Week 13

PHY 402 Atomic and Molecular Physics
Instructor: Sebastian Wüster, IISER Bhopal, 2018

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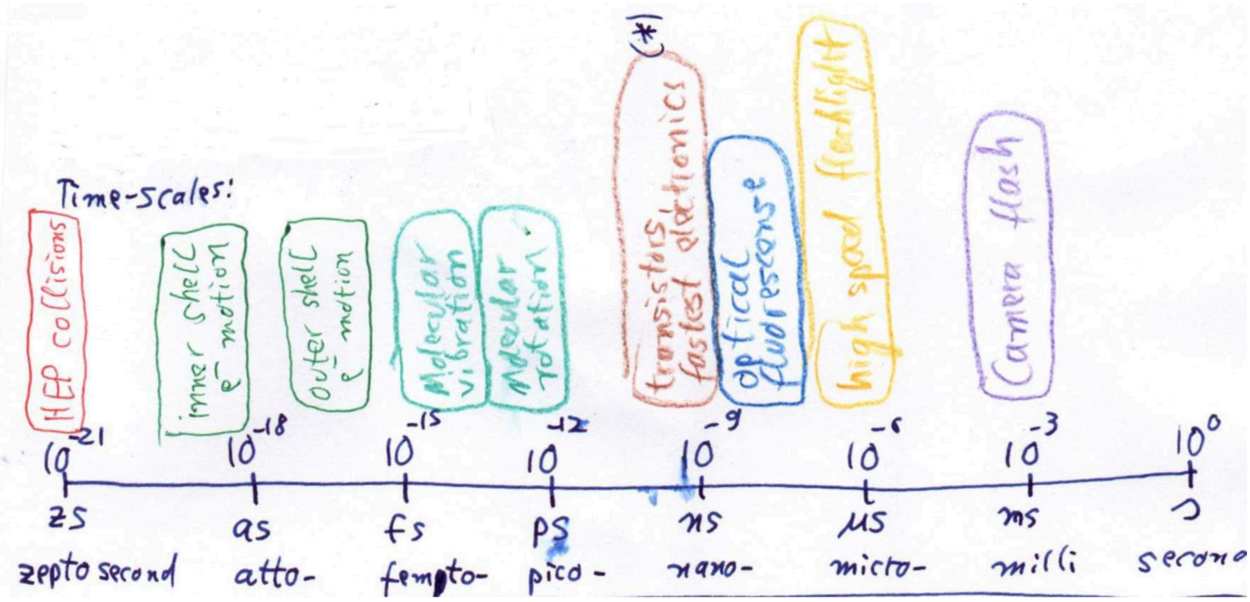
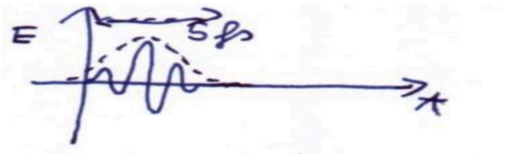
5 Frontiers of Modern AMO physics

We can only cover a small section biased by my own interests.

5.1 Ultrafast

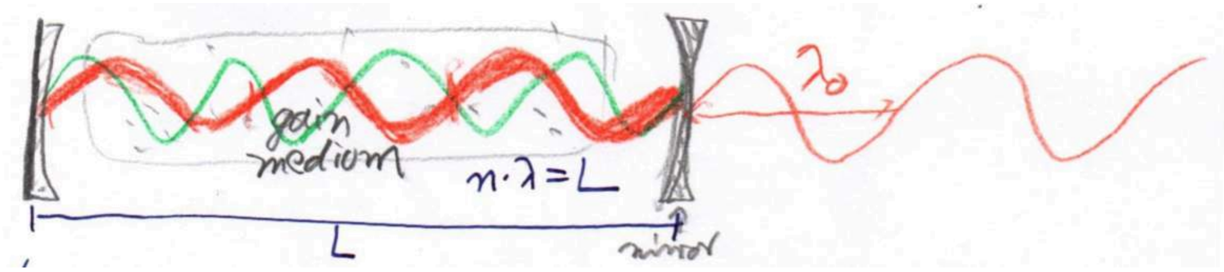


- To resolve e.g., vibrational molecular motion need ∼fs light pulses
- consider visible, e.g. 500nm $\Longrightarrow$ $\nu = 6 \times 10^{14}$Hz and a pulse duration of $\Delta T = 1$fs. In that case $\Delta T\,\nu \sim 0.6$, thus an optical pulse of a few fs duration has only a few oscillation cycles:
- Such short pulses are challenging to generate, we cannot simply switch on and off the laser that fast, since the required electronic processes are much slower, see (*) in time-scale figure above. One solution is portrayed in the following.



5.1.1 Frequency combs/ Femtosecond lasers

Laser resonators have multiple "eigenmodes" numbered with n, such that the light fulfils the boundary conditions at each end-mirror, thus $\lambda_n = 2L/n$.

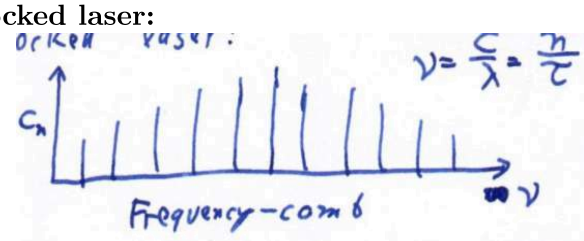


- For a normal laser, we rather want "single-mode" operation, where only a single λ_n is relevant.
- If we use a multi-mode, also called mode-locked, laser, the light field has the following Fourier spectrum

Frequency spectrum of mode locked laser:

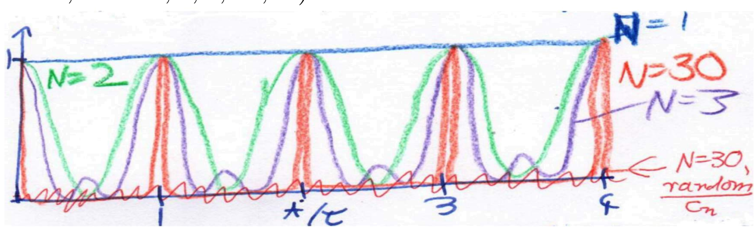
$$\tilde{E}(\omega) = \underbrace{\sum_n}_{N-modes} c_n \delta(\omega - \omega_n)$$

τ=round-trip time [$\sim 2L/c$]



resulting time-domain picture (c_n= constant, $N = 1, 2, 3, 30, ...$)

$$I(t) \sim \langle |E(t)|^2 \rangle$$



- Interpretation: Short pulse is bouncing back and forth in resonator and partially released out each time is hits the right-hand side (exit) mirror. As a result, outside the resonator we see a fs pulse train (large red line).

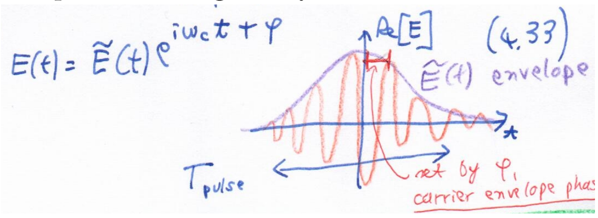
- This crucially results on the mode locking, i.e. all $c_n = 1$. If instead each c_n was a different random number, and we average over that, we get the small red line.

Pulse-waveform:

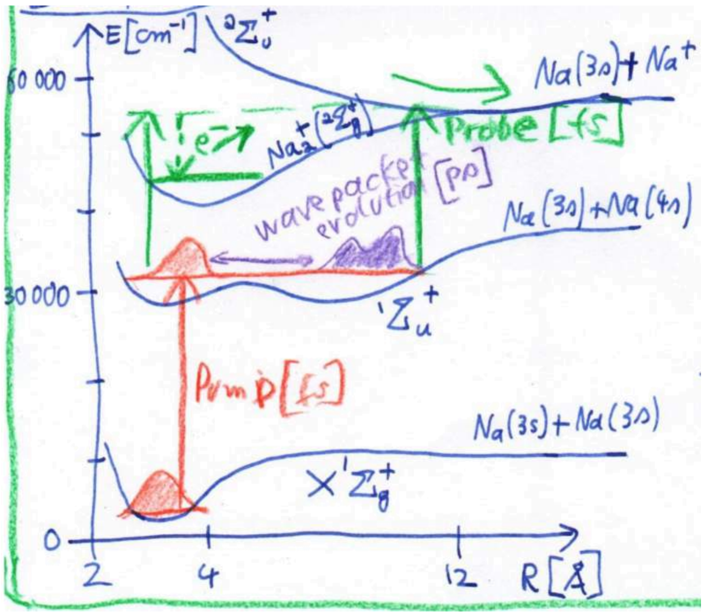
A single fs pulse is described by the waveform

$$E(t) = \tilde{E}(t)e^{i\omega_c t+\varphi} \tag{5.1}$$

where ω_c is the carrier frequency and $\tilde{E}(t)$ an envelope that changes only on slower time-scales than $T = 2\pi/\omega_c$. φ is called carrier-envelope phase.

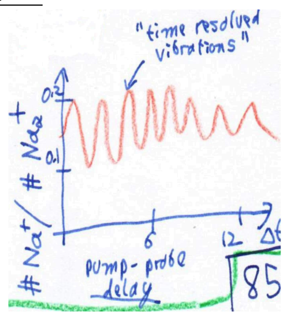


Example 5.1.1. Femtosecond pump-probe spectrosopy of Na_2:



- After pump, vibrational wave packets evolves in excited elec. state.
- Depending on nuclear separation $R(t)$, the probe pulse can dissociate Na_2 or not.

signal



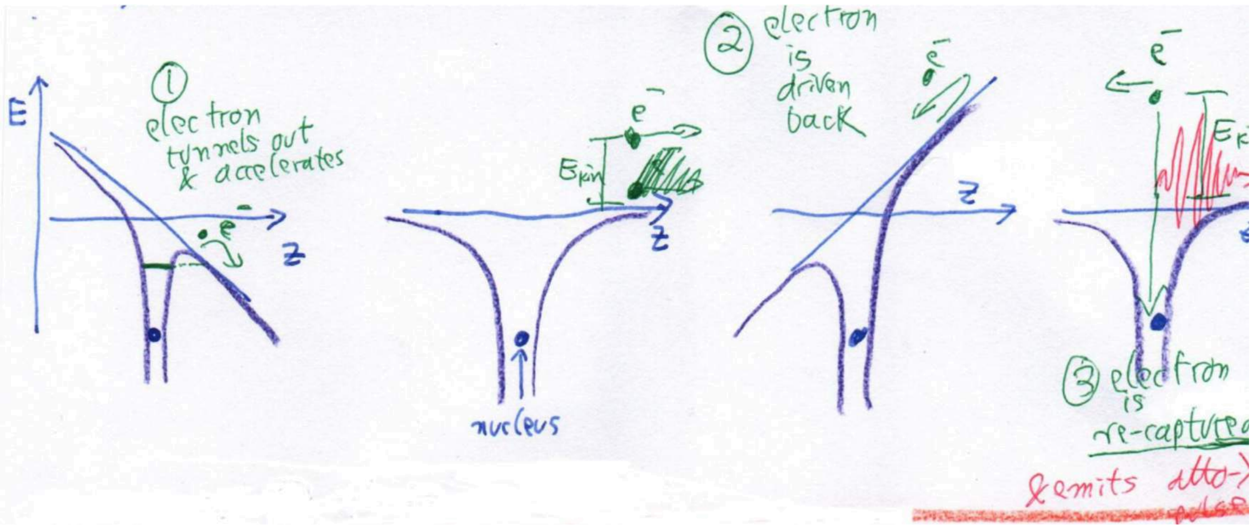
5.1.2 Strong fields, tunnel ionization

- Another consequence of the laser focussing all its energy into very short pulse: Very high intensities.
- In terms of Eq. (3.7), $\hat{H}'(t)$ may no longer be perturbative, $\boldsymbol{E}(t)$ may become comparable to Coulomb-field of nucleus!

> **Example:**
>
> - Electric field strength in hydrogen at a distance $r = a_0$ from the nucleus is $E(a_0) = \frac{Ze^2 m_e}{(4\pi\epsilon_0)^2\hbar^2}$.
> - Creating an equal field with a laser requires an intensity $I = \epsilon_0 |E(a_0)|^2 c$.
> - Assume a continuously running laser that is tightly focussed to $r_{\text{foc}} = 1\mu$m. This then requires a power $P = I \times \pi r_{foc}^2 \sim 2$ GigaWatt. (This is a large nuclear power plant).
> - However using pulsed operation as in a fs laser, with pulse length T_{pulse} and pulse period τ, we only need $P' = P\frac{T_{pulse}}{\tau} \sim$ few $100W$

- These extreme conditions an be used to study interesting electron dynamics, and also to generate even shorter laser pulses than those in section 5.1.1.

Three-step model of HHG (high-harmonic generation)



Through steps (1) ⇔ (2), electron gains an energy corresponding to ....

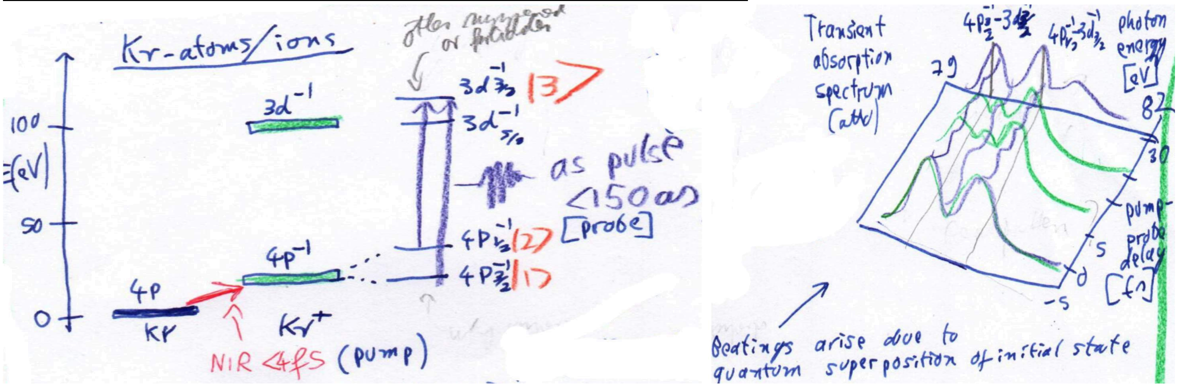
> **Ponderomotive energy**
>
> $$U_p = \frac{e^2 E_a^2}{4m\omega_0^2} \quad \text{(cycle averaged kinetic energy in field} \sim E_a\cos(\omega_0 t)\text{)} \qquad (5.2)$$

Duration of emitted pulse ∼ time-scale of electron motion.

- Classical electron orbit $z = 1$ (outer shell) $t_{orb} \simeq 150as$
  $z = 20$ (inner shell) $t_{orb} = 7as$

⇒ Can in this way (HHG) generate attosecond laser pulses.

Example: 5.1.2: Real-time valence electron motion: (Nature **466** (2010) 739)



$$|\,\Psi(0)\,\rangle \sim |\,1\,\rangle + |\,2\,\rangle$$

$$|\,\Psi(t)\,\rangle \sim e^{-iE_1\frac{t}{\hbar}}|\,1\,\rangle + e^{-iE_2\frac{t}{\hbar}}|\,2\,\rangle$$

$$\Big|\langle\,3\,|\hat{\mathbf{d}}|\,\Psi(t)\,\rangle\Big|^2 = \Big|\langle\,3\,|\hat{\mathbf{d}}|\,1\,\rangle e^{-iE_1\frac{t}{\hbar}} + \langle\,3\,|\hat{\mathbf{d}}|\,1\,\rangle \exp^{-iE_2\frac{t}{\hbar}}\Big|^2$$

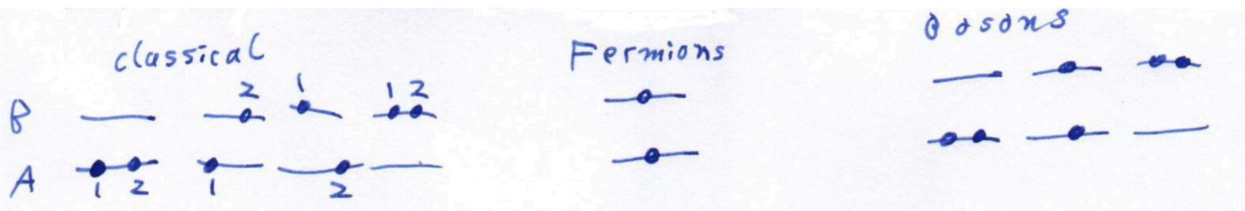
$$= \langle\,3\,|\hat{\mathbf{d}}|\,1\,\rangle^* \langle\,3\,|\hat{\mathbf{d}}|\,2\,\rangle e^{i(E_1-E_2)\frac{t}{\hbar}} + \text{c.c.} + \Big|\langle\,3\,|\hat{\mathbf{d}}|\,1\,\rangle\Big|^2 + \Big|\langle\,3\,|\hat{\mathbf{d}}|\,2\,\rangle\Big|^2$$

5.2 Ultra Cold

We have discussed in section 3.2.3 how thermal motion of atoms Doppler broadens spectral lines. Since manipulations (excitation, trapping) are more controlled for narrow lines, it is appealing to cool atomic gases as much as possible.

5.2.1 Bose-Einstein Condensation

For indistinguishable quantum particles (see section 1.2.6) we need to change the way we count the total number of accessible many-body states. Consider two particles (1,2) distributed over two states (A,B):



This gives rise to quantum-statistics:

Bose-Einstein (-)/ Fermi-Dirac (+) distribution function

$$n_i = \frac{1}{e^{(E_i-\mu)/k_B T} \pm 1} \text{ for mean number } n_i \text{ of particles in a state with energy } E_i. \quad (5.3)$$

- μ is the chemical potential (fixes $N = \sum_i n_i$)
- In comparison the classical (Boltzmann) distribution does not have the ± 1.
- BE- distribution diverges for groundstate $(E_u - \mu) = 0 \Rightarrow$ treat separately
- Find below a certain temperate, need macroscopic occupation of groundstate:

BEC transition temperature

$$k_B T_c \simeq (\hbar\omega) N^{1/3} \quad (5.4)$$

- N particles
- 3D harmonic trap $V(\boldsymbol{x}) = \frac{1}{2} m\omega^2 |\boldsymbol{x}|^2$

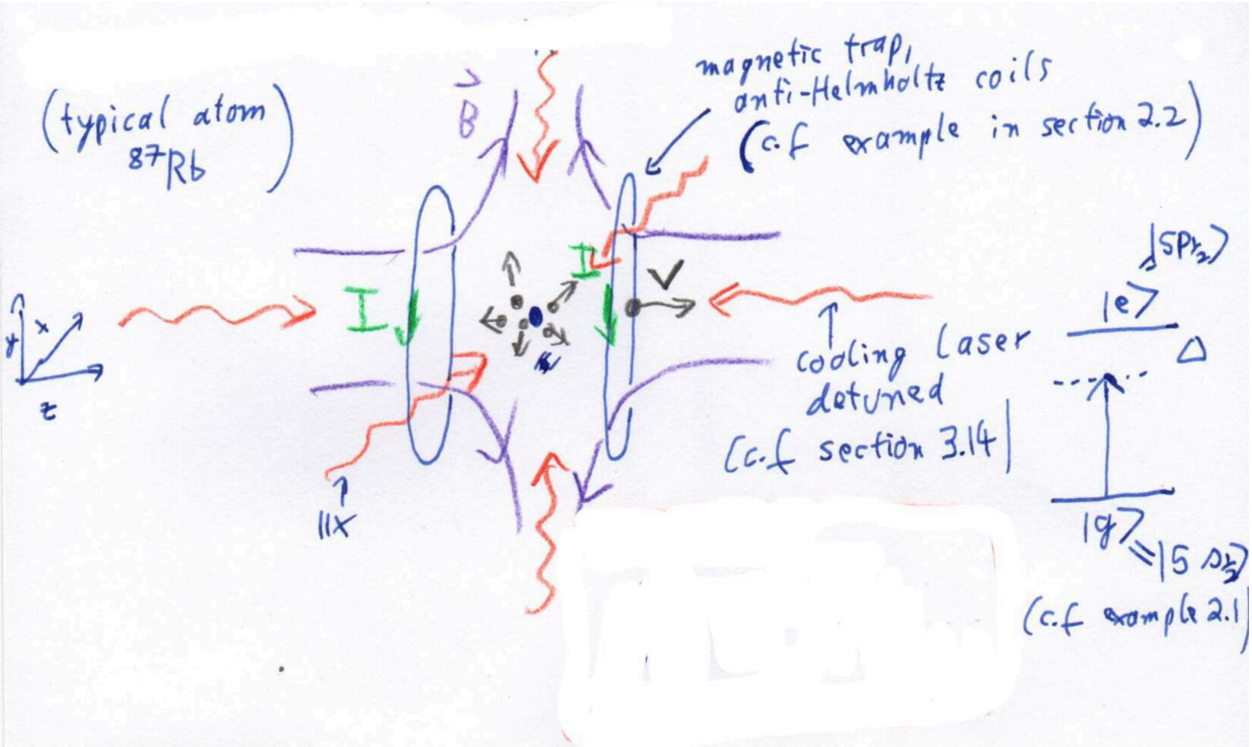
e.g. $N = 10000$
$\omega = (2\pi)100Hz \qquad T_c = 97nK$

Groundstate/Condensate fraction

$$\frac{N_0(T)}{N} = \left[1 - \left(\frac{T}{T_c}\right)^3\right] \quad (5.5)$$

5.2.2 Laser cooling and trapping

Typical ultra-cold atom apparatus



Doppler Shift

$$\omega' = \omega - \boxed{\mathbf{v}} \cdot \mathbf{k}$$

shifts only the fastest atoms into resonance. Photon absorption is most likely from against the motion direction, re-emission into a random direction. The atom thus experiences net cooling through photon recoil (momentum kicks).

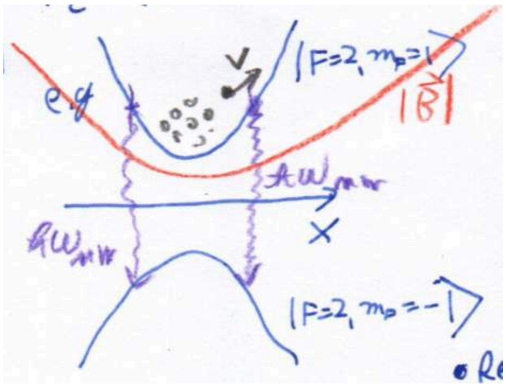
- Can combine magnetic field shifts on $|\, g\,\rangle, |\, e\,\rangle$ to get spatially dependent optical force ⇒ MOT ($\underline{m}agneto - \underline{o}ptical - \underline{t}rap$)
- Laser-cooling can reach $\simeq 100\mu K$ (Doppler limit)
- Improved laser cooling (Sisyphus cooling)

Recoil Limit

$$k_B T = \frac{(\hbar k_{\text{las}})^2}{2M} \simeq 0.1 - 1\mu K \tag{5.6}$$

- To finally reach condensation temperature T_c :

Evaporative cooling:



- Magnetic trap:

$$E = \pm g_L \mu_B m_F |\boldsymbol{B}|, \tag{5.7}$$

see Eq. (2.63).

- Trapped atoms are in
- Drive microwave transition at frequency ω_{mw} to anti-trapped $m_F = -1$ state. This will be only resonant (likely) at large $|\mathbf{x}|$, see diagram ($x = 0$ is in the centre).
- Hence only the most energetic atoms can make a microwave transition to the anti-trapped state and are lost.
- This scheme looses the large majority of all atoms.
- However through collisions, the remaining ones re-thermalize at a much lower temperature $T \simeq nK$.

5.2.3 Condensate mean-field

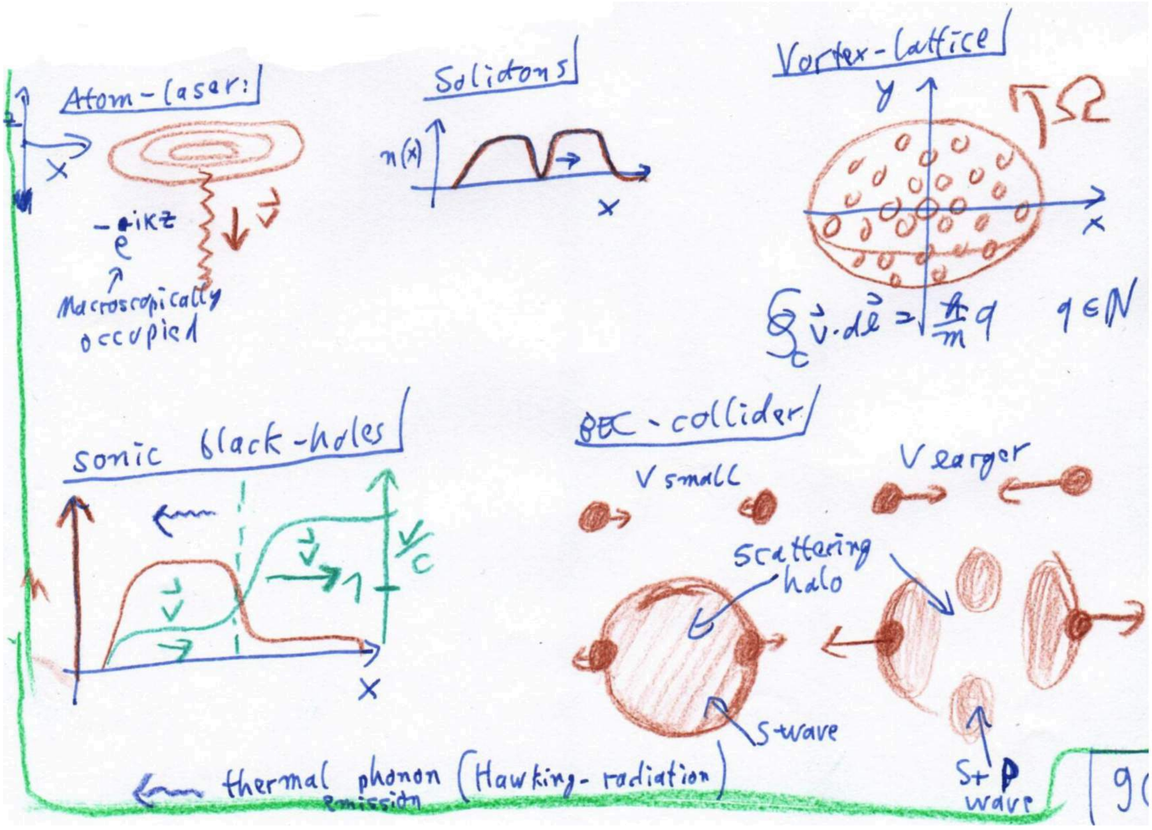
- Prior to condensation, we have to deal with a many-body wavefunction $\Psi(\mathbf{R}_1, ..., \mathbf{R}_N)$ for N atoms. This is intractable for N$\simeq$ 10000
- After condensation, can describe this using a condensate wave-function/order-parameter/mean-field $\phi(\boldsymbol{R})$ which obeys

Gross-Pitaevskii equation

$$i\hbar\dot{\phi}(\boldsymbol{R}) = \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{x}) + U_0|\phi(\boldsymbol{R}|^2 \right]\phi(\boldsymbol{R}) \tag{5.8}$$

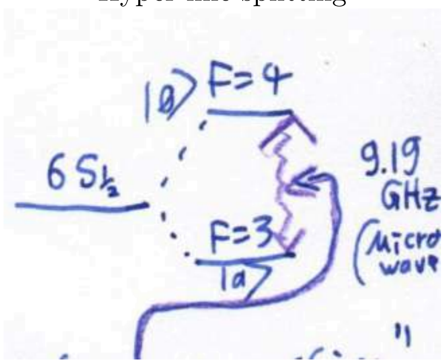
- where $V(\boldsymbol{x})$ is the trapping potential
- $U_0 = \frac{4\pi\hbar^2 a_s}{m}$ describes atomic collisions
- a_s = s-wave scattering length (see QM book, partial-wave treatment of scattering)
- $n(\boldsymbol{R}) = |\phi(\boldsymbol{R})|^2$ is the atom-density, $N = \int d^3\boldsymbol{R}|\phi(\boldsymbol{R})|^2$ the atom number.

Example: BEC Phenomena:



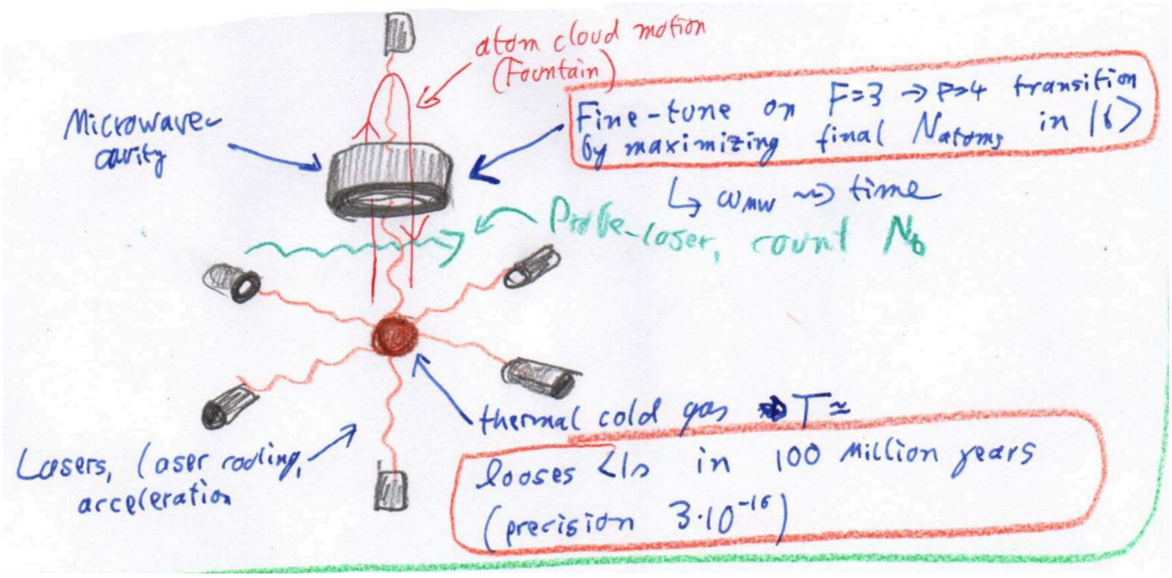
5.3 Atomic clocks

Hyper-fine splitting



Consider a ^{133}Cs atom with nuclear spin $I = \frac{7}{2}$. The current definition of SI-unit "second" is as the "Duration of 9 192 631 770 periods of electromagnetic radiation resonant on the $F = 3$ to $F = 4$ hyperfine transition in the ground-state of that atom, see right.

Example: NIST-F1 Cesium fountain clock: www.nist.gov



5.4 Quantum-simulation

As we have seen when studying multi-electron atoms or molecules: Many-body quantum mechanics is extrememly challenging.

Many-body Hilbert space dimension For N particles that can be in $\boxed{\text{M}}$ states each, the dimension of the many-body Hilbert space is

$$d \sim M^N \tag{5.9}$$

- As N, M increase, this becomes quickly too large to solve anything on classical computers

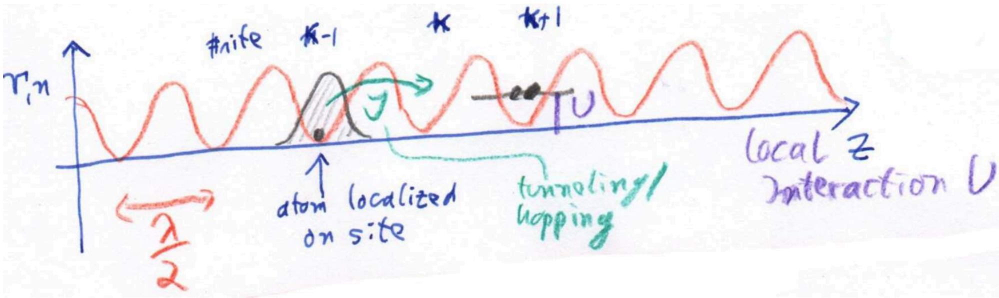
Idea by R. Feynman:

"Find another quantum-system with mathematically equivalent Hamiltonian where all parameters are under experimental control"

$\hookrightarrow$ (experimental) analogue quantum simulator

5.4.1 Bose-Hubbard model

Consider Bose-gas in optical lattice (= standing light wave), see e.g. Nature **415** 39 (2002).

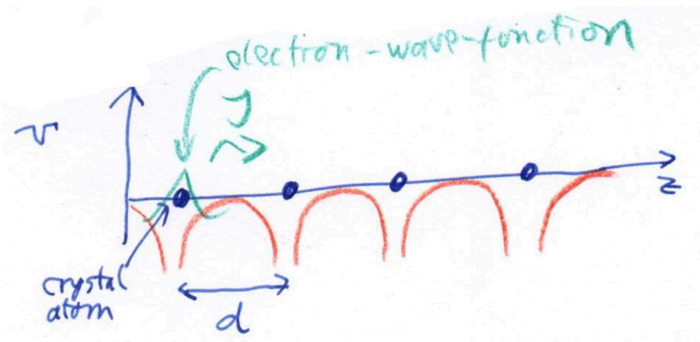


Many-body hamiltonian/Bose-Hubbard model

$$\hat{H} = -J\sum_k(\hat{a}^\dagger_{k+1}\hat{a}_k + \hat{a}^\dagger_{k-1}\hat{a}_k) + \frac{U}{2}\sum_k \hat{n}_k(\hat{n}_k - 1) \tag{5.10}$$

- $\hat{a}_k$, $(\hat{a}^\dagger_k)$ destroys (creates) a Boson at site k.
- $\hat{n}_k = \hat{a}^\dagger_k\hat{a}_k$ is the number operator on site k
- this setting provides.....

Quantum simulator for Hubbard model in condensed matter physics:

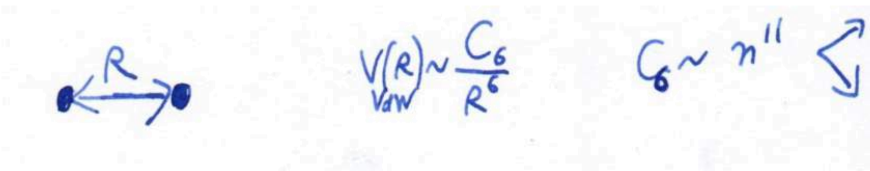


- electrons in a metal crystal (key difference: electrons are fermionic)
- here d, J, U cannot be changed in a given material.

- In cold atoms, J, λ, U can all be tuned.

5.4.2 Strongly interacting Rydberg systems

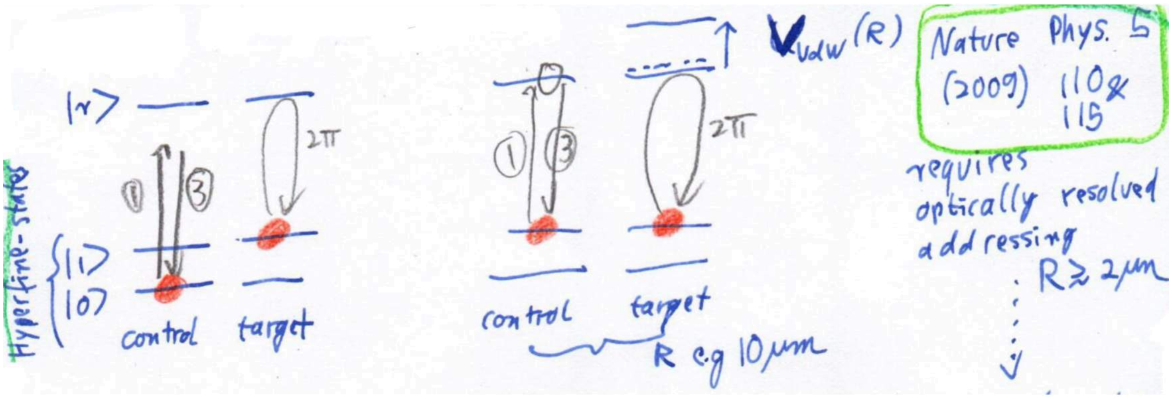
Consider Rydberg atoms, i.e. atoms in electronic states $|\,nlm\,\rangle$ with $n \gg 20$, see section 2.1.5. Two Rydberg atoms interact via Van-der-Waals interactions, see section 4.5.



In the ground state typical interaction ranges are $\sim 20a_0 \sim 0.01\mu m$

For Rydberg states their range is $\sim 10\mu m$

Example: Rydberg C-NOT Gate



Sequence:

In the following $|\,ab\,\rangle$ denotes a two atom state where $a \in \{0, 1\}$ is the state of the control atom and b of the target atom. We list the resulting transition sequence for all four possible initial quantum states.

(i) Rabi-π pulse on $|1> \leftrightarrow |r>$transition for control only

$\|00>$	$\|01>$	$\|10>$	$\|11>$
$\downarrow$			
$\|00>$	$\|01>$	$\|r0>$	$\|r1>$

(ii)Rabi-2π pulse on $|1> \leftrightarrow |r>$transition for target only

$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
$\|00>$	$-\|01>$ $(see Eq.\ (3.51))$	$\|r0>$	$\|r1>$

(iii)Rabi-π pulse on $|1> \leftrightarrow |r>$transition for control only

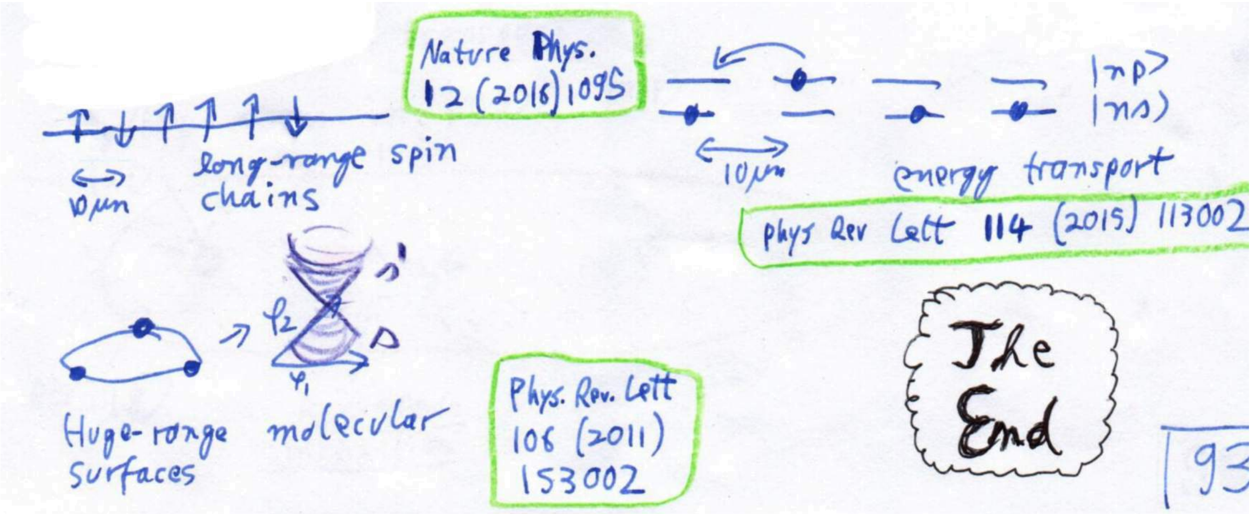
$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
$\|00>$	$-\|01>$	$\|10>$	$\|11>$

Truth Table:

$\|00>$	$\rightarrow$	$\|00>$
$\|01>$	$\rightarrow$	$-\|01>$
$\|10>$	$\rightarrow$	$\|10>$
$\|11>$	$\rightarrow$	$\|11>$

Controlled Z-gate
$\hookrightarrow$ can get C-NOT from here

Other Examples:



Acknowledgements:
Thanks to Abhishek Nandekar, Kaustav Mukherjee, Piyush Jangid, Sarthak Choudhury and Vidit Das for helping to type-set the handwritten lecture notes into Latex.