j_l(kR) \underset{R\to\infty}{\longrightarrow} \sin(kR - l\pi/2)/kR \qquad n_l(kR) \underset{R\to\infty}{\longrightarrow} -\cos(kR - l\pi/2)/kR \quad (13)$$

$$\Phi_l(R) \underset{R\to\infty}{\longrightarrow} A_l \sin[kR - l\pi/2] - B_l \cos[kR - l\pi/2] = A_l \sin[kR - l\pi/2 + \delta_l(k)]\,, \quad (14)$$

Long-range energy normalization:

$$\Phi_l(R) \underset{R\to\infty}{\longrightarrow} \sqrt{\left(\frac{2\mu}{\pi k}\right)}(\sin(kR - l\pi/2) + K_l \cos(kR - l\pi/2)) \quad (15)$$

Scattering phase

$$\delta_l = \arctan\left(\frac{-B_l}{A_l}\right), \qquad K_l = -\tan\delta_l, \qquad S_l = e^{2i\delta_l} \tag{16}$$

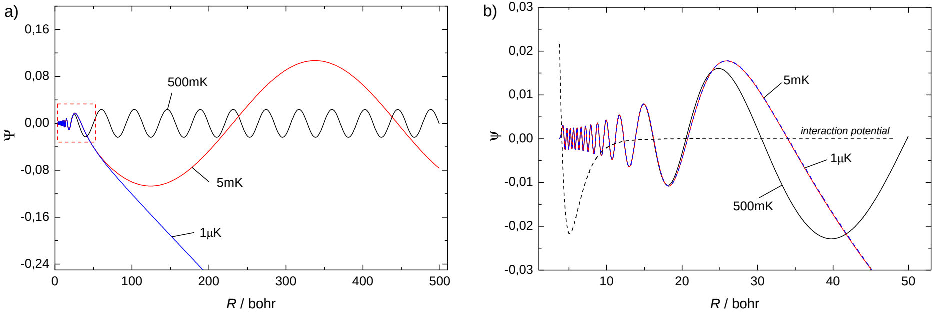
$$\sigma_l = \frac{\pi}{k^2}(2l+1)\sin^2\delta_l = \frac{4\pi}{k^2}(2l+1)|1-S_l|^2 \tag{17}$$

$$\sigma_{\text{tot}} = \sum_{l=0}^{\infty}\sigma_l, \qquad \delta_l(k) \underset{k\to 0}{\longrightarrow} -(ka)^{2l+1} \tag{18}$$

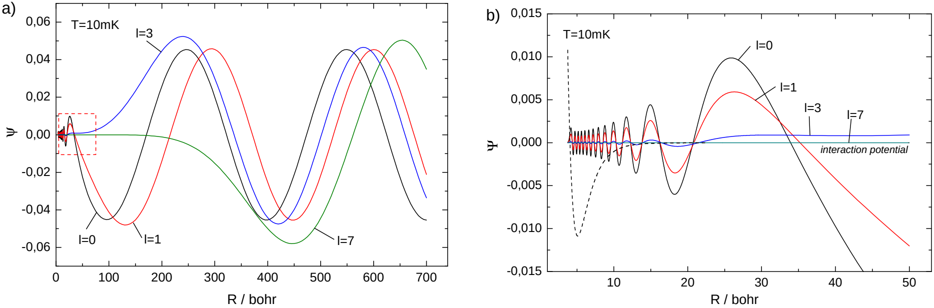
$$a_l(k) = -\frac{\tan\delta_l(k)}{k} = \frac{1}{ik}\frac{1-S_l(k)}{1+S_l(k)} \tag{19}$$

$$a_0(k) \underset{k\to 0}{\longrightarrow} const., \qquad \sigma_0 \underset{k\to 0}{\longrightarrow} 4\pi a_0^2 \tag{20}$$

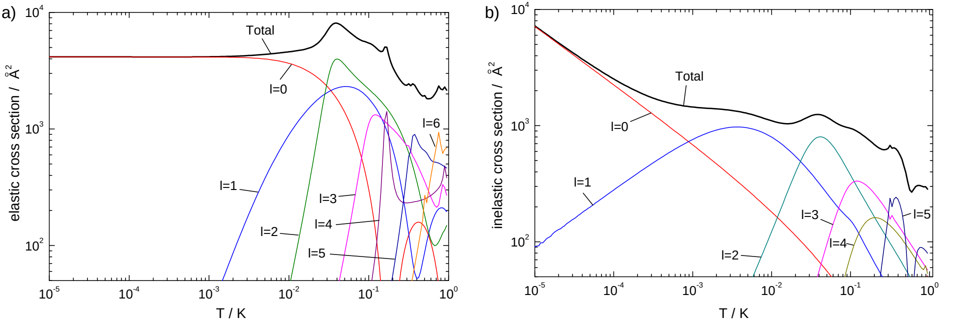
Wave function dependence on the energy



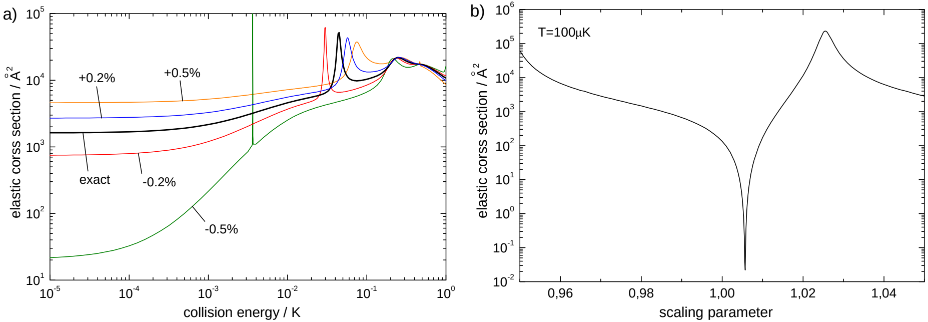
Wave function dependence on the partial wave



Example cross sections for LiH+Li



Example cross sections for LiH+Li



Numerov method

$$\frac{d^2\Phi(R)}{dR^2} + k^2(R)\Phi(R) = 0, \qquad k^2(R) = \frac{2\mu}{\hbar}(E - V_{\rm tot}(R)) \tag{21}$$

Integration of the wavefunction $\Phi(R)$ from R_0 in classically forbidden region to large distance $R_{\rm max}$ on the equidistant grid with step $h = dR$
$R_n \equiv R_0 + nh$, $k_n \equiv k(R_n)$, $\Phi_n \equiv \Phi(R_n)$

$$\Phi_{n+1} = \frac{2(1 - \frac{5h^2k_n^2}{12})\Phi_n - (1 + \frac{h^2k_{n-1}^2}{12})\Phi_{n-1}}{1 + \frac{h^2k_{n+1}^2}{12}} \tag{22}$$

For numerical stability it is better to propagate the ration $F_n = \Phi_{n+1}/\Phi_n$

$$F_n = \frac{2(1 - \frac{5h^2k_n^2}{12}) - (1 + \frac{h^2k_{n-1}^2}{12})/F_{n-1}}{1 + \frac{h^2k_{n+1}^2}{12}} \tag{23}$$

Computer laboratory

Elastic scattering

Task I (1 pt.): Calculate total $\sigma_{\text{tot}}^{\text{el}}$ and partial $\sigma_{\text{l}}^{\text{el}}$ cross sections for elastics scattering of cold spin-polarized heteronuclear mixture of potassium atoms as a function of the collisions energy. Identify the *s*-wave regime and compare it with the height of the *p*-wave barrier. Identify shape resonances and Wigner's threshold laws.

Task II* (0.5 pt.): Calculate total $\sigma_{\text{tot}}^{\text{el}}$ cross sections as a function of the interaction potential scaled by $\lambda = 0.95 - 1.05$: $D_e \to \lambda D_e$ for the collision energies of 1 μK, 100 μK and 10 mK. OR Repeat and analyze the above for the spin-polarized homonuclear bosonic and fermionic gases of potassium atoms. OR Plot and analyze the radial component of the scattering wavefunctions for shape resonances.

Elastic scattering

Interaction potential for the spin-polarized K+K:

$$V(R) = D_e \left[\left(\frac{R_e}{R} \right)^{12} - 2 \left(\frac{R_e}{R} \right)^{6} \right],$$

where $D_e = 0.0011141$ a.u., $R_e = 10.98$ a.u.

$m_{^{39}\mathrm{K}}$=38.963707 u
$m_{^{40}\mathrm{K}}$=39.963999 u
$m_{^{41}\mathrm{K}}$=40.961825 u
1 u = 1822.888 a.u.

R_{min}: $V(R_{\mathrm{min}}) \approx D_e$, R_{max}: $V(R_{\mathrm{max}}) \ll E$
$dR \approx \lambda_{\mathrm{max}} \approx \frac{1}{50} \frac{2\pi}{k(R_e)}$
use atomic units: $\hbar = m_e = 1$