

Laboratoire Kastler Brossel
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Introduction to Ultracold Atoms
Optical lattices – Atoms in artificial crystals made of light

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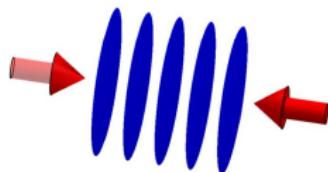
Advanced School on Quantum Science and Quantum Technologies, ICTP
Trieste

September 5, 2017

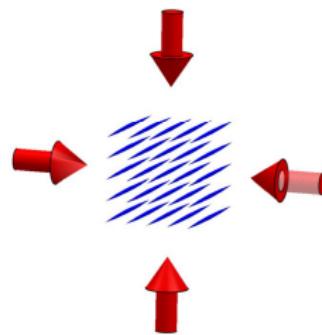
A coherent superposition of waves with different wavevectors results in interferences.

The resulting interference pattern can be used to trap atoms in a periodic structure.

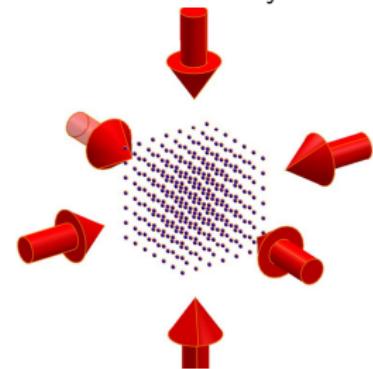
Linear stack of 2D gases



Planar array of 1D gases



Cubic array



Additional, weaker trapping potentials provide overall confinement of the atomic gas.

Many more geometries are possible by “playing” with the interference patterns.

Why is this interesting ?

- ➊ Connection with solid-state physics (band structure and related phenomenon)
- ➋ A tool for atom optics and atom interferometry: coherent manipulation of external degrees of freedom
- ➌ Path to realize strongly correlated gases and new quantum phases of matter

In the next lectures, we will discuss the behavior of quantum gases (mostly bosons, a little about fermions) trapped in periodic potentials.

Outline

- ➊ A glimpse about experimental realizations, and single-particle physics : band structure, Bloch oscillations.
- ➋ Superfluid-Mott insulator transition for bosonic gases

① Realizing optical lattices

② Band structure in one dimension

③ BECs in optical lattices

④ Bloch oscillations

Superposition of mutually coherent plane waves :

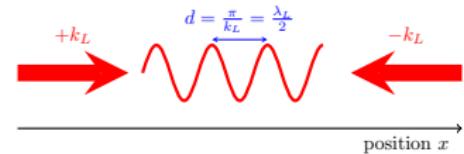
$$|\mathcal{E}(\mathbf{r})|^2 = \left| \sum_n \mathcal{E}_n e^{i\mathbf{k}_n \cdot \mathbf{r}} \right|^2 = \left(\sum_n |\mathcal{E}_n|^2 + \sum_{n \neq n'} \mathcal{E}_n^* \cdot \mathcal{E}_{n'} e^{i(\mathbf{k}_{n'} - \mathbf{k}_n) \cdot \mathbf{r}} \right)$$

Intensity (and dipole potential) modulations with wavevectors $\mathbf{k}_{n'} - \mathbf{k}_n$

Simplest example :

- Standing wave with period $d = \pi/k_L$
- Trapping potential of the form (red detuning):

$$\begin{aligned} V(x) &= -2V_1 (1 + \cos(2k_L x)) \\ &= -V_0 \cos(k_L x)^2 \end{aligned}$$

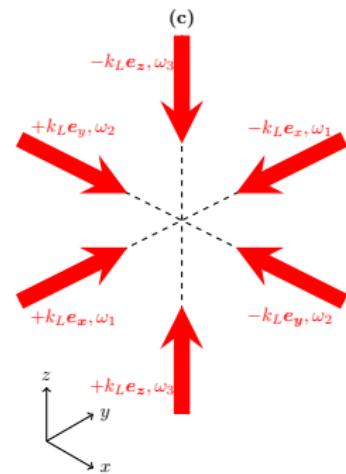
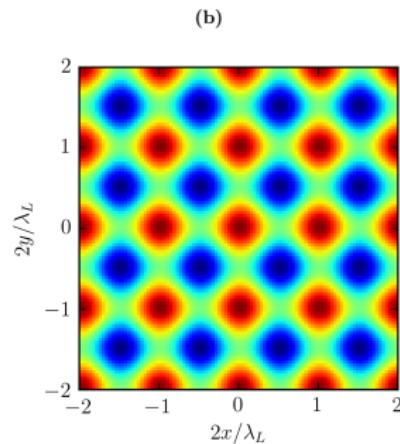
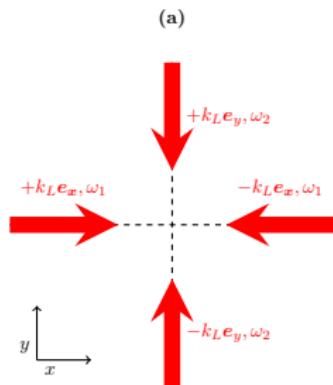


For red detuning (the case assumed by default from now on for concreteness), atoms are trapped near the antinodes where $V \approx -4V_0$.

Two and three-dimensional optical lattices

Two dimensions :

$$|\mathcal{E}(\mathbf{r})|^2 \approx |2E_0 \cos(k_L x)|^2 + |2E_0 \cos(k_L y)|^2$$



Two-dimensional square potential

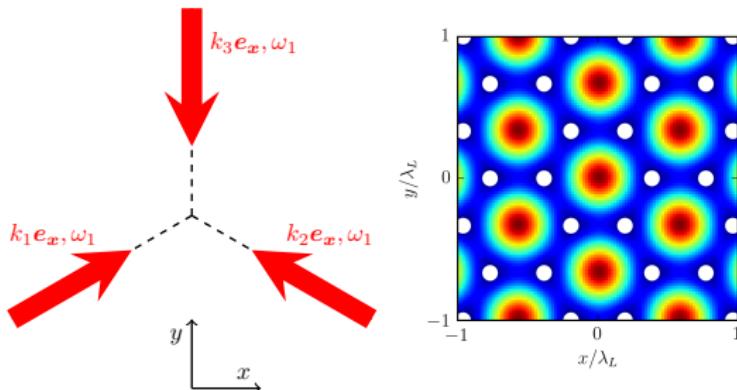
Three-dimensional cubic potential

Square ($d = 2$) or cubic ($d = 3$) lattices : $V_{\text{lat}}(\mathbf{r}) = \sum_{\nu=1, \dots, d} -V_\nu \cos(k_\nu x_\nu)^2$

- Separable potentials : sufficient to analyze the 1D case

Triangular/honeycomb optical lattices

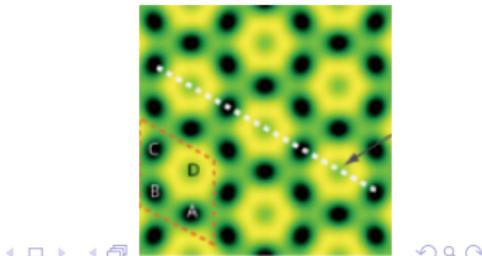
Other lattice geometries are realizable as well. Example with three mutually coherent coplanar beams [Soltan-Panahi *et al.*, Nature Phys. (2011)]:



- intensity maxima on a triangular lattice
- intensity minima on a honeycomb lattice (triangular with two atoms per unit cell)

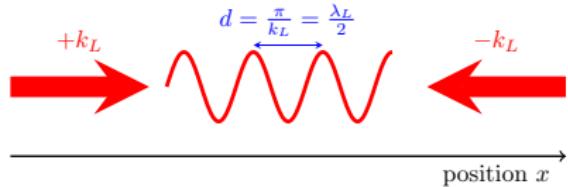
More complex example : the Kagomé lattice

[Jo *et al.*, PRL (2012)]:



- Standing wave with period $d = \pi/k_L$
- Trapping potential :

$$V(x) = V_0 \sin^2(k_L x)$$



Natural units :

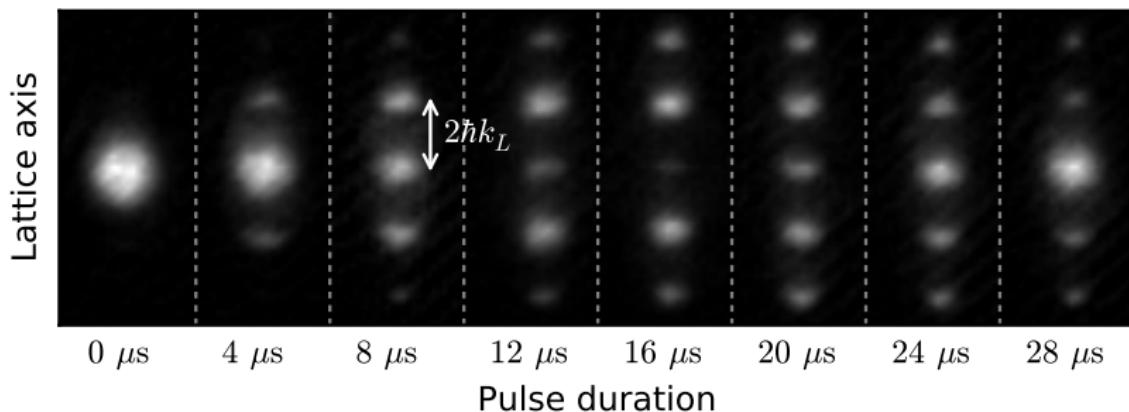
- lattice spacing $d = \lambda_L/2 = \pi/k_L$
- recoil momentum $\hbar k_L$
- recoil energy $E_R = \frac{\hbar^2 k_L^2}{2M}$

^{87}Rb , $\lambda_L = 1064\text{ nm}$:

- $d \approx 532\text{ nm}$
- $E_R \approx h \times 2\text{ kHz}$ ($k_B \times 100\text{ nK}$)

Diffraction from a pulsed lattice

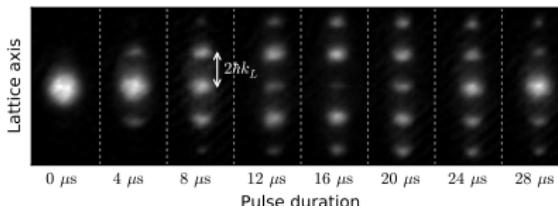
- Apply a lattice potential on a cloud of ultracold atoms (BEC) for a short time,
- look at momentum distribution :



- initial BEC : narrow wavepacket in momentum space (width $\ll k_L$)
- treat it as plane wave with *momentum $k = 0$*

Diffraction from a pulsed lattice : Kapitza-Dirac regime

Pulsing a lattice potential on a cloud of ultracold atoms (BEC) :



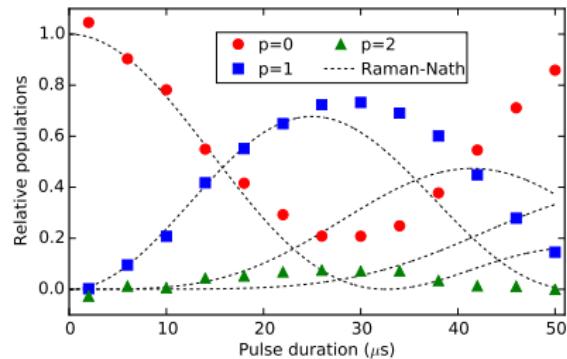
Raman-Nath approximation:

- BEC \rightarrow plane wave with $\mathbf{k} = 0$
- neglect atomic motion in the potential during the diffraction pulse :

$$\begin{aligned}\Psi(x, t) &\approx e^{i \frac{V_0 \cos(2k_L x)}{2\hbar} t} \Psi(x, 0) \\ &\approx \sum_{p=-\infty}^{+\infty} J_p(V_0 t / 2\hbar) e^{i 2p k_L x}.\end{aligned}$$

J_p : Bessel function

- Analogous to phase modulation of light wave by a *thin* phase grating



Raman-Nath approximation valid only for short times

① Realizing optical lattices

② Band structure in one dimension

③ BECs in optical lattices

④ Bloch oscillations

Bloch theorem

Hamiltonian :

$$\hat{H} = \frac{\hat{p}^2}{2M} + V_{\text{lat}}(\hat{x})$$
$$V_{\text{lat}}(x) = -V_0 \sin^2(k_L x)$$

Natural units:

- lattice spacing $d = \lambda_L/2 = \pi/k_L$
- recoil momentum $\hbar k_L$
- recoil energy $E_R = \hbar k_L^2/2M$

Lattice translation operator :

- definition : $\hat{T}_d = \exp(ipd/\hbar)$
- $\langle x | \hat{T}_d | \phi \rangle = \phi(x + d)$ for any $|\phi\rangle$
- $[\hat{T}_d, \hat{H}] = 0$.

Bloch theorem : Simultaneous eigenstates of \hat{H} and \hat{T}_d (*Bloch waves*) are of the form

$$\phi_{n,q}(x) = e^{iqx} u_{n,q}(x),$$

where the $u_{n,q}$'s (*Bloch functions*) are periodic in space with period d .

- q : *quasi-momentum*
- n : band index

$$\hat{H}\phi_{n,q}(x) = \varepsilon_n(q)\phi_{n,q}(x),$$
$$\hat{T}_d\phi_{n,q}(x) = e^{iqd}\phi_{n,q}(x),$$

Bloch waves :

$$\phi_{n,q}(x) = e^{iqx} u_{n,q}(x),$$

where the $u_{n,q}$'s (*Bloch functions*) are periodic in space with period d .

- q : *quasi-momentum*
- n : band index
- Periodic boundary conditions for a system with N_s sites (length $L = N_s d$) :
 $q_j = \frac{2\pi}{L} j = 2k_L \frac{j}{N_s}$ with $j \in \mathbb{Z}, |j| \leq N_s/2$

State labeling :

- Quasi-momentum is defined from the eigenvalue of \hat{T}_d :

$$\hat{T}_d \phi_{n,q}(x) = e^{iqd} \phi_{n,q}(x).$$

- For $Q_p = 2pk_L$ with p integer (a vector of the *reciprocal lattice*),

$$\hat{T}_d \phi_{n,q+Q_p}(x) = e^{i(q+Q_p)d} \phi_{n,q+Q_p}(x) = e^{iqd} \phi_{n,q+Q_p}(x).$$

- To avoid double-counting, restrict q to the

first Brillouin zone: $\text{BZ1} = [-k_L, k_L]$.

Bloch waves :

$$\phi_{n,q}(x) = e^{iqx} u_{n,q}(x)$$

The Bloch function $u_{n,q}$ is periodic with period d : Fourier expansion with harmonics $Q_m = 2mk_L$ of $2\pi/d = 2k_L$.

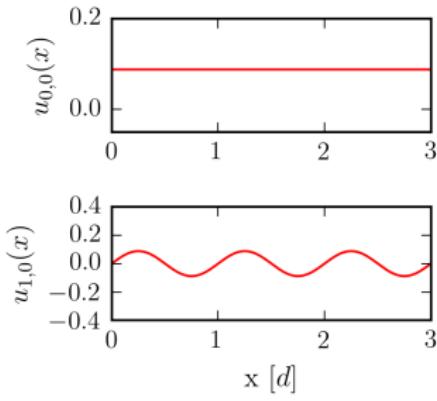
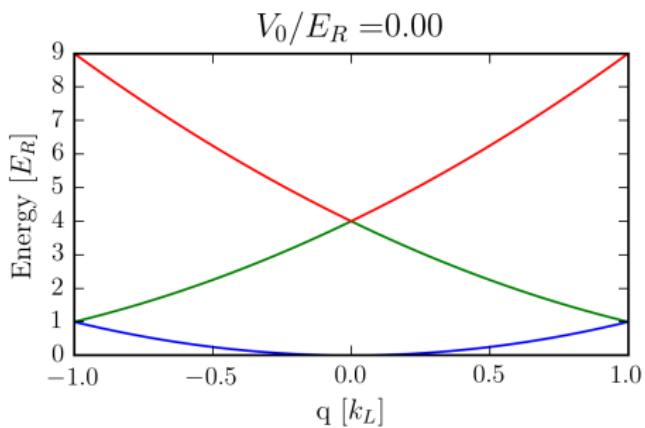
$$u_{n,q}(x) = \sum_{m \in \mathbb{Z}} \tilde{u}_{n,q}(m) e^{iQ_m x},$$

$$V_{\text{lat}}(x) = \sum_{m \in \mathbb{Z}} \tilde{V}_{\text{lat}}(m) e^{iQ_m x} = -\frac{V_0}{2} + \frac{V_0}{4} \left(e^{iQ_{-1}x} + e^{iQ_1 x} \right)$$

- the Bloch functions are **superpositions of all harmonics of the fundamental momentum $2k_L$.**
- the lattice potential couples momenta p and $p \pm 2k_L$.

Useful to solve Schrödinger equation : reduction to band-diagonal matrix equation for the Fourier coefficients $\tilde{u}_{n,q}(m)$ (tridiagonal for sinusoidal potential)

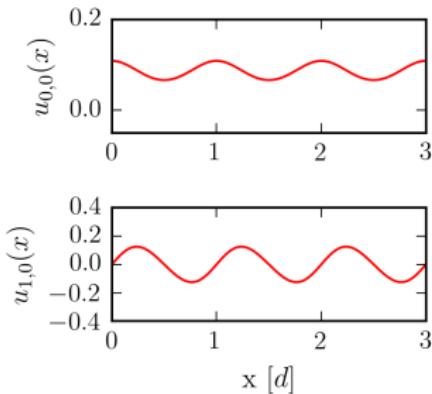
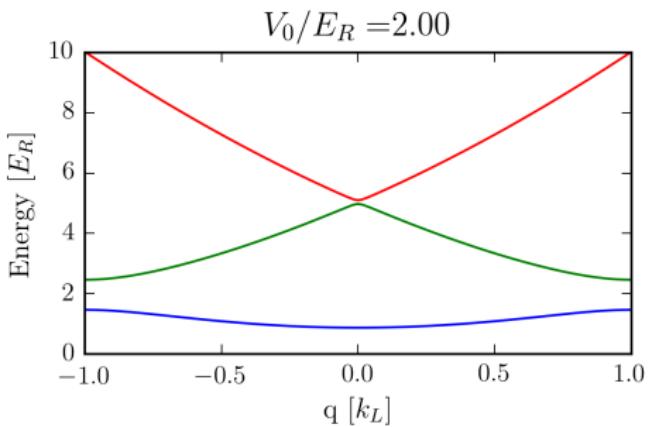
Spectrum and a few Bloch states, $V_0 = 0E_R$



Free particle spectrum : $\epsilon_n(q) = \frac{\hbar^2(q+2nk_L)^2}{2M}$, Momentum : $k = q + 2nk_L$

Degeneracy at the edges of the Brillouin zone : $E_n(\pm k_L) = E_{n+1}(\pm k_L)$

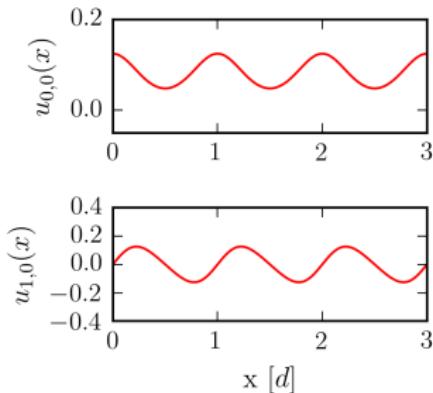
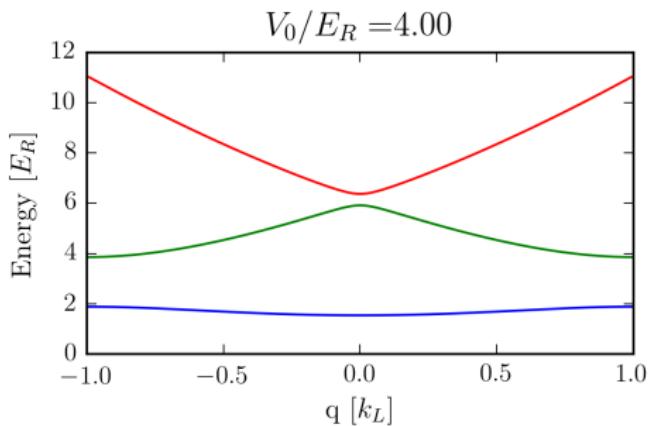
Spectrum and a few Bloch states, $V_0 = 2E_R$



Gaps open near the edges of the Brillouin zones ($q \approx \pm k_L$)

Lifting of free particle degeneracy by the periodic potential

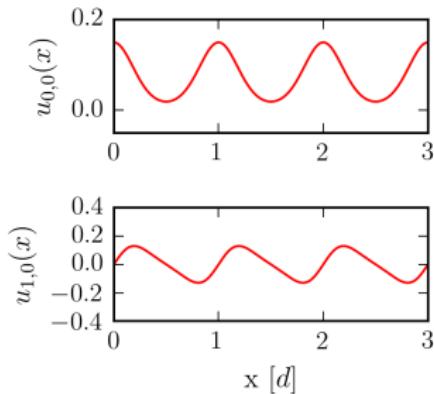
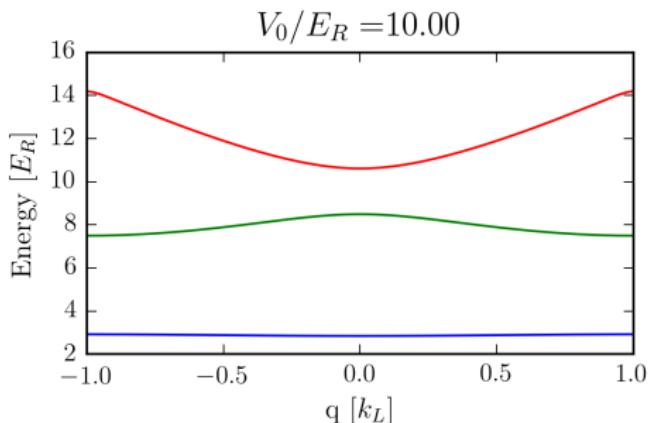
Spectrum and a few Bloch states, $V_0 = 4E_R$



Gaps widen with increasing lattice depth V_0

Bands flatten with increasing lattice depth V_0

Spectrum and a few Bloch states, $V_0 = 10E_R$

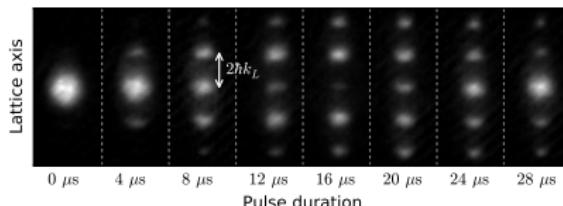


Gaps widen with increasing lattice depth V_0

Bands flatten with increasing lattice depth V_0

Diffraction from a pulsed lattice from band theory

Pulsing a lattice potential on a cloud of ultracold atoms (BEC) :



Bloch wave treatment:

$$|\phi_{n,q}\rangle = \sum_{m=-\infty}^{\infty} \tilde{u}_{n,q}(m) |q + 2mk_L\rangle$$

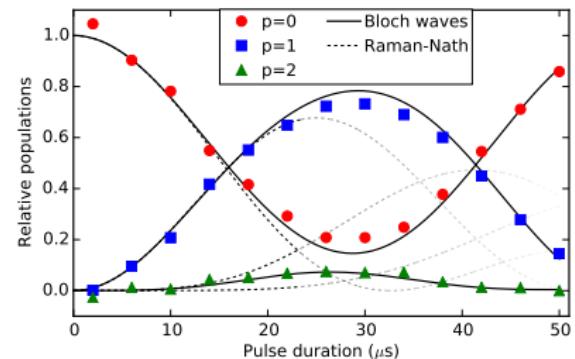
$$\langle k=0 | \phi_{n,q} \rangle = \tilde{u}_{n,q=0}(m=0)$$

Initial state :

$$|\Psi(t=0)\rangle = |k=0\rangle = \sum_n [\tilde{u}_{n,q=0}(m=0)]^* |\phi_{n,q=0}\rangle$$

Evolution in lattice potential :

$$|\Psi(t)\rangle = \sum_n [\tilde{u}_{n,q=0}(m=0)]^* e^{-i \frac{E_{n,q=0} t}{\hbar}} |\phi_{n,q=0}\rangle$$



Raman-Nath approximation valid only for short times

① Realizing optical lattices

② Band structure in one dimension

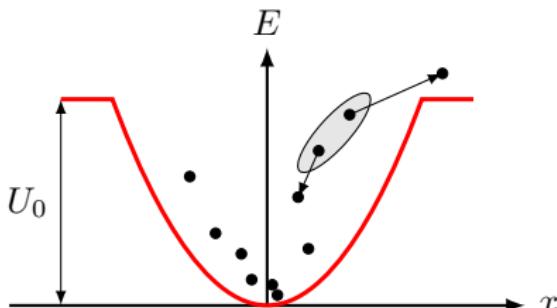
③ BECs in optical lattices

④ Bloch oscillations

Principle of evaporative cooling :

Atoms trapped in a potential of depth U_0 , undergoing collisions :

- two atoms with energy close to U_0 collide
- result: one “cold” atom and a “hot” one with energy $> U_0$
- rethermalization of the $N - 1$ atoms remaining in the trap results in a lower mean energy per atom.



Experimental procedure to prepare a cold atomic gas in a lattice :

- prepare a quantum gas using evaporation in an auxiliary trap,
- transfer it to the lattice by increasing the lattice potential from zero and simultaneously removing the auxiliary trap.

Why not cool atomic gases directly in the periodic potential ? .

- evaporative cooling no longer works due to the band structure as soon as $V_0 \sim a$ few E_R .

The best one can do is to transfer the gas adiabatically, i.e. **at constant entropy**.

Quantum adiabatic theorem

Slowly evolving quantum system, with Hamiltonian $\hat{H}(t)$.

Instantaneous eigenbasis of \hat{H} : $\hat{H}(t)|\phi_n(t)\rangle = \varepsilon_n(t)|\phi_n(t)\rangle$.

Time-dependent wave function in the $\{|\phi_n(t)\rangle\}$ basis:

$$|\Psi(t)\rangle = \sum_n a_n(t) e^{-\frac{i}{\hbar} \int_0^t \varepsilon_n(t') dt'} |\phi_n(t)\rangle,$$

From Schrödinger equation, one gets $[\omega_{mn} = \varepsilon_m - \varepsilon_n]$:

$$\dot{a}_n = -\langle \phi_n | \dot{\phi}_n \rangle a_n(t) - \sum_{m \neq n} e^{-\frac{i}{\hbar} \int_0^t \omega_{mn}(t') dt'} \langle \phi_n | \dot{\phi}_m \rangle a_m(t),$$

- **Berry phase** : $\langle \phi_n | \dot{\phi}_n \rangle = -i\gamma_B$ is a pure phase. Wavefunction unchanged up to a phase evolution after a cyclic change.
- **The adiabatic theorem** : for *arbitrarily slow* evolution starting from a particular state n_0 ($a_n(0) = \delta_{n,n_0}$), and in the *absence of level crossings*, $a_n(t) \rightarrow \delta_{n,n_0}$ (up to a global phase).

Adiabatic approximation for slow evolutions and initial condition $a_n(0) = \delta_{n,n_0}$:

$$a_n(t) \rightarrow e^{i\phi(t)} \delta_{n,n_0}$$

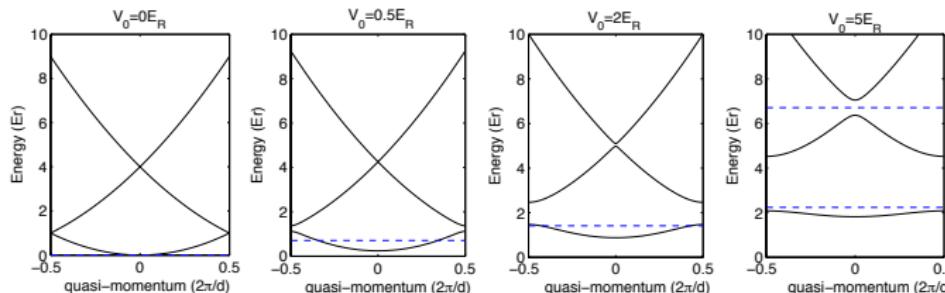
Validity criterion :

$$\langle \phi_n | \dot{\phi}_m \rangle = \frac{\langle \phi_n | \dot{H} | \phi_m \rangle}{\varepsilon_m - \varepsilon_n} \implies \left| \langle \phi_n | \dot{H} | \phi_m \rangle \right| \ll \frac{(\varepsilon_m - \varepsilon_n)^2}{\hbar}.$$

Adiabatic loading of a condensate

- Time-dependent lattice potential : $V_{\text{lat}} = V_0(t) \sum_{\alpha} \sin(k_{\alpha}x_{\alpha})^2$,
- $V_0(t)$ increases from 0 to some final value,
- initial state : BEC in a trap, treated as a narrow wavepacket around momentum $\mathbf{k} = 0$,
- final state : BEC in the OL in the lowest state, $n = 0, \mathbf{q} = 0$.

Quasi-momentum = good quantum number at all times : only *band-changing* transitions are possible



Adiabaticity criterion for the Bloch state ($n = 0, \mathbf{q} = 0$): $|\hbar \dot{V}_0| \ll (\varepsilon_{\mathbf{m}}(0) - \varepsilon_0(0))^2$

Adiabaticity most sensitive for small depths :

- Near band center $n = 0, \mathbf{q} = 0$: $|\varepsilon_1 - \varepsilon_0| \geq 4E_R$
- Near band edge $n = 0, q_{\alpha} = \pi/d$: $|\varepsilon_1 - \varepsilon_0| \geq 0$: never adiabatic !

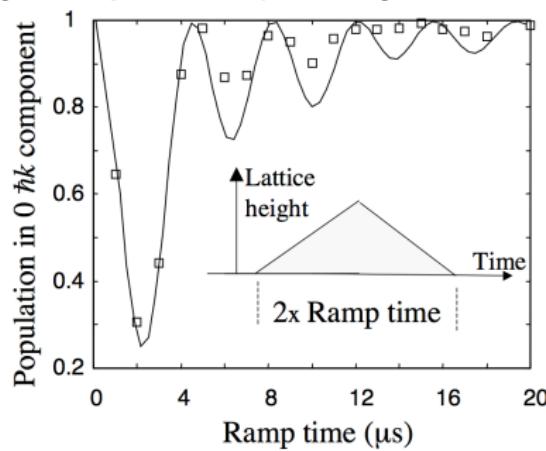
Adiabatic loading of a condensate : experiment

Adiabaticity criterion for a system prepared in a Bloch state ($n = 0, \mathbf{q} = 0$):

$$V_{\text{lat}} = V_0(t) \sum_{\alpha} \sin(k_{\alpha}x_{\alpha})^2$$

Quasi-momentum = good quantum number: $|\hbar \dot{V}_0| \ll (\varepsilon_m(0) - \varepsilon_0(0))^2$

[Denschlag *et al.*, J. Phys. B 2002]:



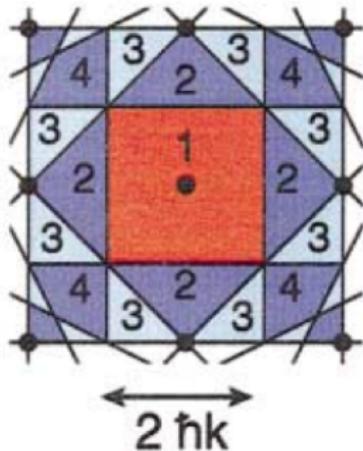
- Near band center $n = 0, \mathbf{q} = 0$:
 $|\varepsilon_1 - \varepsilon_0| \geq 4E_R$
- For Sodium atoms, $E_R/\hbar \approx 20 \text{ kHz}$
 $\left| \frac{\dot{V}_0}{V_0} \right| \sim \frac{1}{T_{\text{ramp}}} \ll \frac{16 E_R^2}{\hbar V_0} \sim \frac{1}{500 \text{ ns}} \frac{E_R}{V_0}$

Caution: for real systems interactions and tunneling within the lowest band are the limiting factors, not the band structure. Adiabaticity requires ramp-up times in excess of 100 ms.

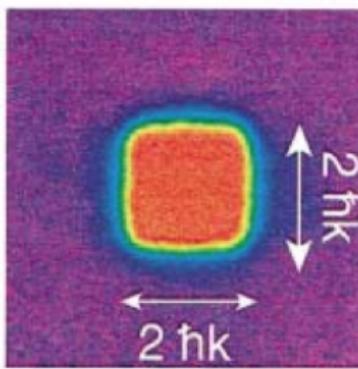
Band mapping : “adiabatic” release from the lattice

- Thermal Bose gas, $J_0 \ll k_B T \ll \hbar\omega_{\text{lat}}$: almost uniform quasi-momentum distribution.
- Mapping by releasing slowly the band structure before time of flight (instead of suddenly) – typically a few ms.
- Qualitative value only if band edges matter.

(a)



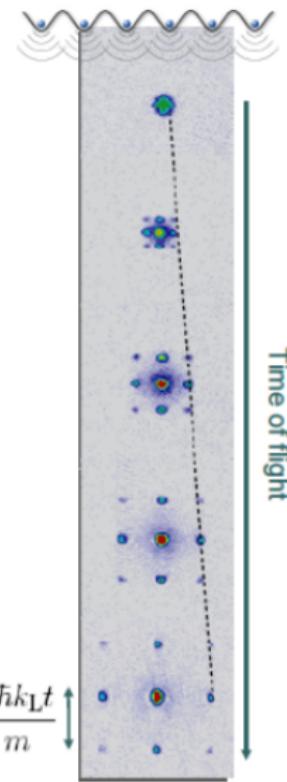
(b)



Greiner et al., PRL 2001

Time-of-flight experiment : sudden release from the lattice

Time-of-flight experiment : suddenly switch off the trap potential at $t = 0$ and let the cloud expand for a time t .



Time of flight (tof) expansion reveals momentum distribution (if interactions can be neglected).

Quantum version: wave-function after tof mirrors the initial momentum distribution $\mathcal{P}_0(\mathbf{p})$ with $\mathbf{p} = \frac{M\mathbf{r}}{t}$.

$$n_{\text{tof}}(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2 \approx \left(\frac{M}{t}\right)^3 \mathcal{P}_0\left(\mathbf{p} = \frac{M\mathbf{r}}{t}\right)$$

- for a condensate : N atoms behaving identically, density profile $n_{\text{tof}}(\mathbf{r}, t) \propto N|\tilde{\psi}(\mathbf{p}, t)|^2$ with $\tilde{\psi}$ the Fourier transform of the condensate wavefunction.
- Analogy with the Fraunhofer regime of optical diffraction: $\frac{\Delta p_0 t}{M} \gg \Delta x_0$ with $\Delta x_0, \Delta p_0$ the spread of ψ_0 in real and in momentum space.

$$\frac{2\hbar k_{\text{L}} t}{m}$$

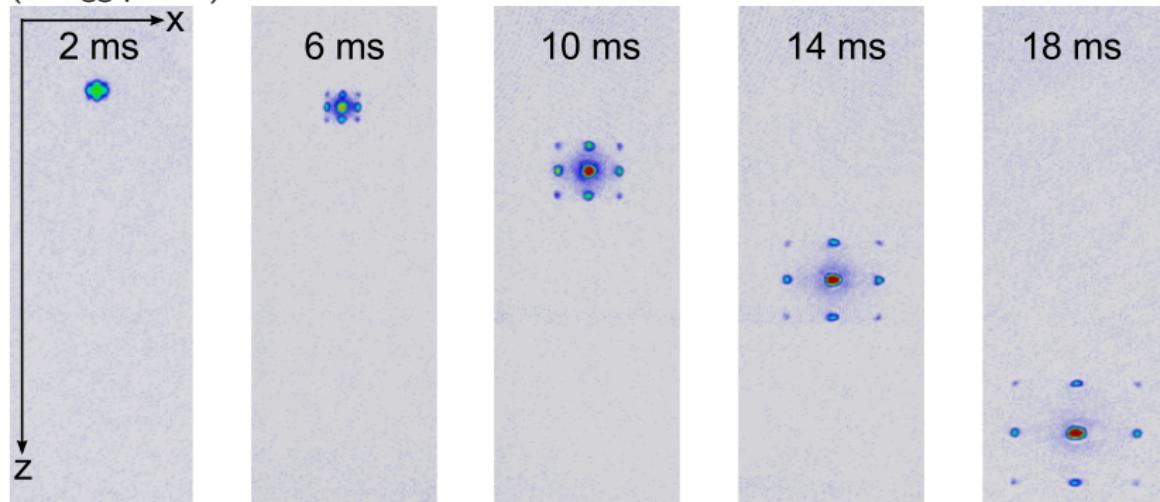
Time-of-flight interferences

Non-interacting condensate: Atoms condense in the lowest band $n = 0$ at quasi-momentum $\mathbf{q} = 0$:

$$\tilde{\phi}_{0,0}(\mathbf{p}) \propto \sum_{\mathbf{m} \in \mathbb{Z}^3} \tilde{u}_{0,0}(\mathbf{m}) \delta(\mathbf{p} - \hbar \mathbf{Q}_\mathbf{m}),$$

$\mathbf{Q}_\mathbf{m} = 2k_L \mathbf{m}$ ($\mathbf{m} \in \mathbb{Z}^3$) is a vector of the reciprocal lattice.

Time-of-flight distribution: comb structure with peaks mirroring the reciprocal lattice ("Bragg peaks").



① Realizing optical lattices

② Band structure in one dimension

③ BECs in optical lattices

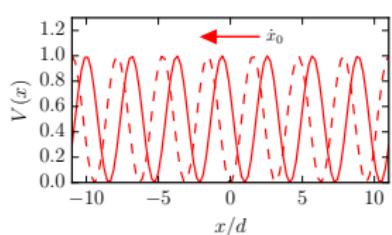
④ Bloch oscillations

Bloch oscillations

Uniformly accelerated lattice : $V_{\text{lat}}[x - x_0(t)]$ with $x_0 = -\frac{Ft^2}{2m}$

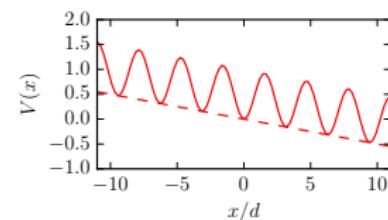
Lab frame:

$$H_{\text{lab}} = \frac{p^2}{2m} + V_{\text{lat}}[x - x_0(t)]$$



Moving frame:

$$H_{\text{mov}} = \frac{p^2}{2m} + V_{\text{lat}}[x] - Fx$$



Unitary
transformation

Bloch theorem still applies : H_{lab} invariant by lattice translations
Upon acceleration (moving frame):

$$|n, q_0\rangle \rightarrow |n, q(t)\rangle : q(t) = q_0 - m\dot{x}_0 = q_0 + \frac{Ft}{\hbar}$$

Quasi-momentum scans linearly across the Brillouin zone.

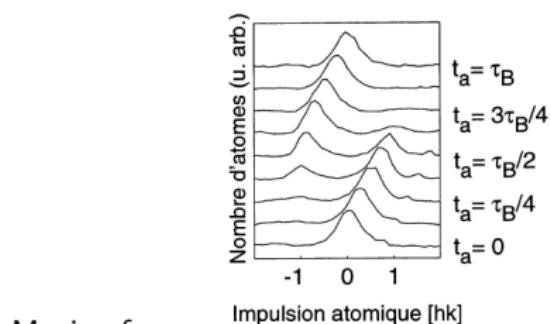
Bloch oscillations

Quasi-momentum scan accross the Brillouin zone : $q(t) = q_0 - m\dot{x}_0 = q_0 + \frac{Ft}{\hbar}$

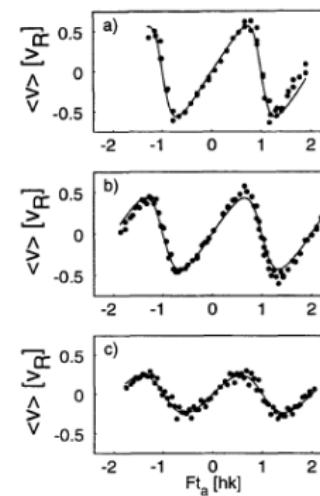
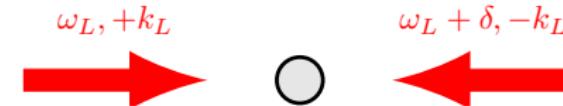
When $q = +k_L$, either non-adiabatic transfer to higher bands or, if adiabatic, Bragg reflection to $q = -k_L$.

Bloch oscillations of quasi-momentum with period $T_B = \frac{2\hbar k_L}{F}$

Experimental observation with cold Cs atoms [Ben Dahan et al., PRL 1995, also in Raizen's group at UT Austin]:



Moving frame

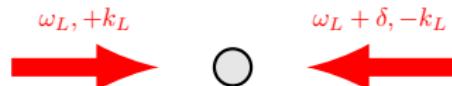


Consider an atomic wavepacket initially at rest and narrow in momentum space (typical velocities $v \ll \hbar k_L/M$).

Accelerated lattice : $V_{\text{lat}} = V_0 \cos^2(k_L x - \delta t)$

Standing wave traveling at velocity $v = \delta/k_L$

Quasi-momentum : good quantum number



Lattice frame : $q \rightarrow q - mv$

For slow (adiabatic) acceleration, a Bloch state $|q\rangle$ evolves to $|q - mv\rangle$.

A wavepacket built from Bloch states propagates with the group velocity :

$v_g = \frac{d\varepsilon(q)}{dq}|_{q=-mv} = \frac{M}{M^*}v$, with $M^* = \frac{d^2\varepsilon(q)}{dq^2}$ the effective mass (for $v \ll \hbar k_L/M$).

Lab frame : group velocity : $v_{\text{BEC}} = v + vg = \left(1 - \frac{M}{M^*}\right)v$

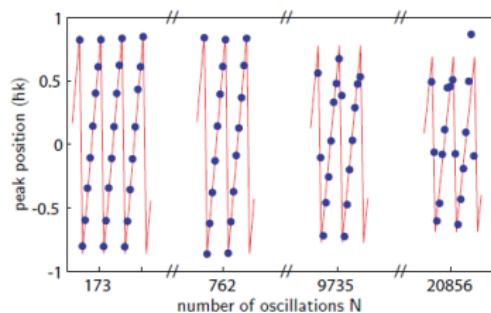
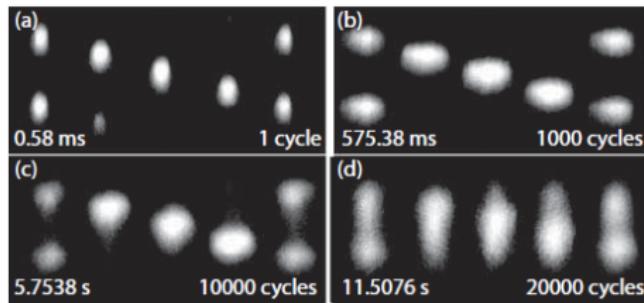
- shallow lattice, $V_0 \ll E_R$: $M^* \approx M$, atoms stand still
- deep lattice, $V_0 \gg E_R$: $M^* \ll M$, atoms dragged by the moving lattice

Bloch oscillations with a BEC

Quasi-momentum scan accross the Brillouin zone : $q(t) = q_0 - m\dot{x}_0 = q_0 + \frac{Ft}{\hbar}$

Bloch oscillations of quasi-momentum with period $T_B = \frac{2\hbar k_L}{F}$

Experimental observation with non-interacting BEC [Gustavsson et al., PRL 2008]:



N.B.: Assume atoms are prepared in a given band $n = 0$, and do not make a transition to higher bands (adiabatic approximation).

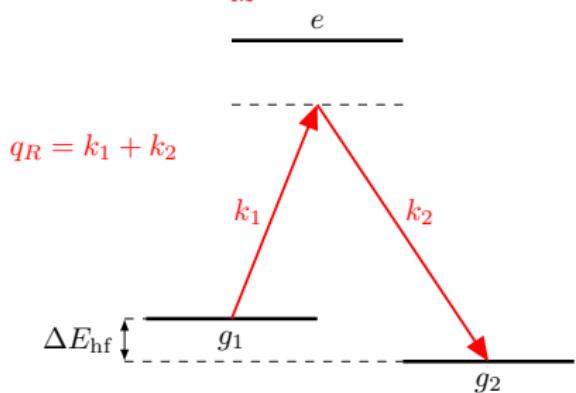
Measurement of the fine structure constant α :

$$\alpha^2 = \frac{4\pi R_\infty}{c} \times \frac{M}{m_e} \times \frac{\hbar}{M}$$

R_∞ : Rydberg constant
 m_e : electron mass
 M : atomic mass

- possible window on physics beyond QED : interactions with hadrons and muons, constraints on theories postulating an internal structure of the electron, ...

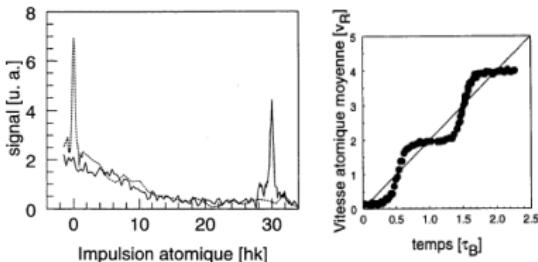
Measurement of $\frac{\hbar}{M}$: Experiment in the group of F. Biraben (LKB, Paris)



Doppler-sensitive Raman spectroscopy :

$$\begin{aligned} \hbar\omega_{\text{res}} &= \Delta E + \frac{\hbar^2}{2M} (p_i + \Delta k + q_R)^2 \\ \implies \frac{\hbar}{M} &= \frac{\omega_{\text{res}}(p_i + \Delta k) - \omega_{\text{res}}(p_i)}{q_R \Delta k} \end{aligned}$$

Large momentum beamsplitter using Bloch oscillations :

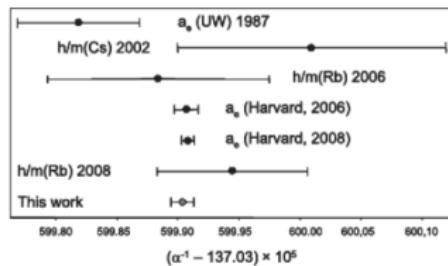


After N Bloch oscillations, momentum transfer of $\Delta k = 2N\hbar k_L$ to the atoms in the lab frame.

This transfer is perfectly coherent and enables beamsplitters where part of the wavepacket remains at rest while the other part is accelerated.

Measurement of $\frac{\hbar}{M}$:

- $N \sim 10^3$: Comparable uncertainty as current best measurement (anomalous magnetic moment of the electron – Gabrielse group, Harvard).
- Independent of QED calculations
- Other applications in precision measurements: measurement of weak forces, e.g. Casimir-Polder [Beaufils et al., PRL 2011].



[Bouchendira et al., PRL 2011]