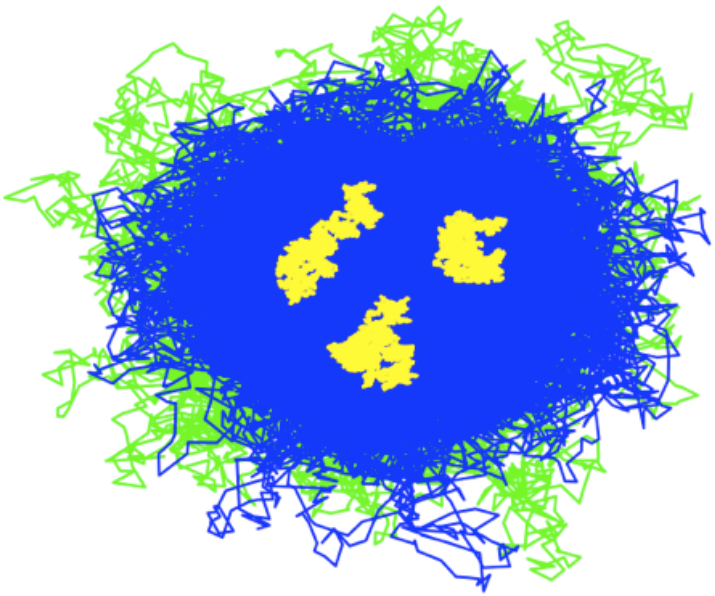
KVANTTIFYSIIKKA JA MATERIAALIFYSIIKKA

Tapio Rantala
Fysiikka, Tampereen yliopisto

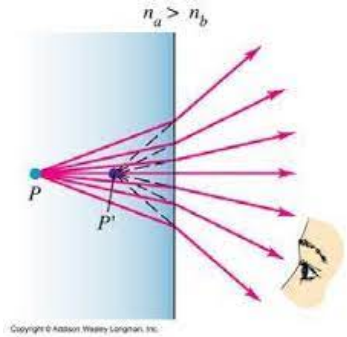
SISÄLTÖ

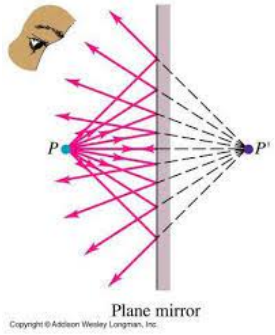
- AALTOJEN OMINAISUUKSIA
  - DIFFRAKTIO JA INTERFERENSSI
  - KLASSILLINEN MEKANIIKKA JA KVANTTIMEKANIIKKA
  - POLKUINTEGRAALIT
- KVANTITTUMINEN
  - SYMMETRIAT
  - ORBITAALIT JA VETYATOMI
- MATERIAALIFYSIIKKAA
  - ELEKTRONIRAKENNETEORIA
  - KVANTTIKEMIA



OPTIIKAN JA VALON DIFFRAKTIO- JA INTERFERENSSI-ILMIÖT

Geometrinen optiikka ja Fermat'n periaate:



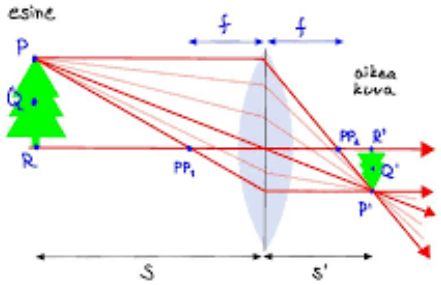


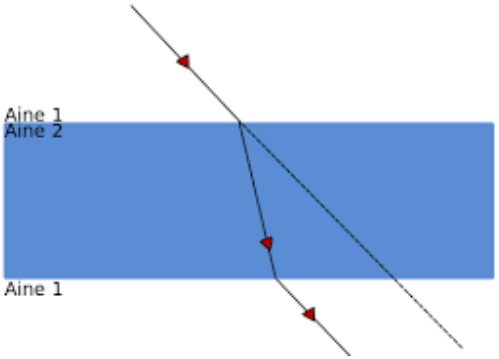
Valonsäde kulkee nopeinta reittiä suoraviivaisesti.

$$S = \int_a^b n \, \mathrm{d}s$$

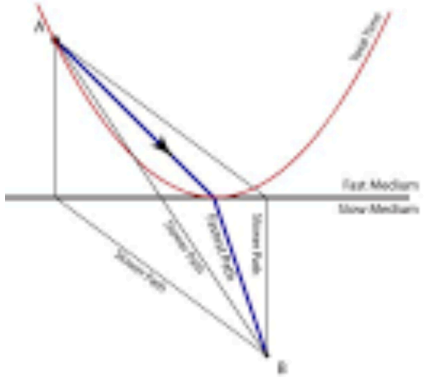
Siksi valonsäde voi taittua pinnassa

$$n = \frac{c}{v}$$



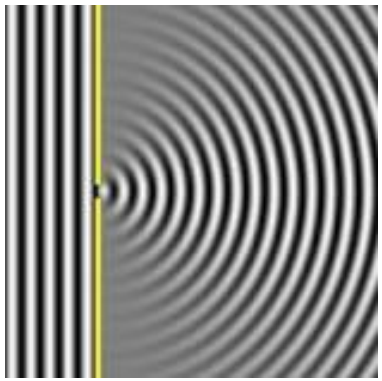


$\delta S = 0$ $\quad$ $\delta S \neq 0$

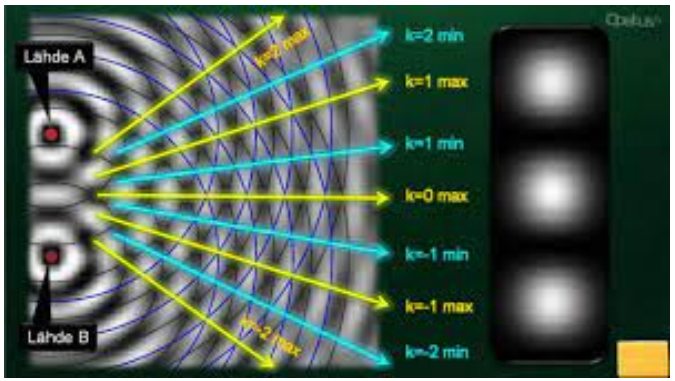


Fysikaalinen optiikka ja diffraktio sekä interferenssi-ilmiöt

Huygensin periaate: Valonsäde lähtee jokaisesta pisteestä kaikkiin suuntiin

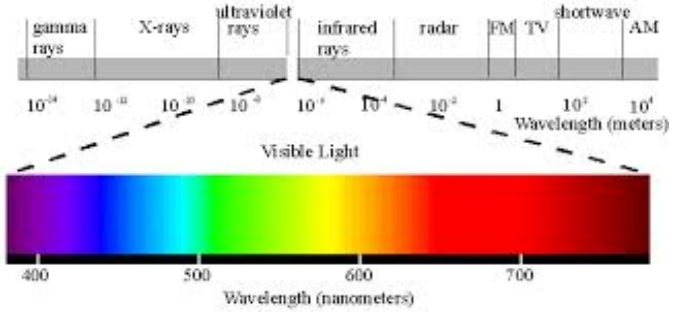


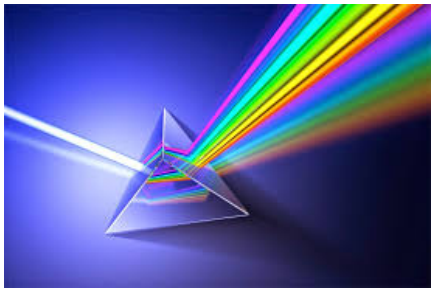
Kahden raon interferenssi

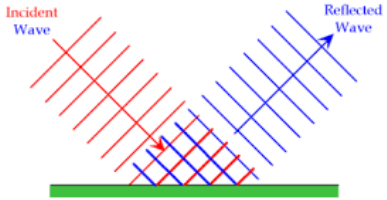


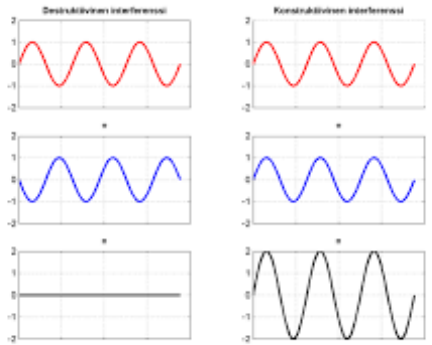
ETENEVÄT AALLOT, HEIJASTUMINEN TAITTUMINEN, DIFFRAKTIO JA INTERFERENSSI

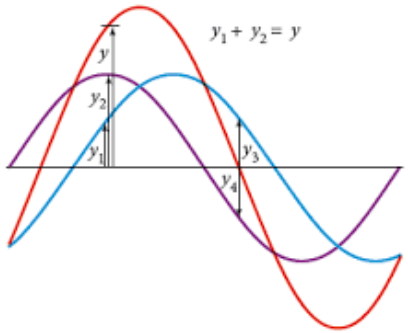
Valoaallot



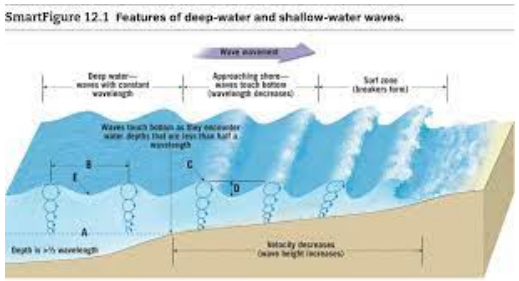








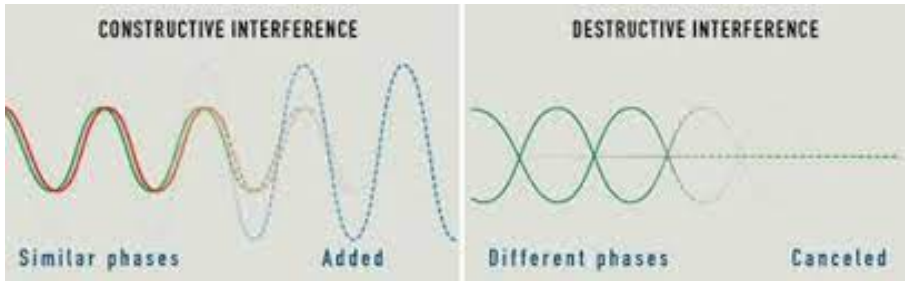
Mekaaniset aallot











KLASSILLINEN MEKANIIKKA JA LAGRANGEN FUNKTIO

Klassillinen mekaniikka ja pienimmän vaikutuksen periaate:

Hiukkanen kulkee (nopeinta) reittiä suoraviivaisesti, jos

$$L = T - V$$

on vakio.

$$T = \tfrac{1}{2}mv^2$$

Newtonin liikeyhtälö

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial v}\right) - \frac{-\partial V}{\partial x} = 0$$

$$\frac{\mathrm{d}}{\mathrm{d}t}mv - F = 0$$

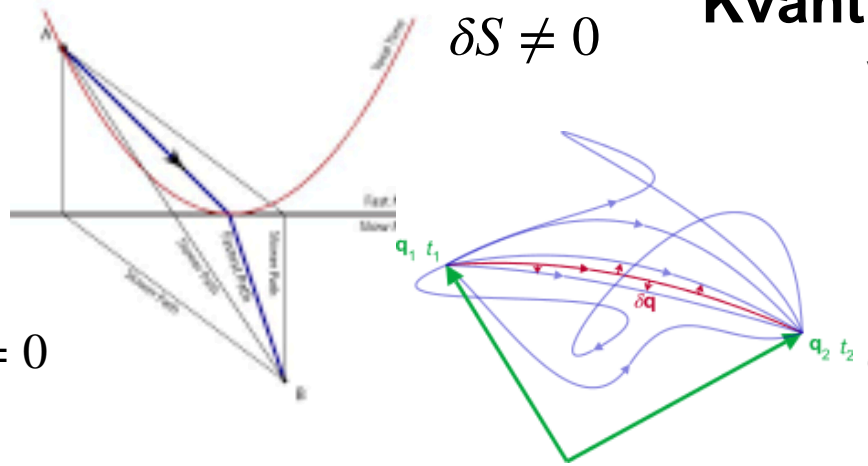
$$ma = F$$

Lagrangen funktio $L = T - V$

Vaikutus (engl. **action**) $S = \int_a^b L \, \mathrm{d}t$

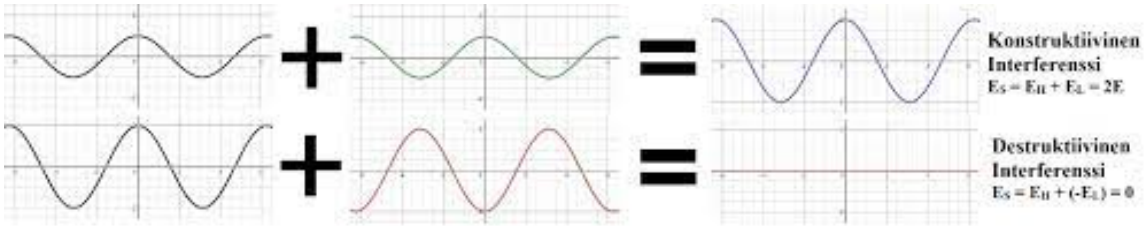
Eulerin yhtälö $\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0$

$\delta S = 0$ $\delta S \neq 0$



Kvanttimekaniikka

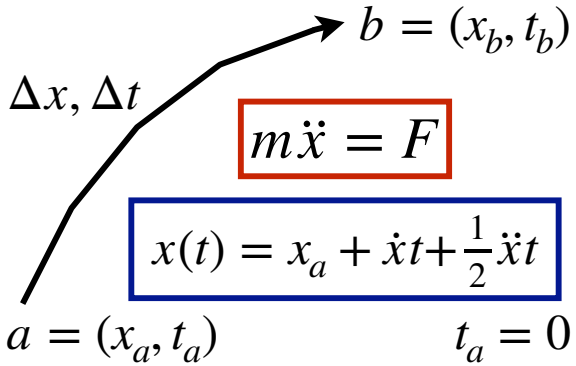
Vertaa Huygensin periaatteeseen: Eteneminen 1 -> 2 kaikkia mahdollisia polkuja pitkin. Sekä konstruktiivista että destruktiivista interferenssiä.



TODENNÄKÖISYYSAMPLITUDI Ψ, VERTAILUA JA YHTEENVETOA

Klassillinen dynamiikka

$\delta S = 0$



$$m\ddot{x} = F$$

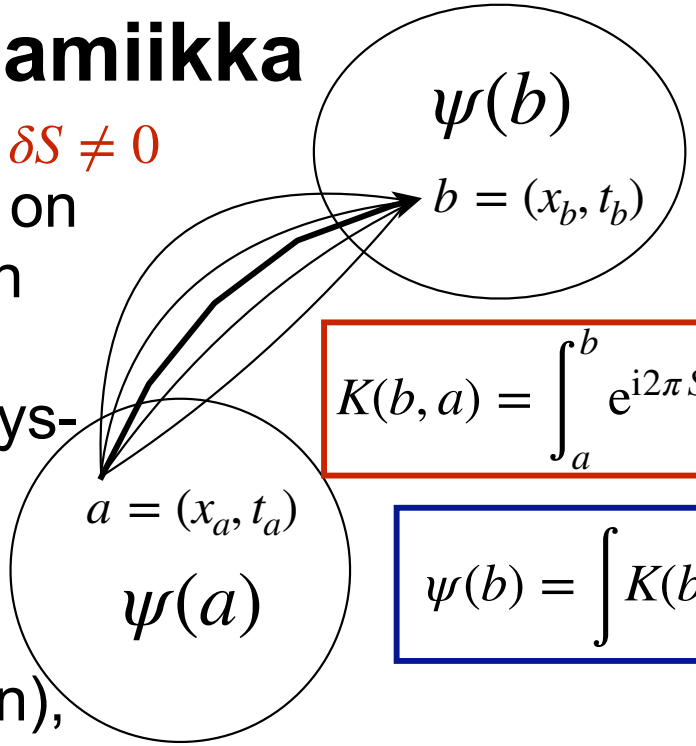
$$x(t) = x_a + \dot{x}t + \frac{1}{2}\ddot{x}t$$

Kvanttidynamiikka

$\delta S \neq 0$

- aallon paikka on epämääräinen

- todennäköisyys-amplitudi eli aaltofunktio on $\psi(x,t)$ (kompleksinen), joka on ratkaistavissa Schrödingerin yhtälöstä tai vastaavasta integraaliyhtälöstä



$$K(b,a) = \int_a^b \mathrm{e}^{\mathrm{i}2\pi\, S[a,b]/h}\, D[x(t)]$$

$$\psi(b) = \int K(b,a)\,\psi(a)\ \mathrm{d}a$$

$$H\psi(x,t) = \mathrm{i}\frac{\partial\psi(x,t)}{\partial t} \quad \Leftrightarrow \quad \psi(x,t) = \int K(x,t;x_a,t_a)\psi(x_a,t_a)\mathrm{d}x_a$$

QUANTUM MECHANICS
THE CONVENTIONAL APPROACH

QM – WHY AND WHAT

- was needed to interpret and explain new experimental observations more than 100 years ago
- replaces Newton's equation of motion by Schrödinger equation, which is kind of "equation of motion" of very small particles by "replacing zero by Planck's constant h"
- yields classical mechanics for macroscopic objects as a limiting case, if $h \to 0$.
- leads to the concept **wave function** and **quantization** of energy, and consequently, particle–wave dualism, uncertainty relation, probability interpretation and quantum state
- all experimental observation, so far, support quantum theory

Quantum theory and relativity are called modern physics.

QM – WHY AND WHAT

Postulate1: The state of a system is fully described by its **wave function** $\Psi_{m,n,\ldots}(\mathbf{r}_1, \mathbf{r}_2, \ldots ; t) \equiv |m, n, \ldots ; t\rangle$.

Postulate 2: Observables are represented by hermitian operators chosen to satisfy certain **commutation relations.**

Postulate 3: For a system in state ψ, repeated measurements of an observable Ω amounts to the **expectation value** $\langle\Omega\rangle$.

Postulate 3': When ψ is an eigenfunction of the operator Ω, determination of the value of the observable yields the correspondig eigenvalue ω. When ψ is not an eigenfunction, then the measurement yields one of the eigenvalues ω_n with the probability $|c_n|^2$.

Postulate 4: **Probability**, that the particle will be found in the volume element $d\tau$ at the position $\mathbf{r}$ is $|\psi(\mathbf{r})|^2\, d\tau$, if ψ is normalized.

Postulate 5: The wavefunction $\Psi_{m,n,\ldots}(\mathbf{r}_1, \mathbf{r}_2, \ldots ; t)$ evolves in time according to the **Schrödinger equation**.

ELECTRONIC STRUCTURE

Schrödinger equation – for stationary states

$$\left[\sum_{i=1}^{N}\left(-\frac{1}{2}\nabla_i^2\right) + \sum_{i<j=1}^{N}\frac{1}{r_{ij}} + V(\mathbf{R})\right]\Psi_k(\mathbf{R}) = E_k\,\Psi_k(\mathbf{R}) \qquad \text{where} \quad \mathbf{R} = \{\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, \}.$$

and/or for time evolution

$$\left[\sum_{i=1}^{N}\left(-\frac{1}{2}\nabla_i^2\right) + \sum_{i<j=1}^{N}\frac{1}{r_{ij}} + V(\mathbf{R},t)\right]\Psi(\mathbf{R},t) = i\frac{\partial}{\partial t}\Psi(\mathbf{R},t)$$

The wavefunction $\Psi(\mathbf{R},t) = \Psi(\mathbf{r}_1,\mathbf{r}_1,\ldots,\mathbf{r}_N,t)$

is what we need to fully understand and evaluate the properties of materials.

This is a ***many-body problem!***

EXCHANGE OF IDENTICAL PARTICLES AND CORRELATIONS

Exchange of identical particles

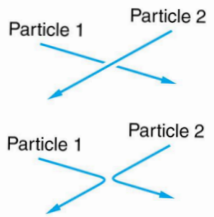
Identical particles may exchange, which must be taken into account

–> symmetry requirements:

Bosons $\psi_S(\mathbf{r}_1,\mathbf{r}_2) = 2^{-1/2}\,(\,|\mathrm{lm}\rangle + |\mathrm{mn}\rangle\,) = +\psi_S(\mathbf{r}_2,\mathbf{r}_1)$

and

Fermions $\psi_A(\mathbf{r}_1,\mathbf{r}_2) = 2^{-1/2}\,(\,|\mathrm{lm}\rangle - |\mathrm{mn}\rangle\,) = -\psi_A(\mathbf{r}_2,\mathbf{r}_1).$



Many-body effects (sc. correlations)

There are no exact solutions to the many-body problems, in general

–> approximations or simulations

PATH INTEGRAL APPROACH: 1/3 CLASSICAL PATH AND QUANTUM PATHS

Let us consider particle dynamics from a to b.

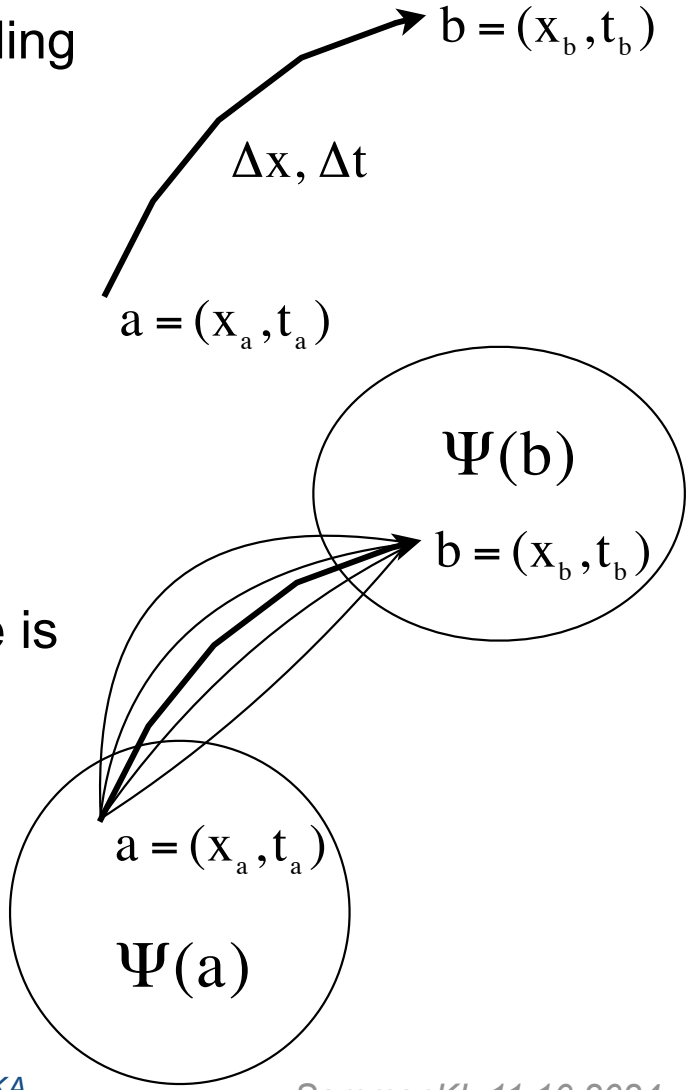
Lagrangian formulation of classical mechanics for finding the path/trajectory leads to equations of motion from minimization (extremum) of action

$$S=\int_{t_a}^{t_b} L(\dot{x},x,t)\,dt, \qquad \text{where the Lagrangian } L = T-V.$$

$$\delta S = 0 \quad \Rightarrow \quad \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 \quad \Rightarrow \quad -\frac{\partial V}{\partial x} = m\ddot{x}$$

For example, the classical **action of the free-particle** is

$$S = \frac{1}{2}m\left(\frac{\Delta x}{\Delta t}\right)^2 \Delta t = \frac{1}{2}m\frac{(x_b - x_a)^2}{(t_b - t_a)}.$$



PATH INTEGRAL APPROACH: 2/3 QUANTUM PATHS AND PROBABILITY

Usually, **the most probable quantum path is the classical one, but other paths contribute, too, with a certain probability.** Quantum probability of the particle propagation from a to b is

$$P(b,a) = |K(b,a)|^2 ,$$

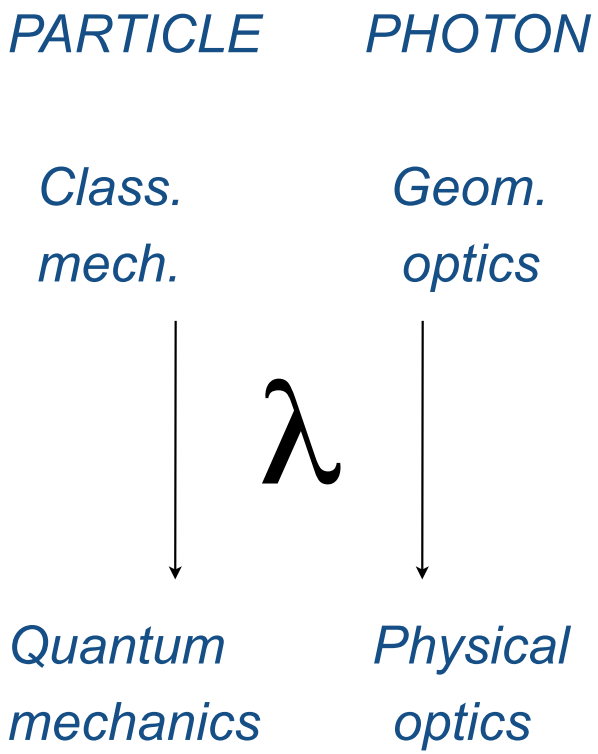
the absolute square of the **probability amplitude** K.

The probability amplitude is the sum over all oscillating phase factors ϕ (or interference) of the paths x_{ab} as

$$K(b,a) = \sum_{\text{all } x_{ab}} \phi[x_{ab}]$$

where the phase is proportional to the exponential of the action

$$\phi[x(t)] = A \times \exp\left(\frac{i}{\hbar} S[x(t)]\right)$$

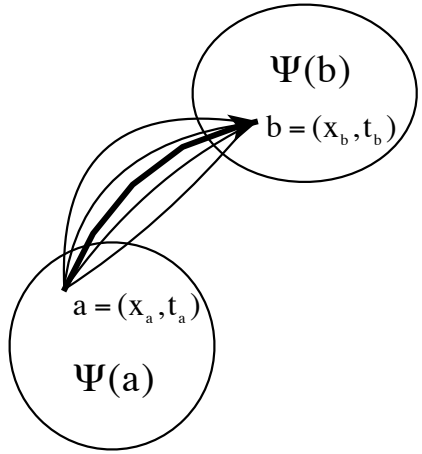


PATH INTEGRAL APPROACH: 3/3 PATH INTEGRAL

Now, let us define the sum over all paths as the path integral

$$\mathrm{K}(\mathrm{b},\mathrm{a}) = \int_{\mathrm{a}}^{\mathrm{b}} \mathrm{e}^{(\mathrm{i}/\hbar)\mathrm{S}[\mathrm{b},\mathrm{a}]}\, \mathcal{D}\mathrm{x}(\mathrm{t}).$$

$$\Psi(b) = \int K(b,a)\Psi(a)\, da$$



We call this ”kernel” or ”propagator” or ”Green’s function”.

In terms of stationary eigenstates $\{\varphi_n\}$ it can be written as

$$K(b,a) = \sum_n \varphi_n^*(a)\varphi_n(b)\mathrm{e}^{-(i/\hbar)E_n(t_b,t_a)}.$$

The kernel **satisfies the Schrödinger equation** in space and time $\{\mathrm{x_b},\mathrm{t_b}\}$.

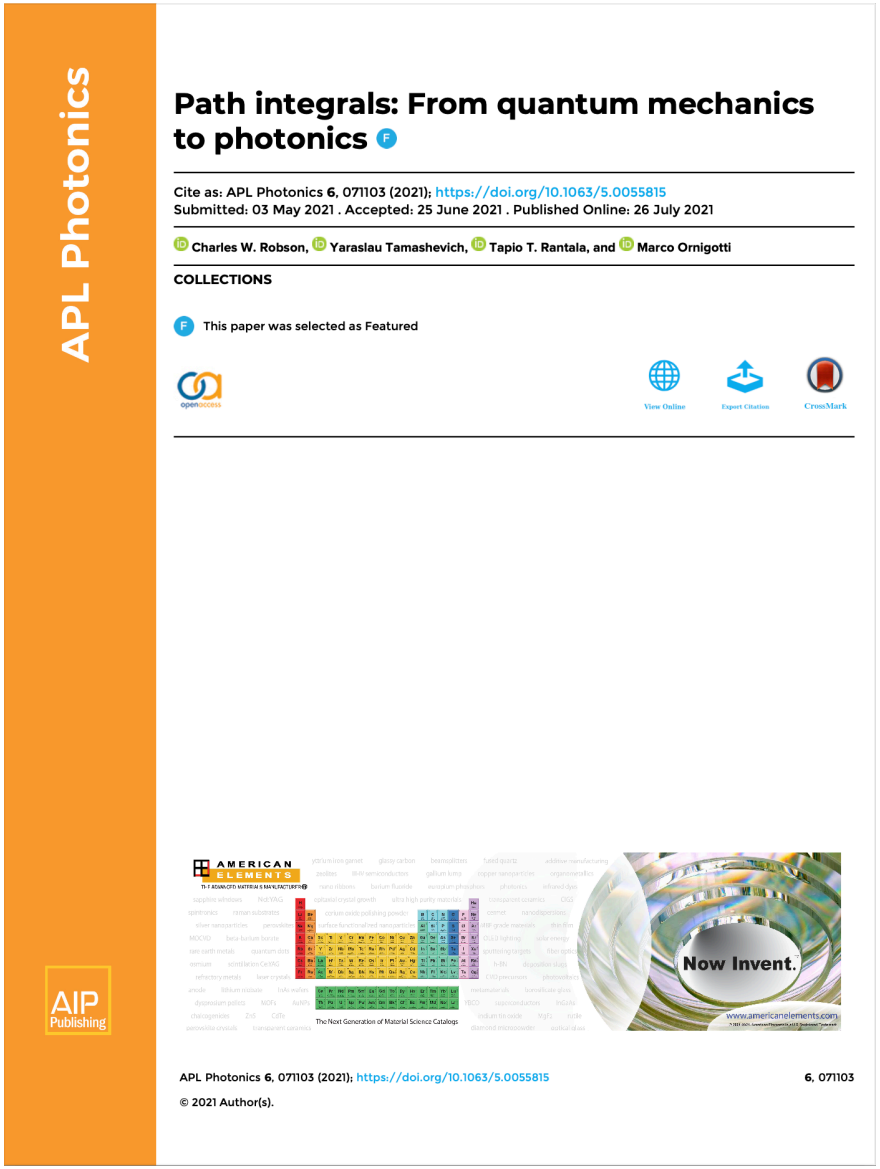
For example, the **free-particle propagator** takes now the form

$$\mathrm{K}_0(\mathrm{b},\mathrm{a}) = \left(\frac{\mathrm{m}}{2\pi\mathrm{i}\hbar(\mathrm{t_b}-\mathrm{t_a})}\right)^{1/2} \exp\left(\frac{\mathrm{im}(\mathrm{x_b}-\mathrm{x_a})^2}{2\hbar(\mathrm{t_b}-\mathrm{t_a})}\right).$$

Classical action is $\mathrm{S} = \frac{1}{2}\mathrm{m}\left(\frac{\Delta\mathrm{x}}{\Delta\mathrm{t}}\right)^2 \Delta\mathrm{t} = \frac{1}{2}\mathrm{m}\frac{(\mathrm{x_b}-\mathrm{x_a})^2}{(\mathrm{t_b}-\mathrm{t_a})}.$

POLKUINTEGRAALIPAPERIT

iki.fi/trantala/paths


APL Photonics

Path integrals: From quantum mechanics to photonics

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Charles W. Robson, Yaraslau Tamashevich, Tapio T. Rantala, and Marco Ornigotti

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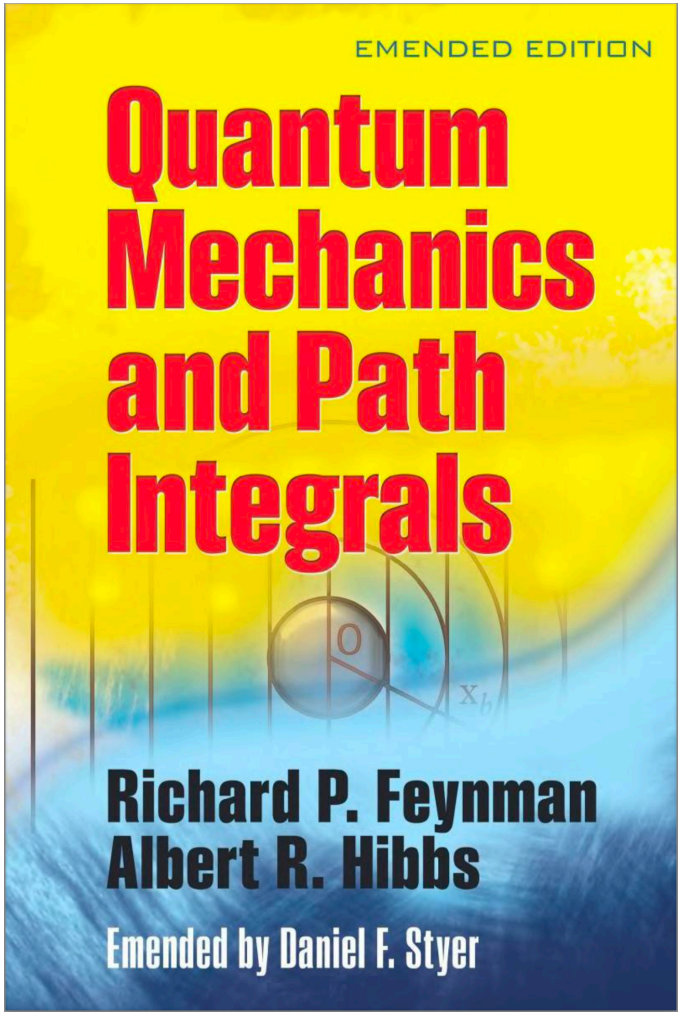
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Feynman–Hibbs, *Quantum Mechanics and Path Integrals,* (McGraw-Hill, 1965)

AALTOJEN KVANTITTUMINEN

EDELLÄ OLEVAN YHTEENVETO

PARTICLE *PHOTON*

Class. mech. *Geom. optics*

λ

Quantum mechanics *Physical optics*

HIUKKANEN LAATIKOSSA

Particle in a box

2.10.–2.13. 1D and 2D confinements

The particle-in-a-box is very useful confining model potential for nanostructures, such as *quantum dots (QD)*, and in particular, for non-spherical parallel piped geometries.

The *quantum well (QW)* is a modified case: A thin layer with an attractive potential for charge carriers.

We consider here an infinite square-well potential, only. Its solutions are those of the free particle waves, which fit to the boundary conditions

$$\psi_n \propto \sin\left(\frac{\pi x}{L} n\right) = \sin(k_n x) \Rightarrow k_n = \frac{\pi}{L} n \quad (2.31)$$

The energies are the corresponding free particle energies

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{h^2}{8mL^2} n^2 \quad (2.30)$$

$n = 1, 2, 3, 4, \ldots$

The two and three dimensional problems trivially separate to one dimensional problems.

We will consider the particle in a spehre, later.

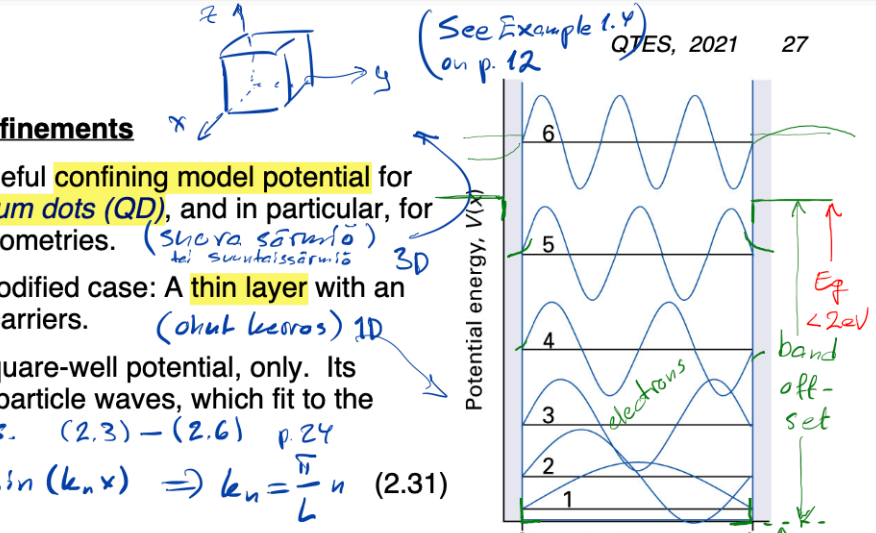


Fig. 2.19.

Fig. 2.22.

RYHMÄTEORIA JA SYMMETRIAT

Symmetria

Symmetriaominaisuuksien systemaattinen tarkastelu perustuu symmetriaoperaatioiden muodostamien ryhmien ominaisuuksiin ja ryhmäteoriaan.

5.1. Symmetriaoperaatiot

Symmetriaoperaatio on toimenpide, joka jättää toimenpiteen kohteen näennäisesti muuttumattomaksi, ja siten se voi ainoastaan vaihtaa kohteen identtisten osien paikkoja.

Mitä enemmän kohteella, esim. molekyylillä, on symmetriaoperaatioita sitä korkeampi on sen symmetria. Symmetriaoperaatioita ovat mm. rotaatio, translaatio, heijastus ja inversio, ja ne suoritetaan jonkin *"symmetriaelementin"* (akseli, suunta, taso tai piste) suhteen.

Molekyylien ja atomien symmetriaoperaatiot muodostavat ns. *pisteryhmiä* (point group), jotka eivät sisällä translaatioita kuten kiteiden symmetriaoperaatioiden yleisemmät *avaruusryhmät* (space group). Pisteryhmien symmetriaoperaatiot jättävät aina yhden pisteen (molekyylin keskellä) ennalleen.

Pisteryhmät sisältävät viidenlaisia operaatioita:

E, **identiteetti** (yksikkö- tai ykkösoperaattori), joka ei tee mitään.

C_n, **n-lukuinen rotaatio** (n-fold rotation) on $360°/n$ kierto *symmetria-akselin* ympäri. Voidaan erottaa erikseen kierto myötäpäivään C_n^+ ja vastapäivään C_n^-. Huomaa, että $C_2^+ = C_2^-$. Jos molekyylillä on useampia symmetria-akseleita, sanotaan *pääakseliksi* (principal axis) sitä, jonka lukuisuus on suurin.

σ, **heijastus** (reflection) *heijastustason* (mirror plane) suhteen. Jos pääakseli on heijastustasossa, sanotaan tasoa vertikaaliseksi ja heijastusoperaatiota merkitään σ_v, ja jos pääakseli on heijastustasoa vastaan kohtisuora on taso horisontaalinen ja heijastus σ_h. Diedrinen (dihedral) taso ja heijastus on erikoistapaus vertikaalisesta heijastuksesta, jossa heijastustaso puolittaa kahden pääakselia vastaan kohtisuoran C_2-akselin välisen kulman.

i, **inversio** (inversion) symmetriakeskuksen suhteen. Inversiossa origon suhteen jokainen piste (x, y, z) siirretään paikaltaan pisteeseen $(-x, -y, -z)$.

S_n, **kiertoheijastus** (improper rotation, rotary–reflection) kiertoheijastusakselin suhteen. Kiertoheijastus koostuu n-lukuisesta kierrosta (rotaatiosta) ja horisontaalisesta heijastuksesta akselia vastaan kohtisuoran tason suhteen. Huomaa, että $S_1 = \sigma_h$ ja $S_2 = i$.

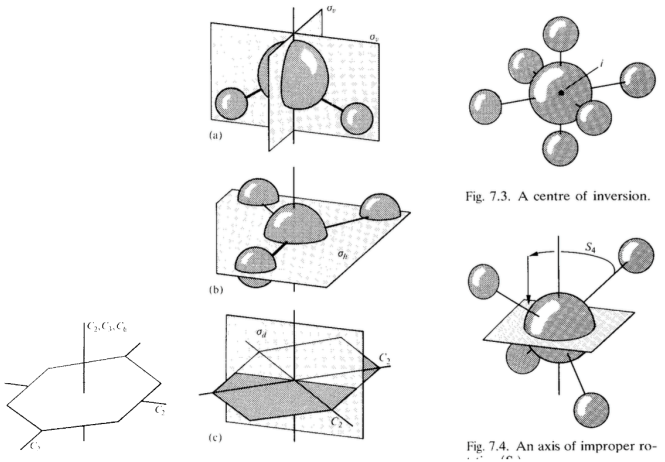


Fig. 7.3. A centre of inversion.

Fig. 7.4. An axis of improper ro-

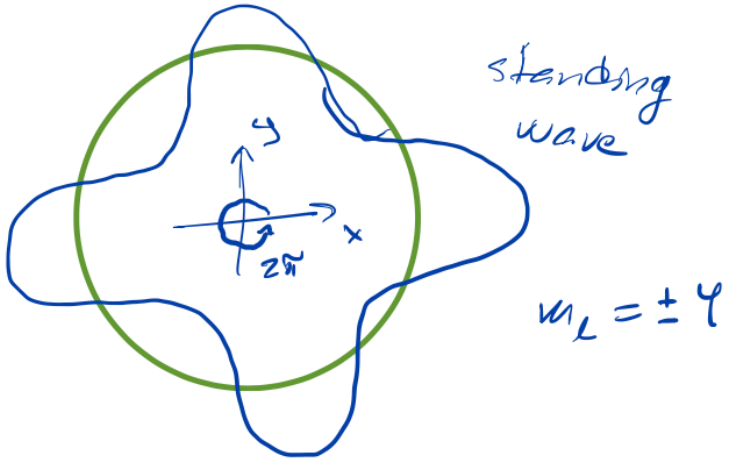
YMPYRÄSYMMETRIA

3.3. Shape of the wavefunction

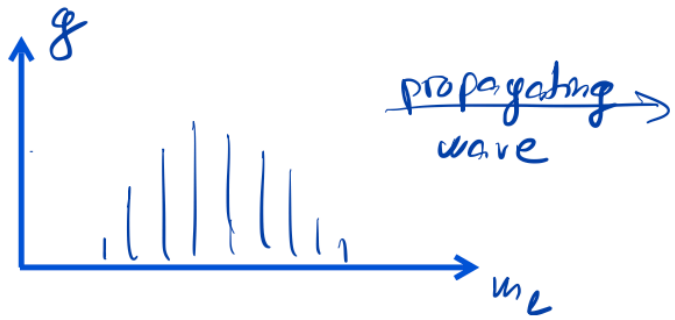
Thus, Φ_A has an angular momentum $m_\ell \hbar$, which indicates rotation. Similarly, $\Phi_B = B\, e^{-im_\ell \phi}$ has an angular momentum $-m_\ell \hbar$ and rotates to the opposite direction. Wavefunctions Φ_A (or Φ_B) are orthonormal with different values of m_ℓ with the normalization constant

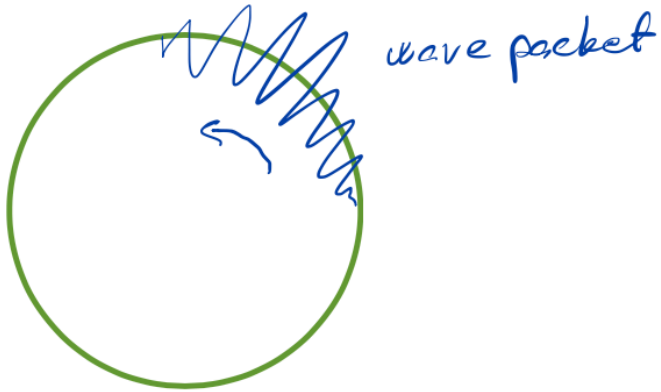
$$A = B = \sqrt{\frac{1}{2\pi}} \,. \qquad (3.12)$$

It should be noted that these states are stationary with constant probability density, but the angle (or position on the ring) is not defined at all, *i.e.*, fully uncertain.



3.4. Classical limit





PALLOSYMMETRIA JA VETYATOMI

3.13. Solutions of the radial equation

For $\ell = 0$, the solution of equation (3.58) behaves as $u \sim Ar + Br^2$, when $r \to 0$, and then $R = u/r \to A$, which means that the probability density of the electron at nucleus is $A^2 \neq 0$.

For $\ell \neq 0$, $u \to A\, r^{\ell+1}$ and $R = u/r \to A\, r^{\ell}$, when $r \to 0$.

The wavefunctions of the hydrogen atom can be written in terms of associated Laguerre functions:

$$R_{n\ell}(r) = -\left(\frac{2Z}{na}\right)^3 \frac{n-\ell+1}{2n(n+\ell)!^2}\, \rho^{\ell}\, L^{2\ell+1}_{n+\ell}(\rho)\, e^{-\rho/2}$$

TABLE 3.4 Radial functions for hydrogen

$n=1$	$l=0$	1s	$R_{10} = \frac{2}{\sqrt{a_0^3}} e^{-r/a_0}$
$n=2$	$l=0$	2s	$R_{20} = \frac{1}{\sqrt{2a_0^3}}\left(1-\frac{r}{2a_0}\right)e^{-r/2a_0}$
	$l=1$	2p	$R_{21} = \frac{1}{2\sqrt{6a_0^3}}\frac{r}{a_0} e^{-r/2a_0}$
$n=3$	$l=0$	3s	$R_{30} = \frac{2}{3\sqrt{3a_0^3}}\left(1-\frac{2r}{3a_0}+\frac{2r^2}{27a_0^2}\right)e^{-r/3a_0}$
	$l=1$	3p	$R_{31} = \frac{8}{27\sqrt{6a_0^3}}\frac{r}{a_0}\left(1-\frac{r}{6a_0}\right)e^{-r/3a_0}$
	$l=2$	3d	$R_{32} = \frac{4}{8\sqrt{30a_0^3}}\frac{r^2}{a_0^2} e^{-r/3a_0}$

The unit of length, sc. *Bohr radius*

$$a_0 = (4\pi\varepsilon_0\hbar^2)/(m_e e^2), \qquad (3.65)$$

is the radius of the electron in Bohr atomic model (infinite nuclear mass).

For the hydrogenic atoms, in general, it is often used

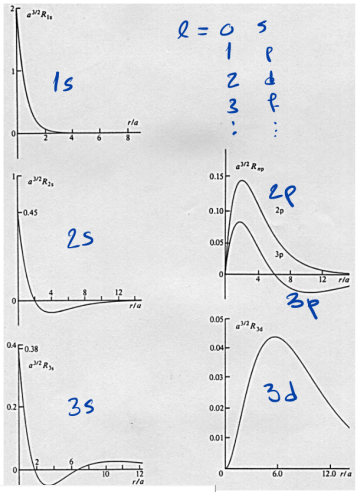
$$a = (4\pi\varepsilon_0\hbar^2)/(\mu e^2)$$

and

$$\varrho = (2Z/na)\, r.$$

(replace $-r/na_0$ by $-\varrho/2$)

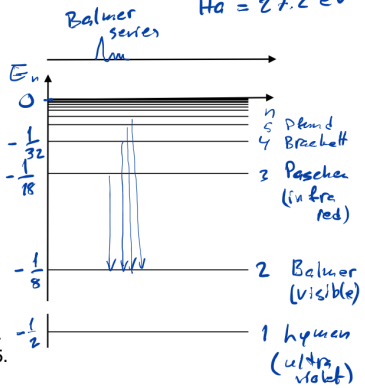
The radial wavefunctions hydrogen atom:



Eigenenergies of the hydrogenic atoms are

$$E_n = -\frac{1}{2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{\mu}{\hbar^2}\frac{1}{n^2};\ n = 1, 2, \ldots . \qquad (3.66)$$

$|E_1| = 1$ Ry (Rydberg) $= 13.6$ eV
$= 1/2$ Ha (Hartree).



Cf. 0.4 on p. 5.

3.14. Probabilities and radial distribution function

$P(r) = 4\pi r^2 \langle|\psi(r)|^2\rangle$ is called the *radial distribution function*. It is the particle probability density as a function of r. For a spherical wavefunction $\psi(r)$

$$P(r) = u^2(r) = R^2(r)\, r^2 = 4\pi r^2 |\psi(r)|^2 \qquad (3.69)$$

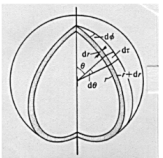


Fig. 4.16. The volume element in spherical polar coordinates.

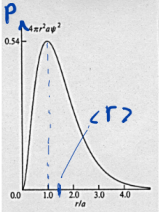


Fig. 4.17. The radial distribution function for the hydrogen 1s-orbital.

3.15. Atomic orbitals

The hydrogenic wavefunctions

$$\psi_{n\ell m_l}(r,\theta,\phi) = R_{nl}(r)\, Y_{lm_l}(\theta,\phi)$$

are called orbitals. Their degeneracy is n^2 and including the spin $2n^2$.

The $(2\ell+1)$ degeneracy arises from symmetry, but n degeneration is accidental.

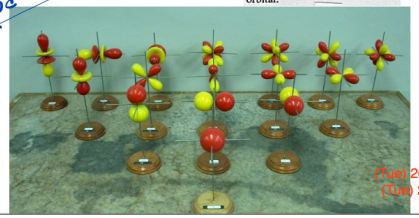
ℓ =	0 (s)	1 (p)	2 (d)	3 (f)	$(0, 1, \ldots, n-1)$
deg.	1	3	5	7	$(2\ell+1)$
n = 1	1s				
2	2s	2p			
3	3s	3p	3d		
4	4s	4p	4d	4f	

The s orbitals are spherical. The p_0 orbital is a real function and the same as p_z orbital. The p_{+1} ja p_{-1} are complex combinations of real p_x and p_y,

$p_{+1} = (p_x - i\, p_y)/\sqrt{2}$ and $p_{-1} = i\,(p_x + i\, p_y)/\sqrt{2}$,

see also the example on p. 8.

The hydrogenic orbitals are simplified models for atomic orbitals. They are used for classification in the periodic table of elements.



(Tue) 20.9.22
(Tue) 2.2.21

MATERIAALIFYSIIKKA

Tampere University

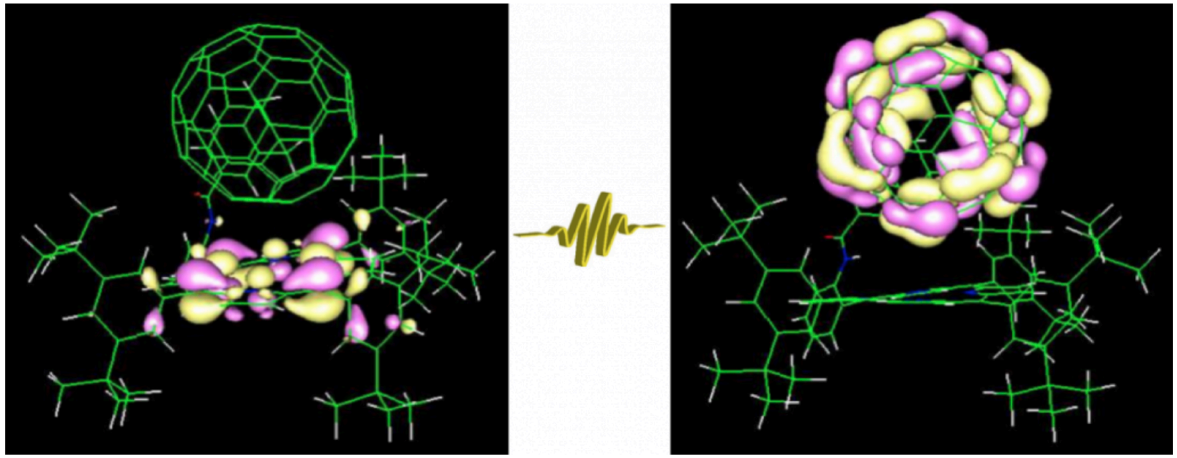
Electronic Structure Theory, Theoretical and Computational Materials Physics

SUOMEKSI SEARCH...

HOME CONTACT

Light–matter interaction

We develop and use electronic structure calculation methods, the fundamental tools for understanding and utilizing the game of electrons and photons



Materials physics

Materials are the most important premise for engineering technology. Therefore, we develop and use electronic structure calculation methods and other modeling approaches for materials physics, the fundamental tools for understanding materials properties and development of better and new materials.

ENGINEERING AND TECHNOLOGY

Challenge

Technology:

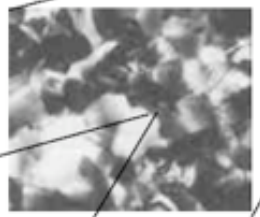
Connection of atomistic and macroscopic scales

and new materials based on materials physics



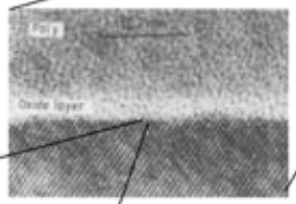
MACRO

10^{-2}m, 10^{8}s



MESO

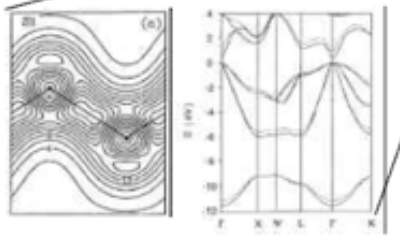
10^{-6}m, 10^{0}s



10 nm

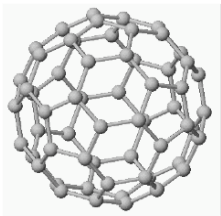
ATOMS

10^{-9}m, 10^{-12}s

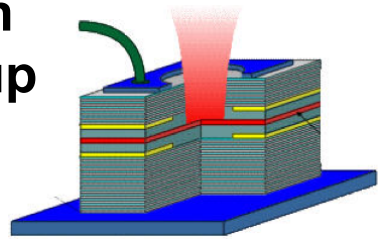


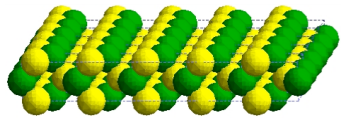
ELECTRONS

10^{-10}m, 10^{-15}s



nano technology:
top–down
bottom–up



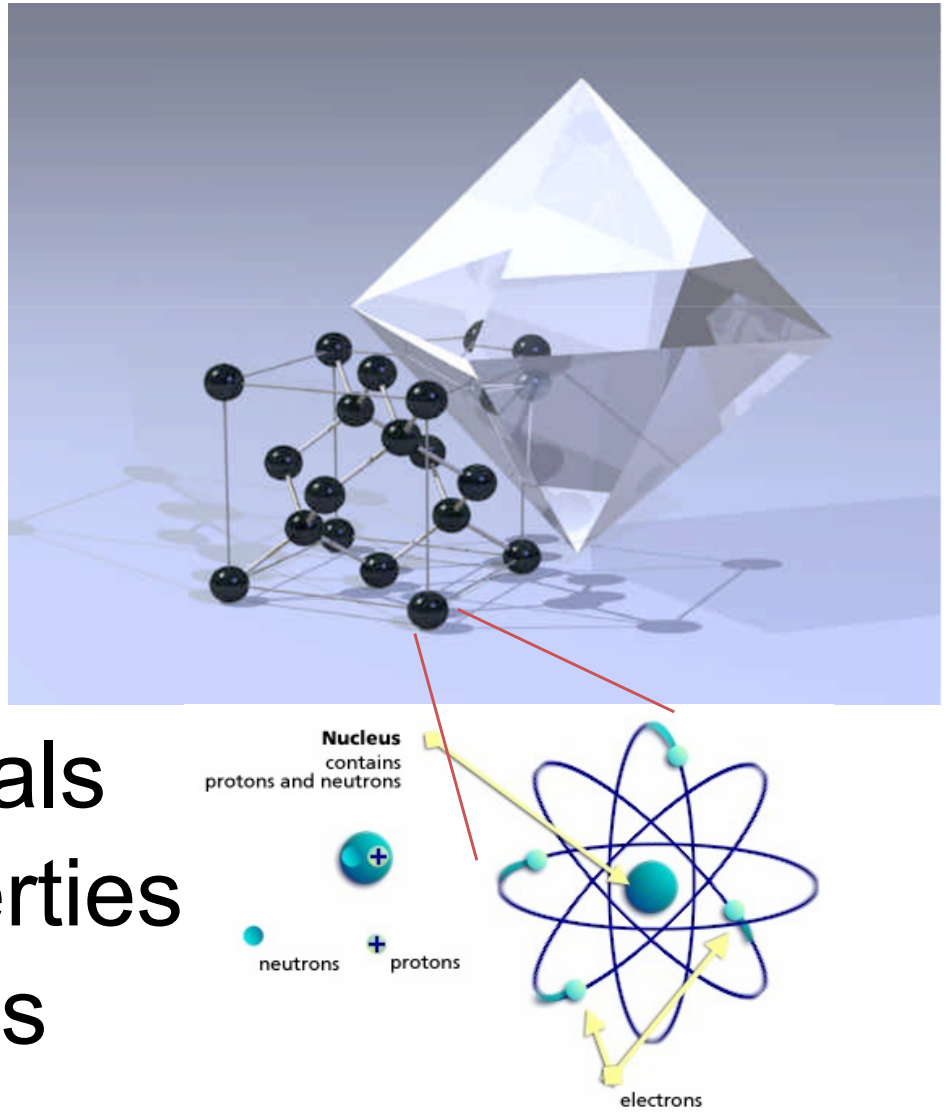


MATERIALS PHYSICS

EST field of science

Materials physics

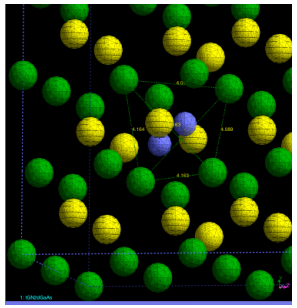
- properties of matter
- understanding with intuitive models
- prediction
- design of new materials with controlled properties or upgrading old ones

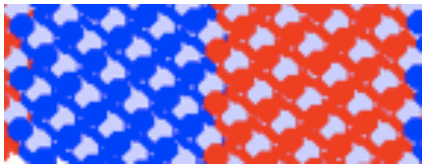


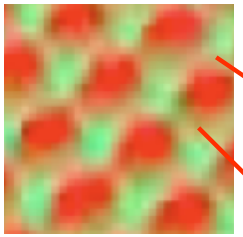
THEORETICAL AND COMPUTATIONAL MATERIALS PHYSICS @ EST

H-P. Komsa: PhD Thesis (2008)

Compound semiconductor physics





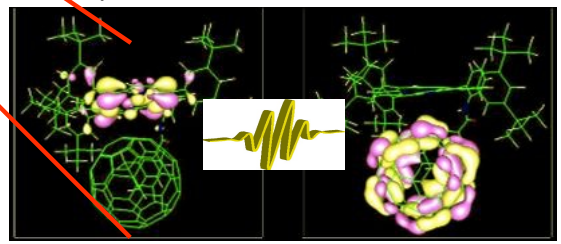


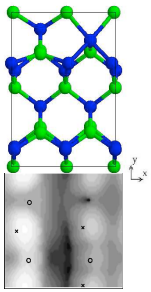
O. Cramariuc: PhD Thesis (2006)

(Bio)molecular

O. Kontkanen: PhD Thesis (2018)

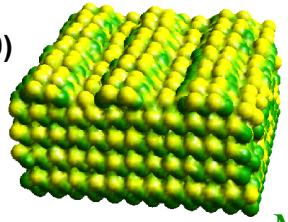
(opto)electronics

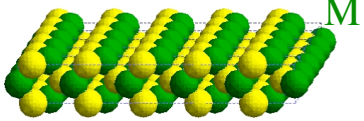


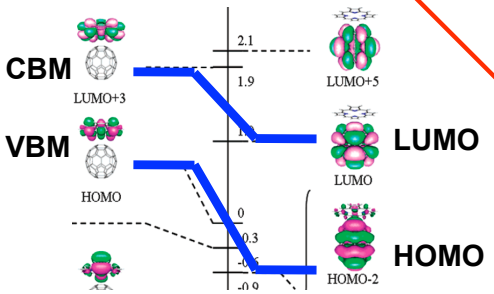


(100)

(110)





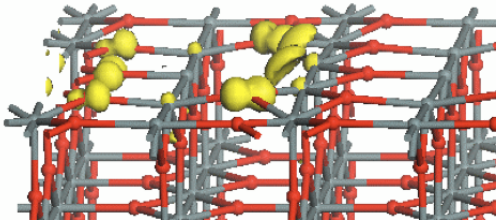


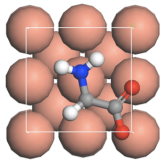
M. Kuisma: PhD Thesis (2014)

GPAW!

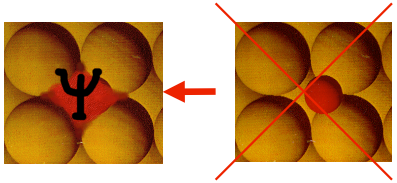
Surface science

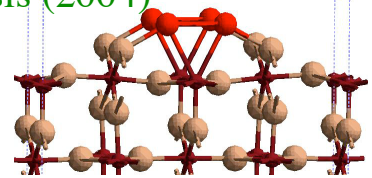
M. Viitala: PhD Thesis (2012)



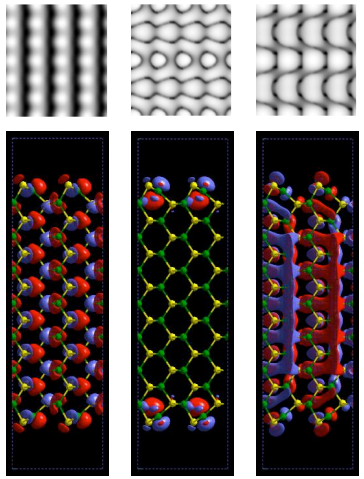


M. Mäki-Jaskari: PhD Thesis (2004)



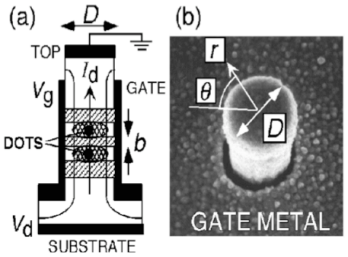


M. Leino: PhD (2007)

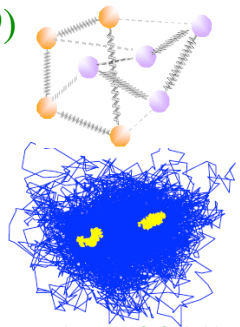


Path-Integral Quantum Monte Carlo

I. Ruokosenmäki: PhD (2019)



J. Tiihonen: PhD (2019)



I. Kylänpää: PhD (2011)

SOFTWARE: DFT

ACADEMIC/COMMERCIAL CODES:

- PlaneWave basis
- localized (atomic) basis
- Real-space grid
- (Gromacs for molecular dynamics)

PBC

finite

PBC and finite

ASE:

MOTIVATION FOR METHOD DEVELOPMENT

Electronic structure is the key quantity to materials properties and related phenomena:
Mechanical, thermal, electrical, optical,... .

Conventional *ab initio* / first-principles type methods

- suffer from laborious description of electron–electron **correlations** (CI, MCHF, DFT-functionals)
- typically ignore nuclear quantum and thermal dynamics and coupling of electron–nuclei dynamics (**Born–Oppenheimer approximation**)
- give the **zero-Kelvin description, only.**
- are typically good for **stationary states, only.**

QMC FOR PHOTONICS

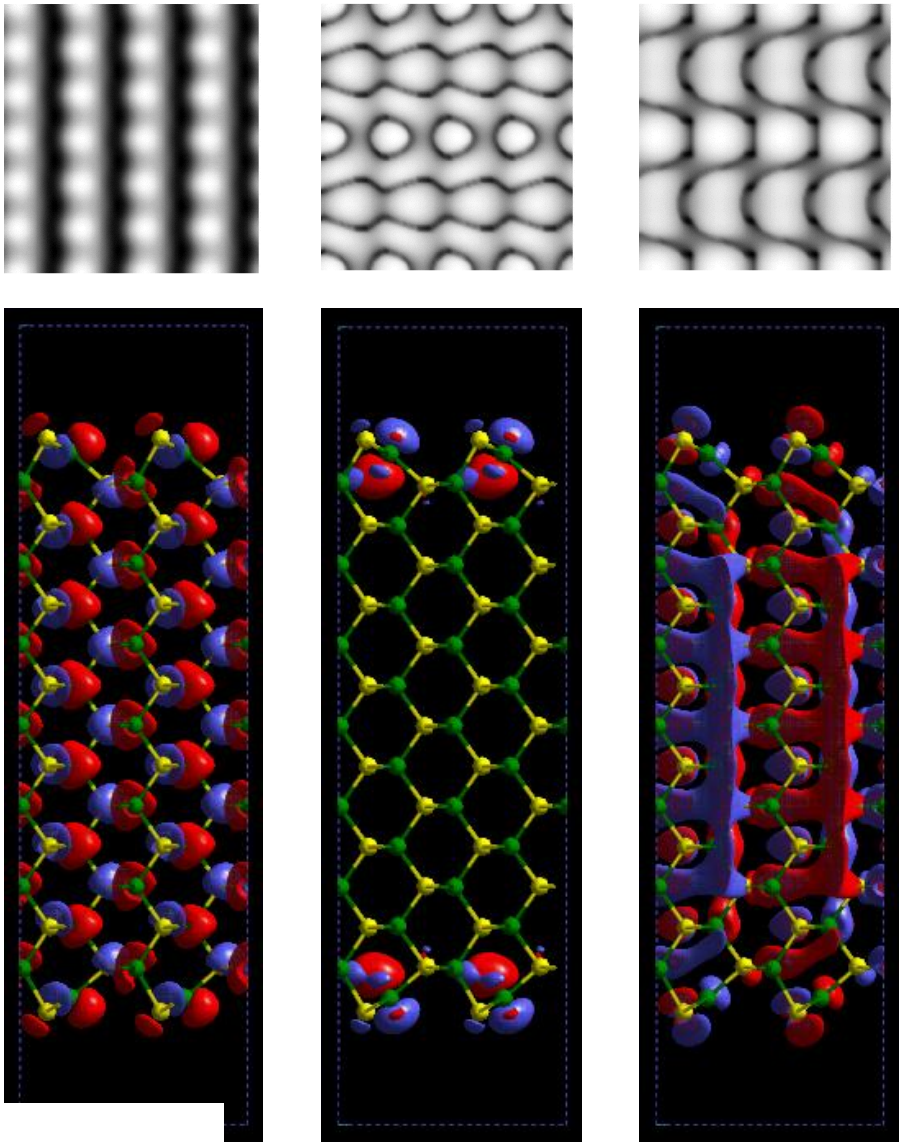
QMC evaluation of optical hyper polarizabilities of 2D materials for photonics:

Materials response to the external electric field, mainly with PIMC, i.e., at *ab initio* level for
- photonics relevant materials like ENZ
- nanostructures, structured light
- dynamics: pulses

David Trejo Garcia (QMC, PIMC)

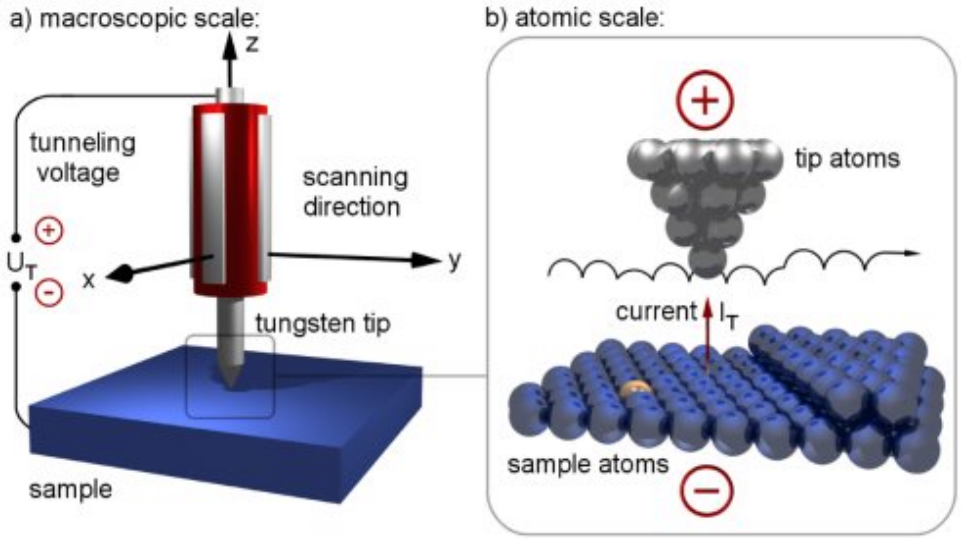
Saijad Ahmadi (QMC, RTPI)
int. collaborators (DFT, QMC)

STM IMAGE SIMULATION OF GaAs (110) SURFACE



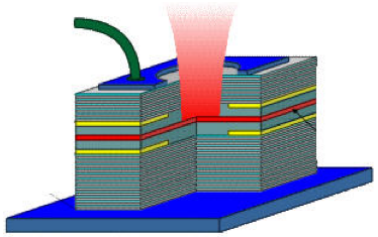
Ville Arpiainen, Jouko Nieminen and Tapio T. Rantala, *Interpretation of orientational contrast in STM images of GaAs(110) cleavage surface*, **Surface Science, 584/1, 27–34 (2005).**

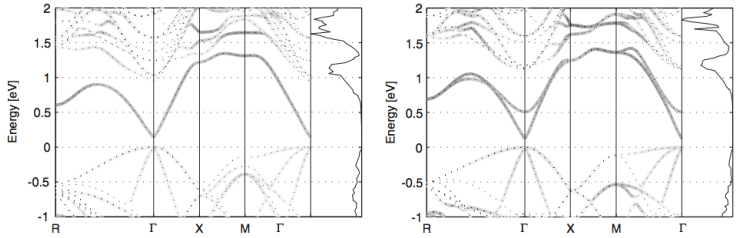
SCANNING TUNNELING MICROSCOPE (STM)

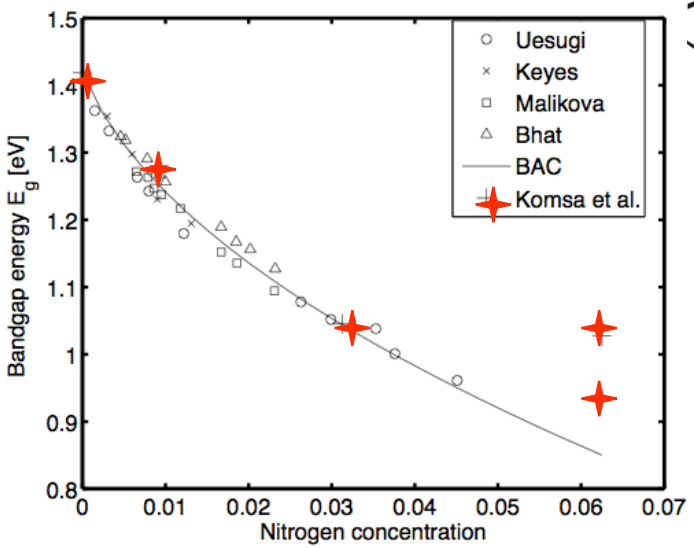


$GaAs_{1-x}N_x$ AND $GaN_{1-y}As_y$

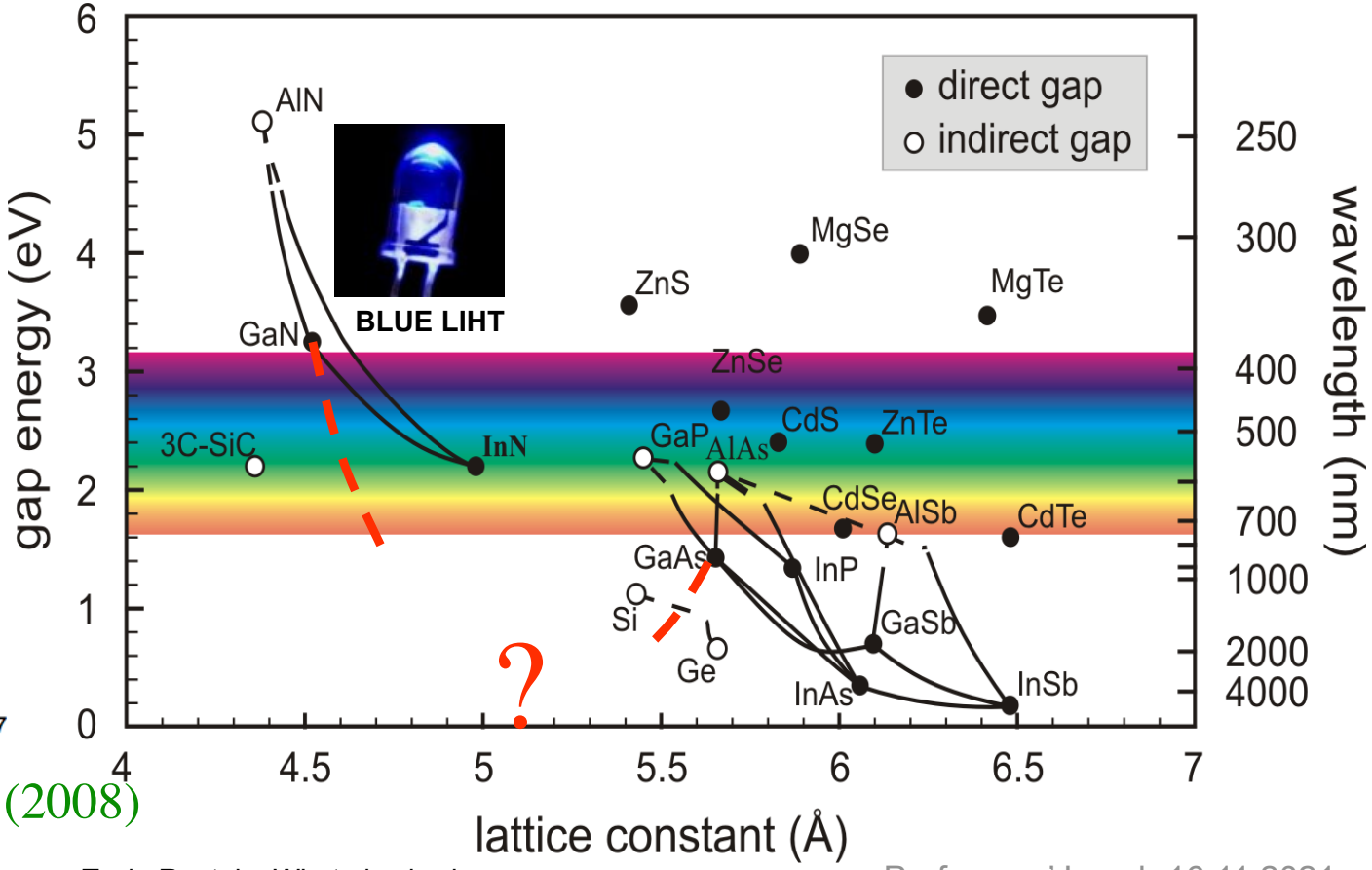
Central compounds in optoelectronic applications,
GaAs: opt. comm.
GaN: blue light
GaAsN: band bowing







H-P. Komsa: PhD Thesis (2008)



QUANTUM DOTS IN QCA

- Finite temperature and electron delocalization

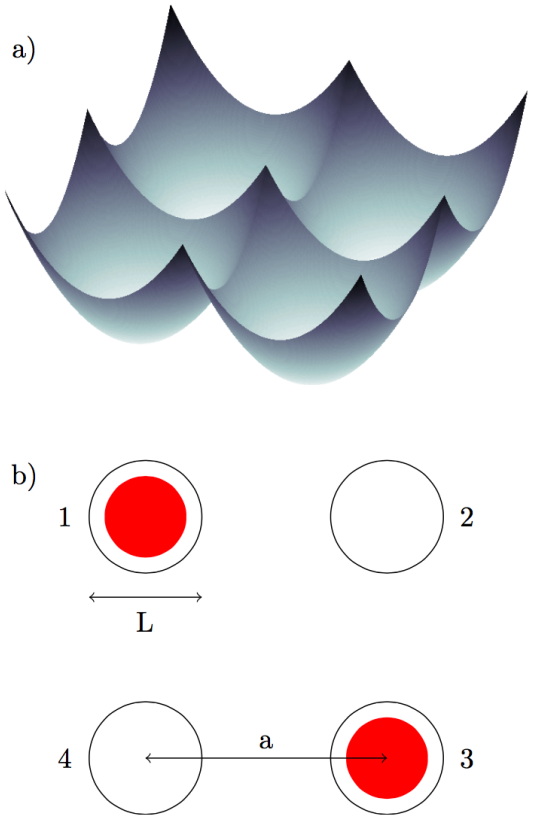


FIG. 1. (a) A visualization of harmonic confinement potential of our QCA cell model. (b) Schematic picture of an ideal QCA setup, where the two electrons occupy either "0" bit (sites 1 & 3) or "1" bit (sites 2 & 4). The site separation a and QD size L are marked.

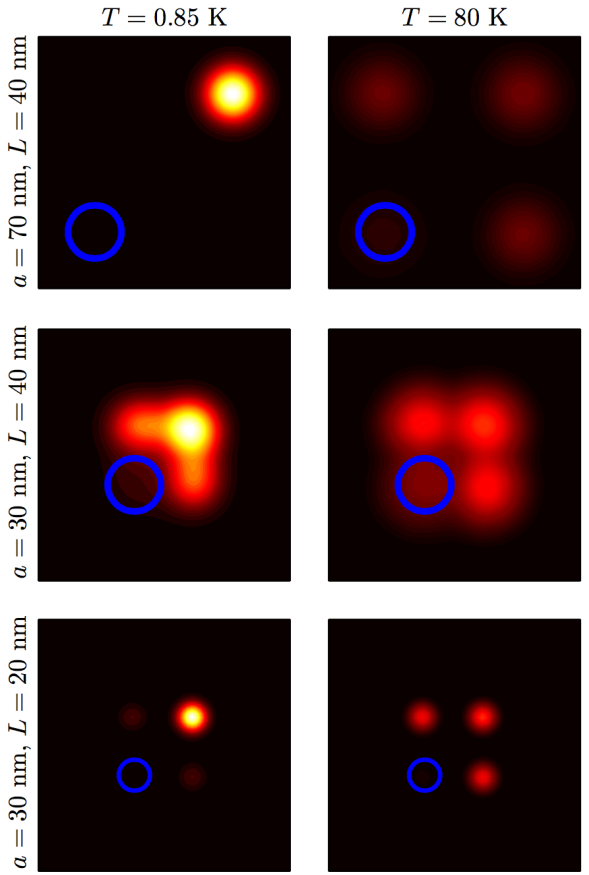


FIG. 3. The density distribution of one electron is plotted according to the reference electron (blue circle) at $T = 0.85$ K (left) and $T = 80$ K (right) with different separation distances and QD sizes. The normalization is the same in both temperatures.

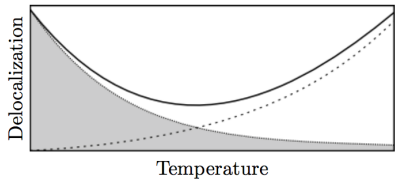


FIG. 6. A schematic separation of the total delocalization (solid line) to thermal part (dashed) and quantum mechanical part (dotted) as functions of temperature. The gray area causes the difference in fidelity between full quantum and classical data.