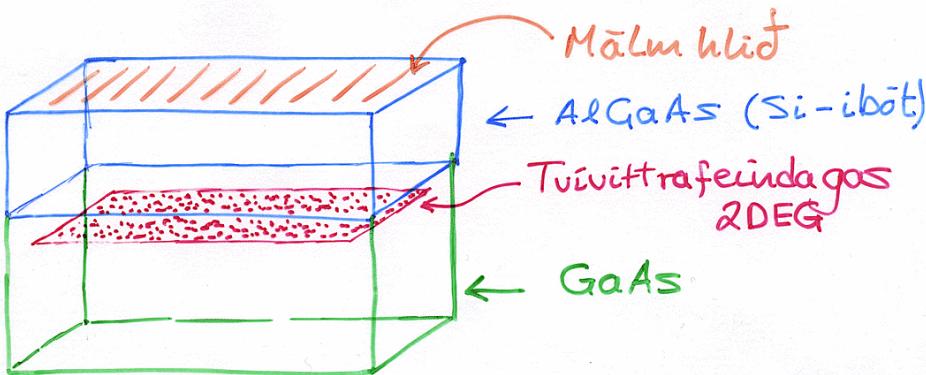


Rafeindakerfi í skertum Uiddum í hálfleidurum

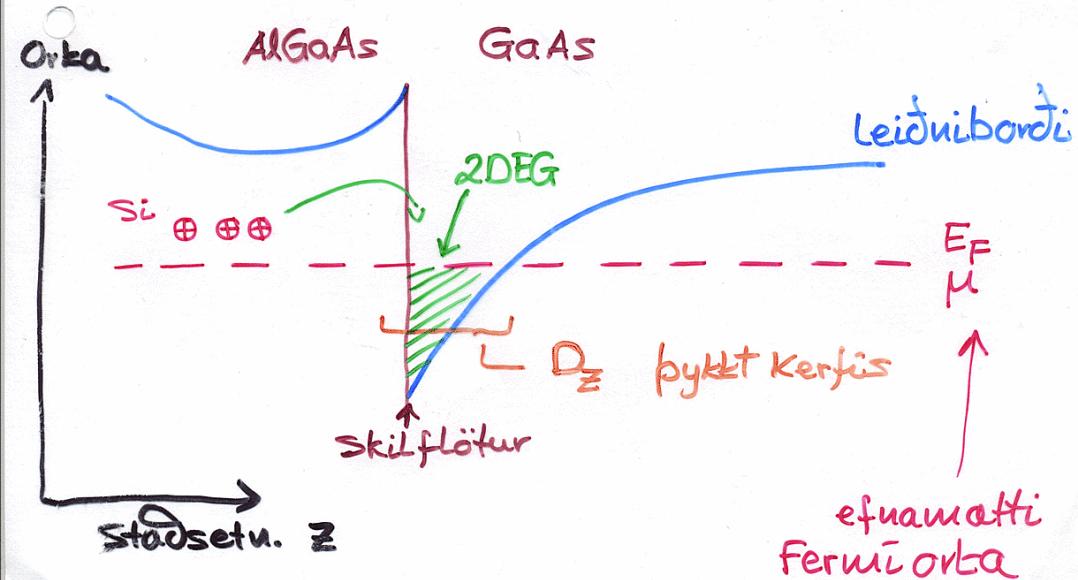
①

- Óvenjuleg hrif
- Tækni, töl

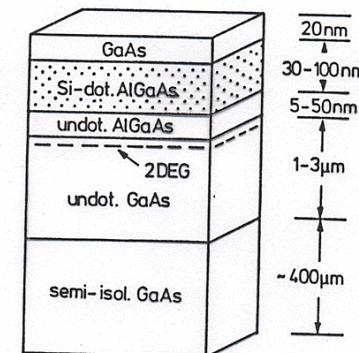
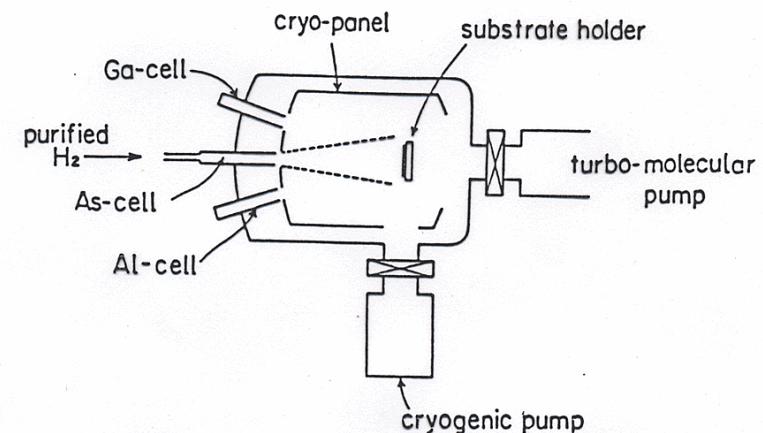
MBE - sameindaúðun

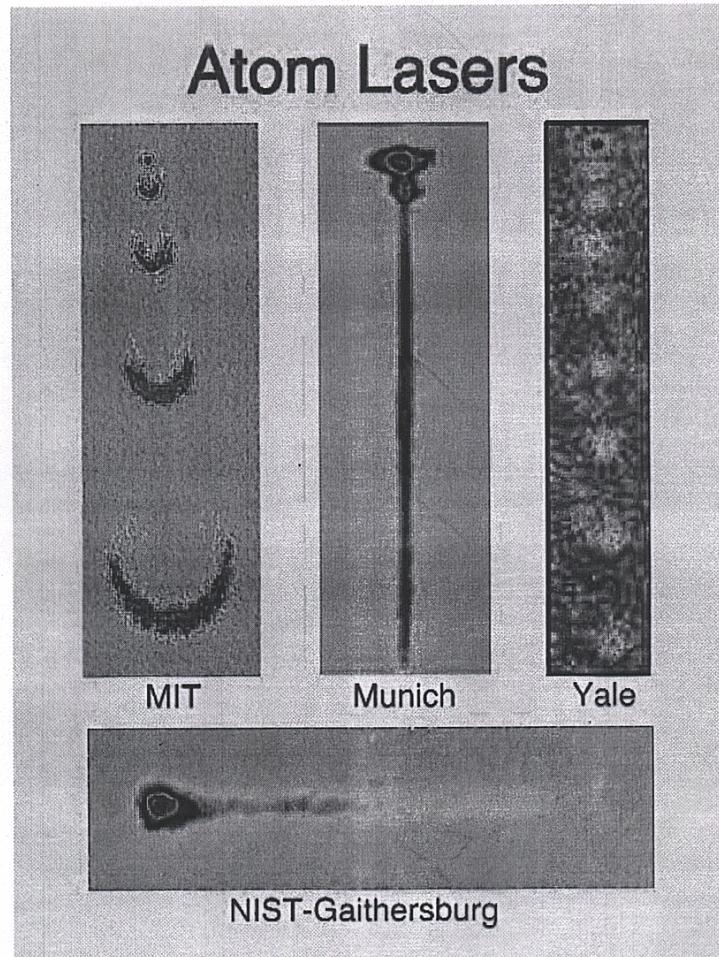


Gegusær kristallur á innrauða suðinu



1 Sameindaúðun (MBE)



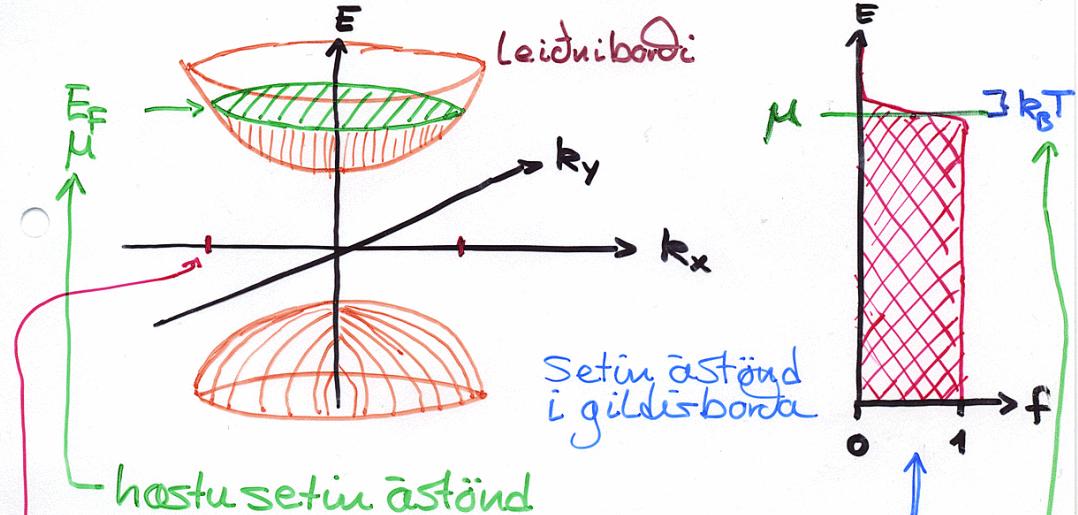
Atom Lasers: The Next Generation

Atom lasers produce highly controlled beams of atoms with desirable properties similar to the light beams produced by optical lasers. The raw ingredients for such devices are ultracold clumps of atoms called "Bose-Einstein condensates," which overlap with one another and fall into the same quantum state, which means that the atoms are highly coordinated with each other. Atom laser devices simply extract beams or pulses of atoms from these BECs.

Frjólsar hreyfingar með fram skilfleti

$$\text{Orkaða óstönd } E(E) = E_z^0 + \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2)$$

skóðum vixLverkun einda síðar



höstu setin óstönd

hösti setui
bylgjuvígur k_F
i Leiduiborda

Pauli einsætui
Fermidreifing

klassisk varmaðra

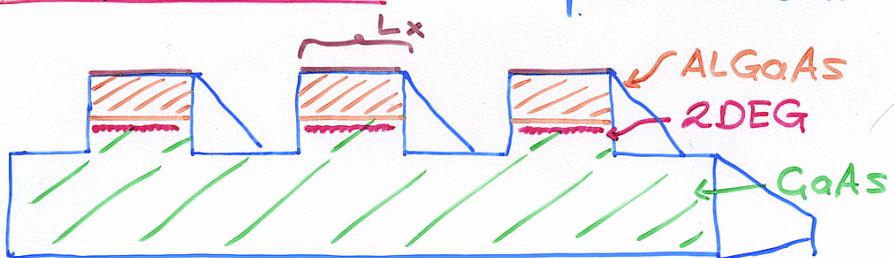
$$\text{Fermi skrifþungi } p_F = \hbar k_F$$

$$\text{Fermi bylgjulengd } \lambda_F = \frac{2\pi}{k_F}$$

$$E_F \quad \lambda_F \gg D_z \rightarrow 2\text{DEG}$$

Afl fræðilega

1DEG - einvidd

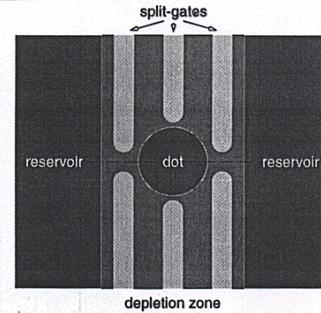
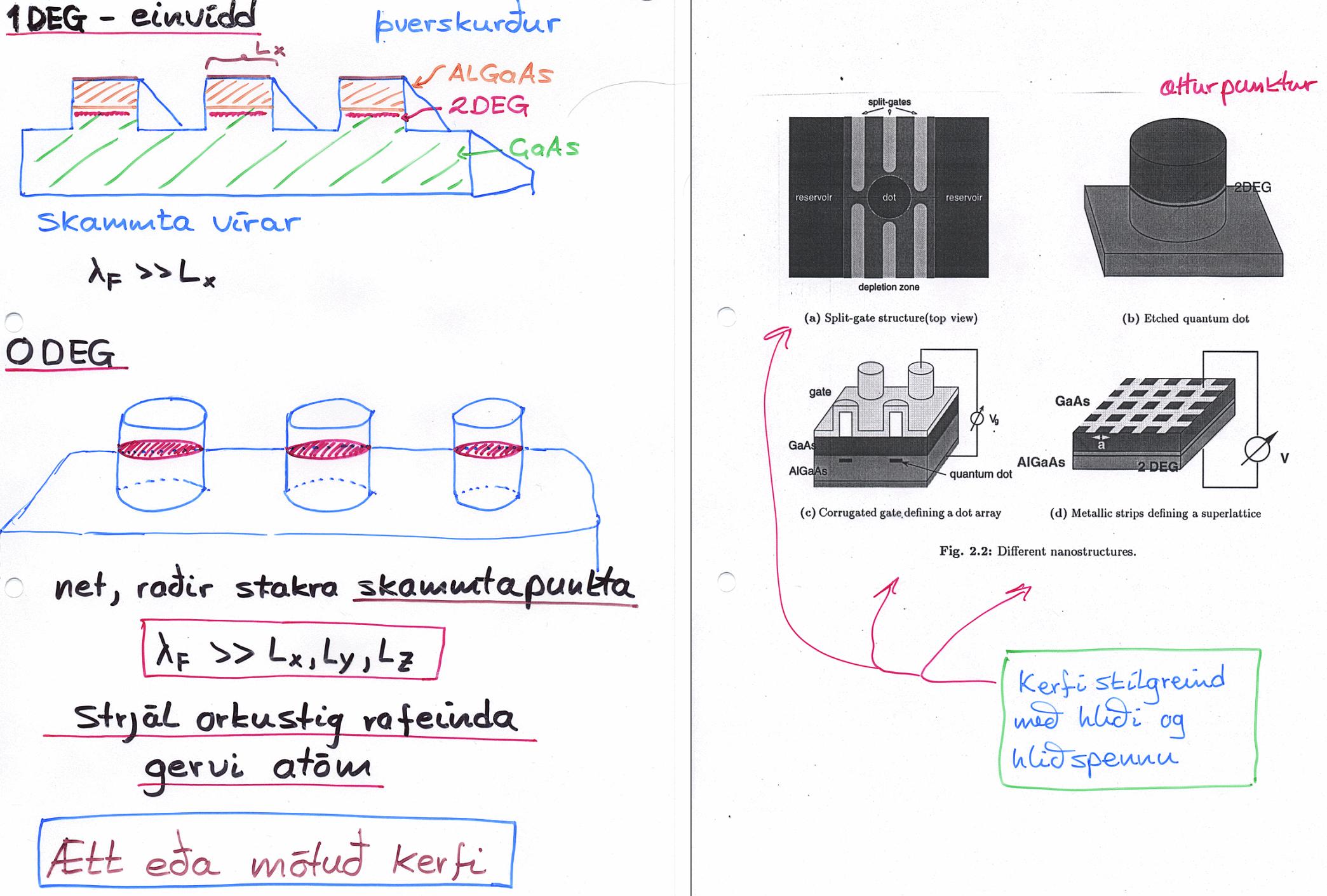


Skamulta virar

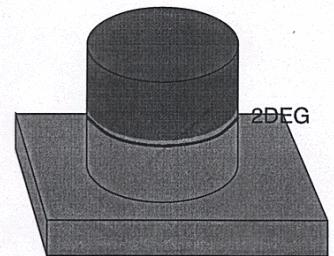
$$\lambda_F \gg L_x$$

(3)

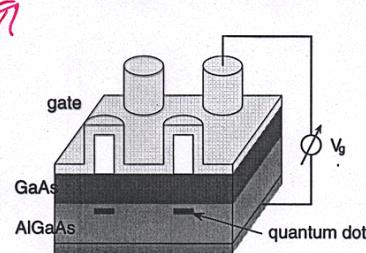
bverskurdur



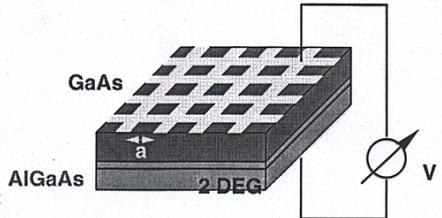
(a) Split-gate structure (top view)



(b) Etched quantum dot



(c) Corrugated gate defining a dot array



(d) Metallic strips defining a superlattice

Fig. 2.2: Different nanostructures.

Kerfi stílgreind
með hluti og
hlidspennu

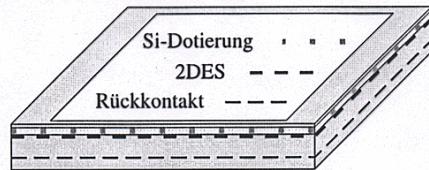
Fraunhofer Vira

2.1. Ausgangsmaterial

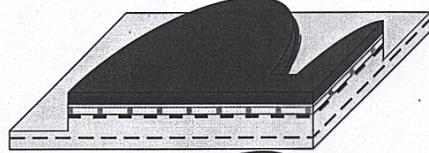
3

4,2 K werden Beweglichkeiten von mehreren Hunderttausend cm²/Vs erreicht.

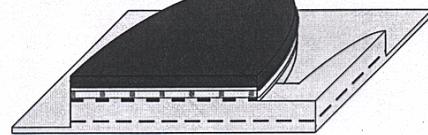
2D-
Ausgangsmaterial



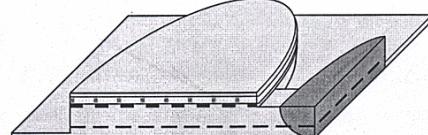
Photolithographie
und erster Ätzschritt



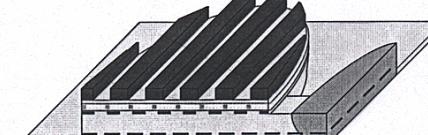
Teilweise Entfernung
des Photolackes und
zweiter Ätzschritt



Einlegen der Kon-
takte und Wedgen
der Probe



Aufbringen von
Photolack und
Erzeugung von Lack-
stegen mittels ho-
lographischer Litho-
graphie



Aufdampfen
des Gates

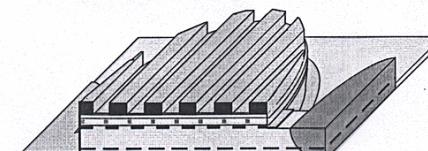
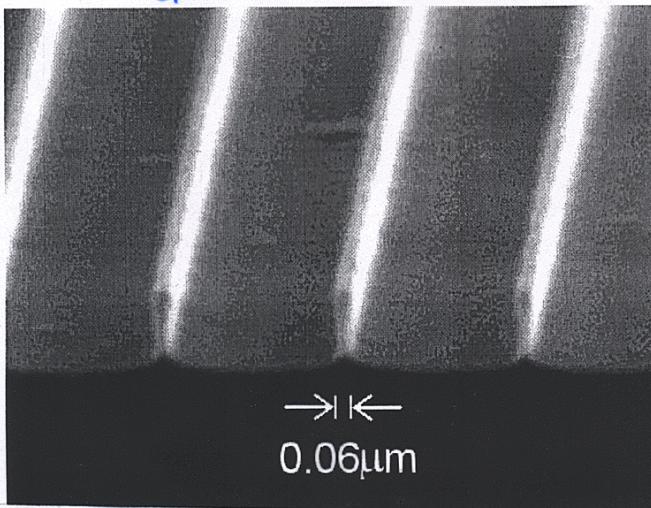


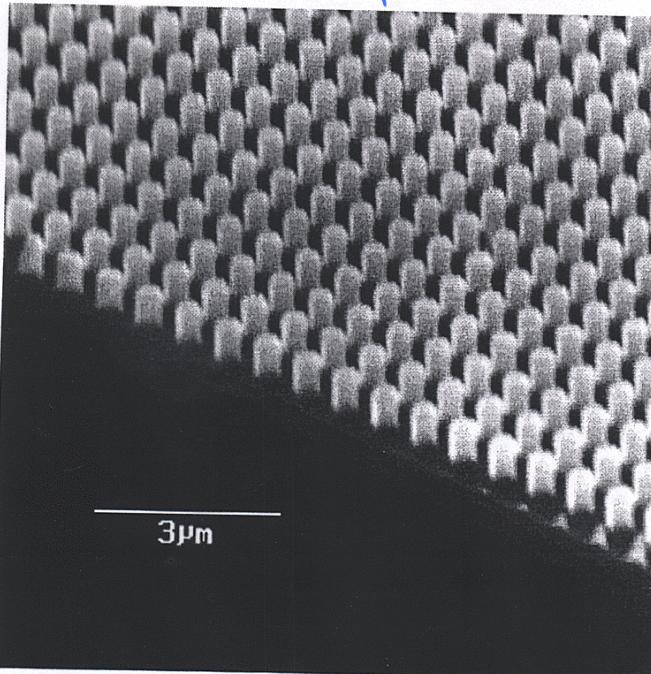
Abb. 2.1: Schematische Darstellung der Prozeßabfolge bei der Präparation von Proben mit Rückkontakte Schicht und moduliertem Gate für FIR-Messungen.

Bei der Herstellung von Proben mit Gate bietet sich die Verwendung von Ausgangs-

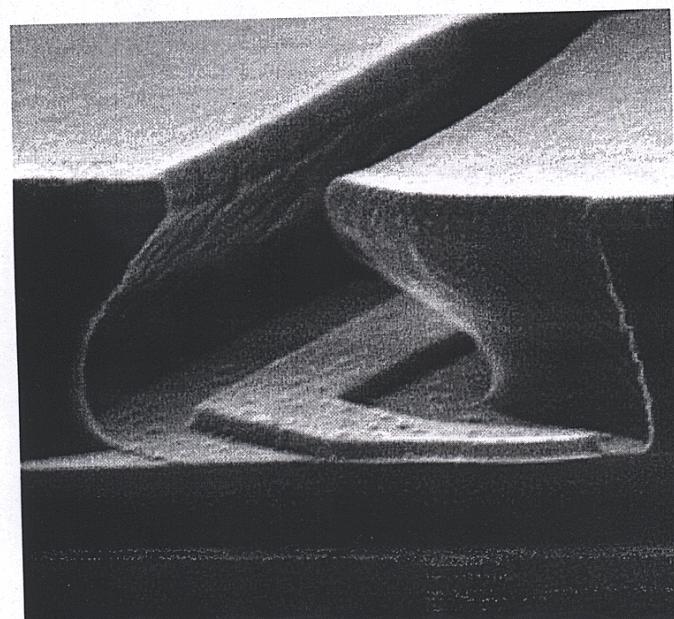
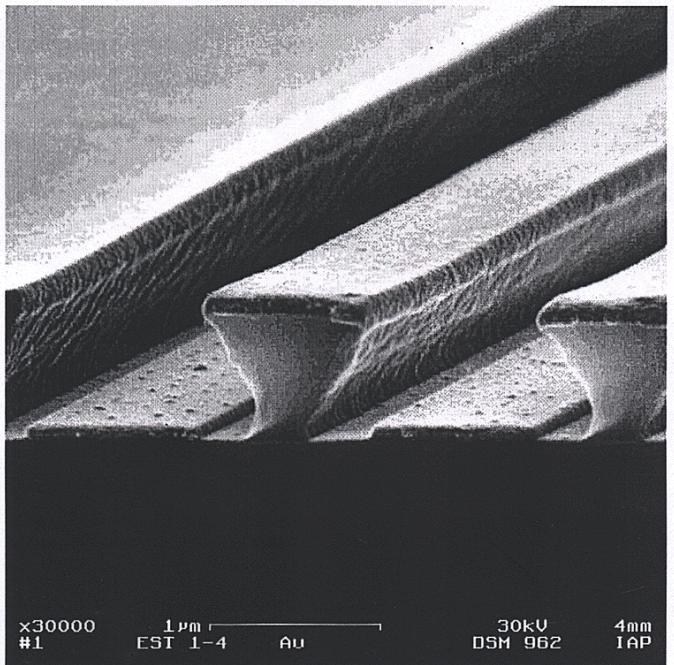
Grauer Stammtavirat



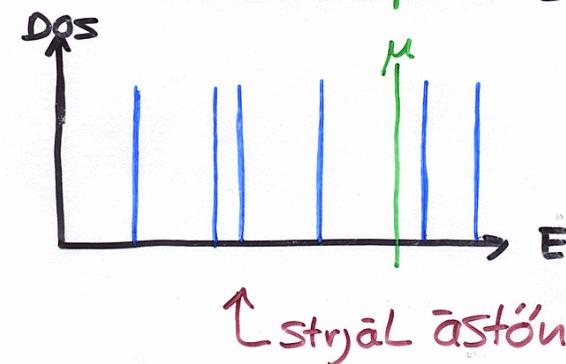
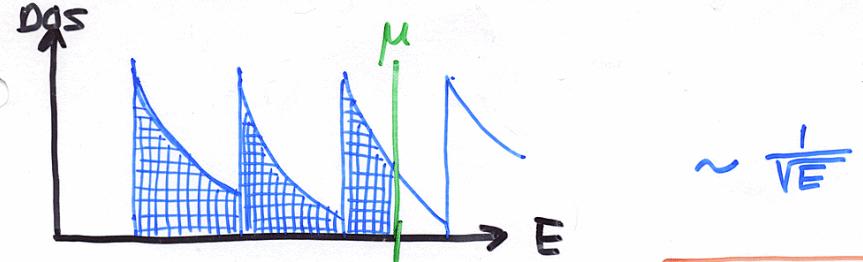
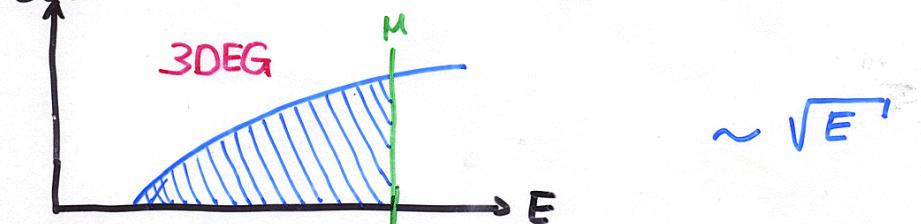
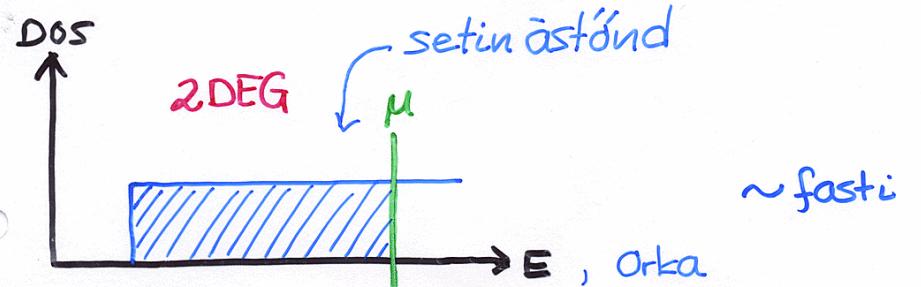
net puncta



Astandabéttleiki DOS



Fjöldi rafeinda ástanda
Orkubil * flatareiniingu = DOS

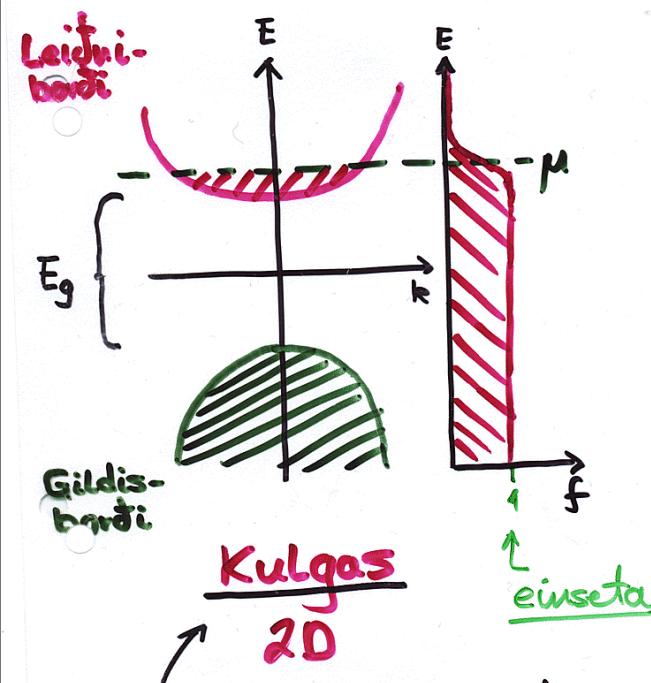


margin eiginleikar tengjast DOS

②

Hlígas — Kulgas
2D — 3D

Rafeindagas í hölfleidara



breyta má þéttleikan! ← ekki hægt í 3DEG.

⑤

Vixlverkun

Coulomb vixlverkun

beinn báttur



$$V(r) = +\frac{e^2}{4\pi\epsilon_0 r}$$

Stöðuorka
frährinding

skipta báttur

Fermi eindir með spuna (skammtatröði)



enginn Skiptakraftur



skiptakraftur
addrættarkraftur

flokkið form
(eindir þekkjast ekki
í sundur)

en reiknulegt
(östurbundin)

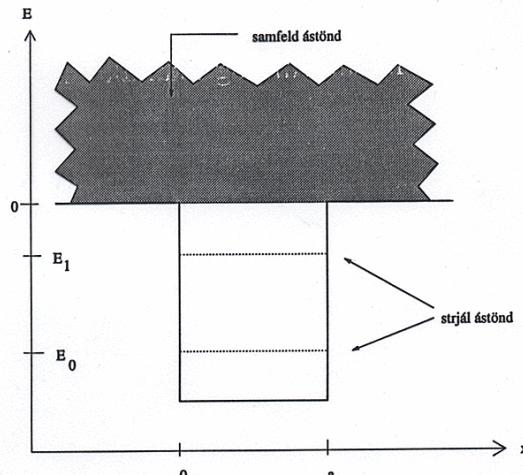
2 Skammtafræði

$$(\Delta x)(\Delta p) \geq \hbar$$

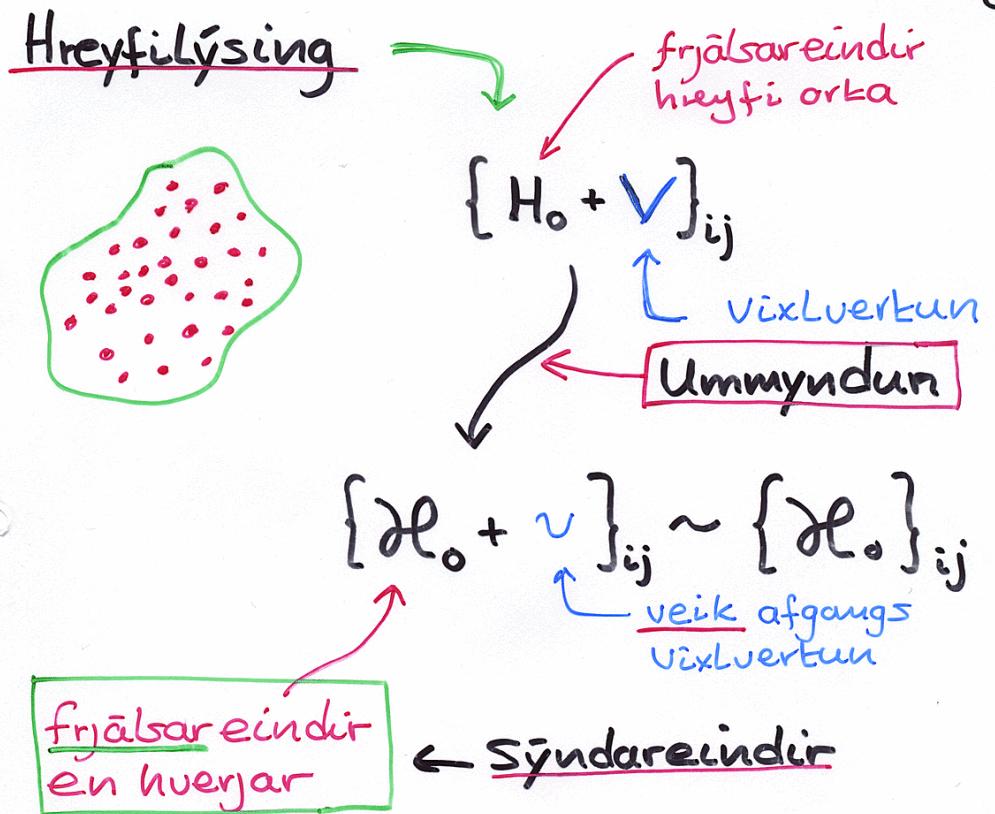
Ekki er hægt að staðsetja rafeind nákvæmlega
→ líkindadreifing.

Hreyfilýsing fyrir líkindabylgjur
sem ferðast um efnið.

2.1 Orkubrunnur - bundin ástönd



Mynd 1: Orkubrunnur.



Kerfi

Rafeindir

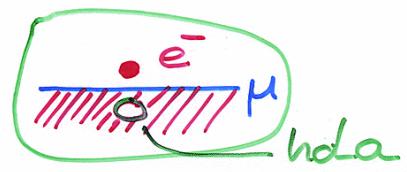
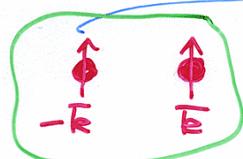
Málmi

Ofurleitara

Hálfleitara

⋮

plasma eindir
Cooperpör
plasma. breyttur massi...
holur.....



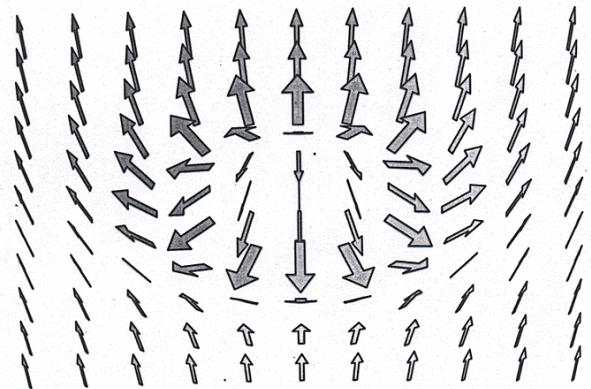
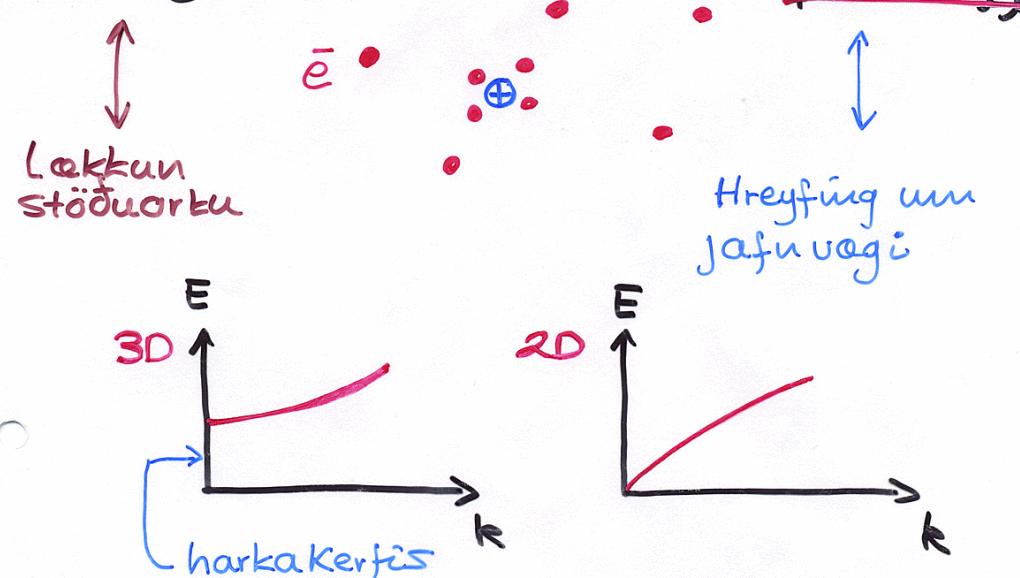


Fig. 9.2: Spin orientation of a skyrmion. The flipped spin sits at its center.

Dæmi um síndareind:

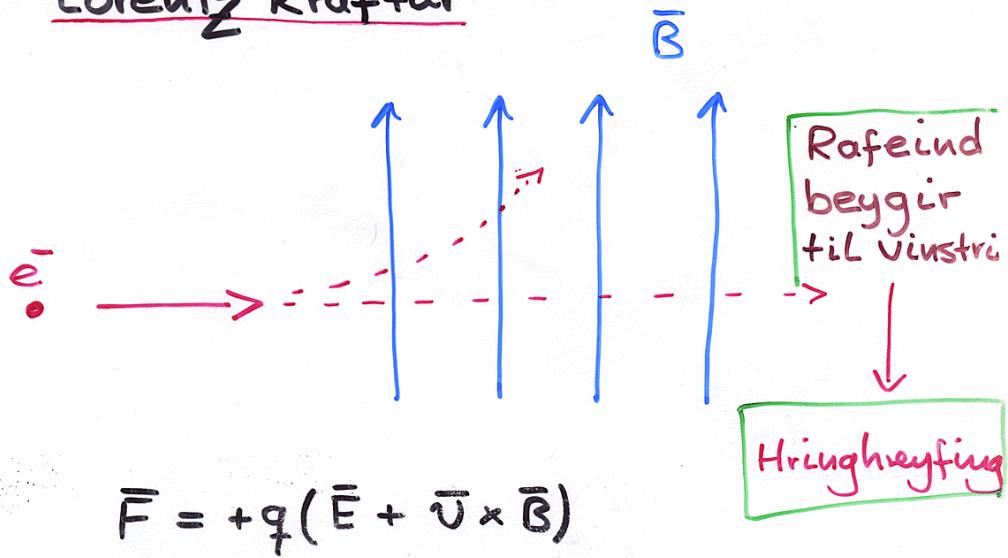
Skyrmie-eind

Skyling



Segulsvid

Lorentz kraftur



Sigild Hall hrit

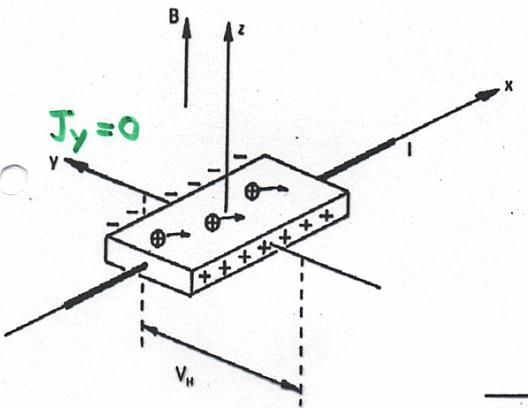
①

1879

$$E_x = g_{xy} J_y + g_{xx} J_x$$

$$E_i = \sum_j g_{ij} J_j$$

$$J_i = \sum_j T_{ij} E_j$$



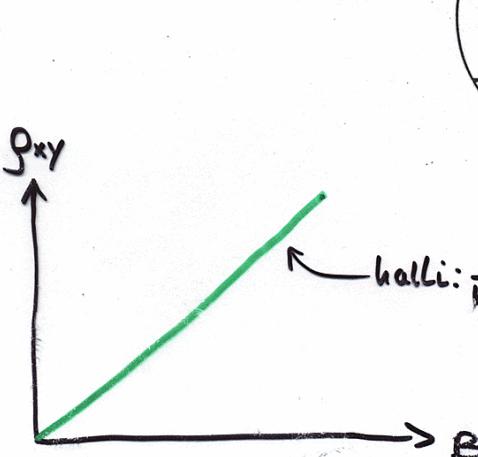
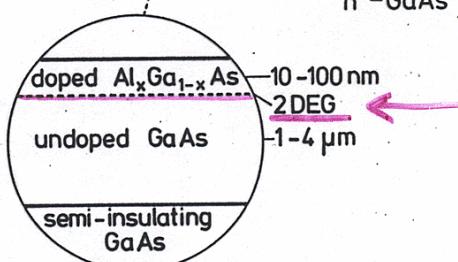
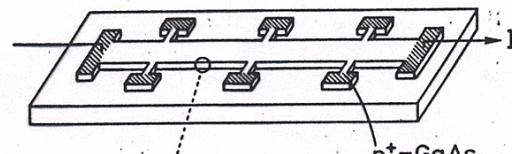
Molt

$$J_y = 0$$

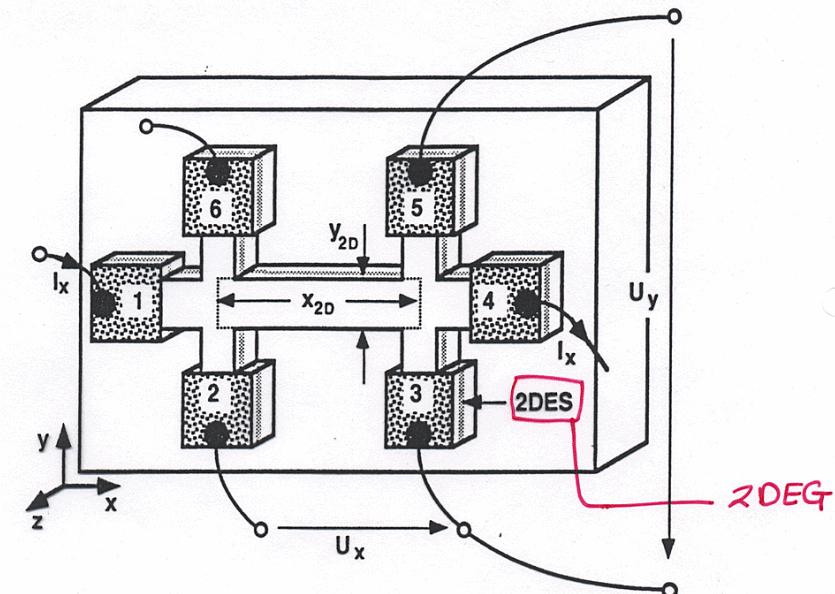
$$R_H = \frac{E_y}{J_x B} = \frac{g_{yx}}{B}$$

$$= -\frac{1}{nec}$$

$$g_{xx} = \frac{E_x}{J_x}$$



$$g_{xy} = -g_{yx}$$



Hall sýni med
molishertum

(3)

New Method for High-Accuracy Determination of the Fine-Structure Constant
Based on Quantized Hall Resistance

K. v. Klitzing
Physikalisches Institut der Universität Würzburg, D-8700 Würzburg, Federal Republic of Germany, and
Hochfeld-Magnetlabor des Max-Planck-Instituts für Festkörperforschung, F-38042 Grenoble, France

and

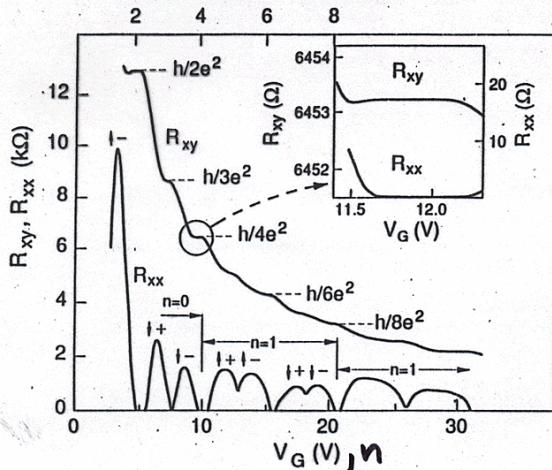
G. Dorda
Forschungslabore der Siemens AG, D-8000 München, Federal Republic of Germany

and

M. Pepper
Cavendish Laboratory, Cambridge CB3 0HE, United Kingdom
(Received 30 May 1980)

Measurements of the Hall voltage of a two-dimensional electron gas, realized with a silicon metal-oxide-semiconductor field-effect transistor, show that the Hall resistance at particular, experimentally well-defined surface carrier concentrations has fixed values which depend only on the fine-structure constant and speed of light, and is insensitive to the geometry of the device. Preliminary data are reported.

LANDAU - LEVEL FILLING

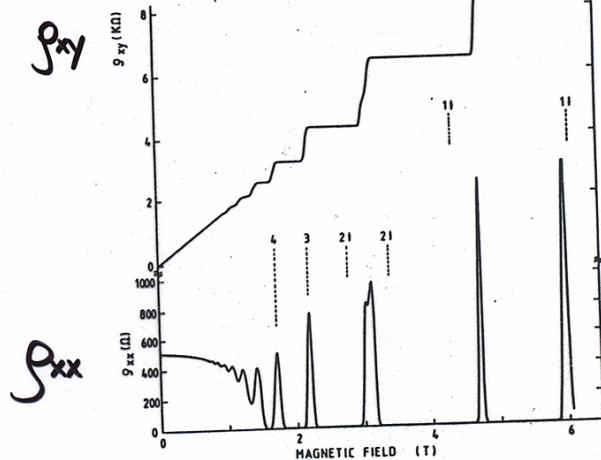


$$g_{xy} \rightarrow \frac{h}{ie^2} \quad i = 1, 2, 3, \dots$$

$$g_{xx} \rightarrow 0$$

$$\tau_{yx} = i \frac{e^2}{h}$$

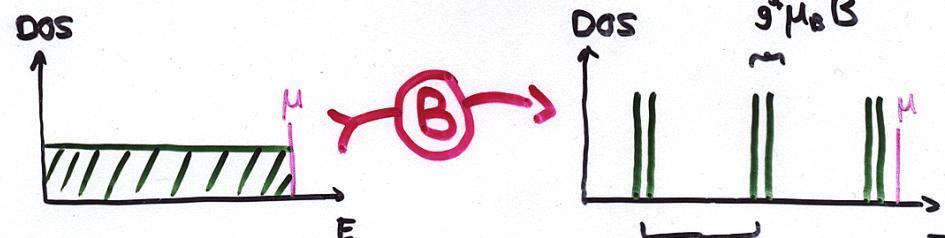
$$\tau_{xx} \rightarrow 0 !$$



Kawaji
Ghezzi
naturwiss

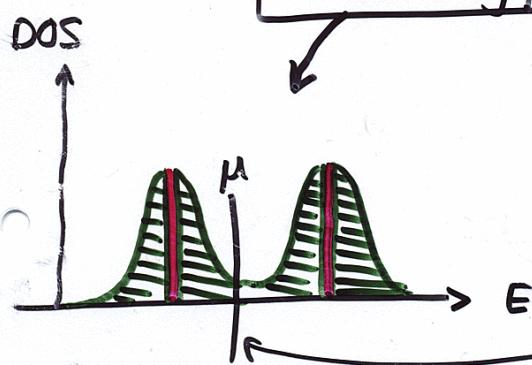
Skyring, 2D

(4)



$$[\text{'Astanda-battleiki}] = \frac{1}{L^2 E}$$

Landau-stig

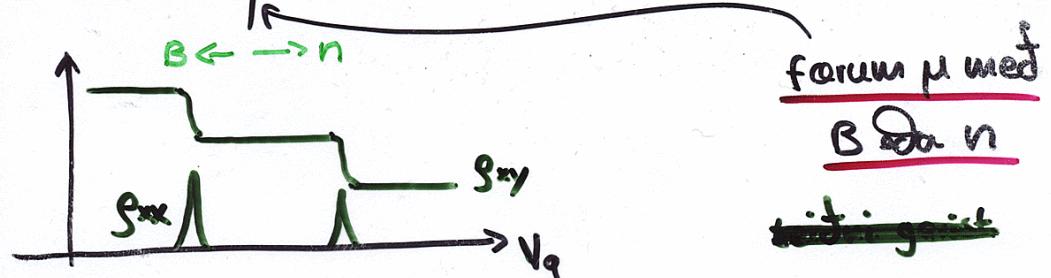


$$\omega_c = \frac{eB}{m^* c}$$

GeAs
 $m^* = 0.067$
 $g^* = -0.44$

Hatt B.....

Margfeldni: $n_0 = \frac{eB}{hc}$
Fylling: $\Delta = \nu/n_0$



förum μ med

B da n

sitjagist

vitnäm ↔ ledni

Staðbünding

2DEG → engin Ohmisk leidni

smá mættis fruflur
→ staðbünding ástanda

Leidni viðurkar með lengd
samkvæmt Lografalli

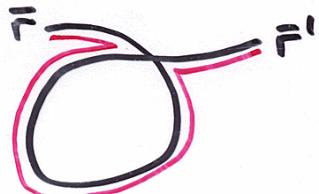
skammta → klassist
staðbünding

linulegt i 3DEG ↔ Ohm

veldisvísíssfalls viðurkar i 1DEG

2D, 1D staðbündingar lengd ξ .

Segulsvid dregur úr staðbündingu
Lotubundin

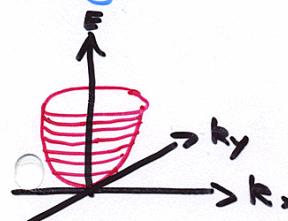


Lokadár brautir
→ vixLurif
háð B

Landau stig

$$\frac{\hbar^2 k^2}{2m^*}$$

Samf.
stig

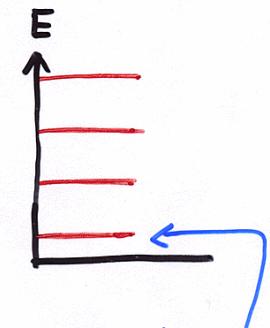


Segulsvid

$$\omega_c = \frac{eB}{m^*}$$

$$t\omega_c(n + \frac{1}{2})$$

Stjórlandau stig



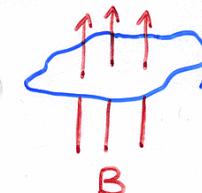
margfeldni

$$n_0 = \frac{eB}{h}$$

fjöldi ástanda á
flatareiningu

segulfloði

$$\Phi = \vec{B} \cdot \vec{A}$$



Segulfloði skammtur

$$\Phi_0 = \frac{h}{e} \rightarrow n_0 = \frac{B}{\Phi_0}$$

fiiling Landau stigs

$$\mathcal{V} = \frac{n}{n_0} = \frac{N}{A} \frac{\Phi_0}{B} = N \frac{\Phi_0}{\Theta}$$

fjöldi rafeinda

: fjöldi rafeinda
á fjölda
segulfloði-
einingu

1982

Wigner 1930

(5)

VOLUME 48, NUMBER 22

PHYSICAL REVIEW LETTERS

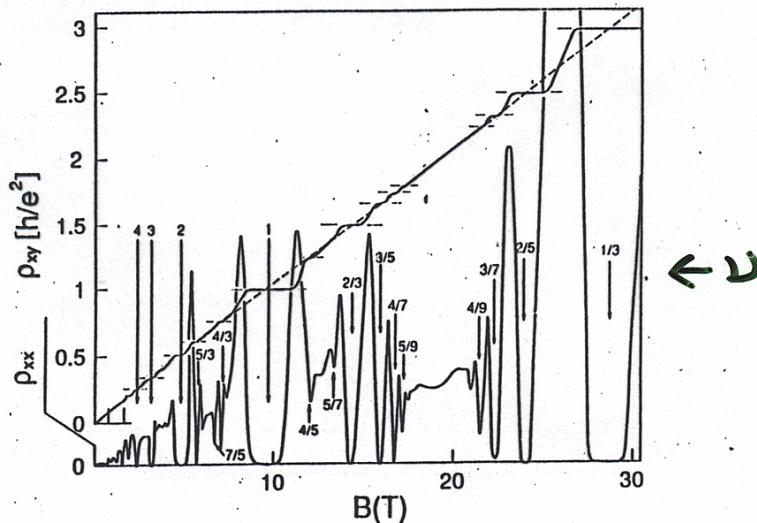
31 MAY 1982

Two-Dimensional Magnetotransport in the Extreme Quantum Limit

D. C. Tsui,^{(a), (b)} H. L. Stormer,^(a) and A. C. Gossard
Bell Laboratories, Murray Hill, New Jersey 07974
 (Received 5 March 1982)

A quantized Hall plateau of $\rho_{xy} = 3h/e^2$, accompanied by a minimum in ρ_{xx} , was observed at $T < 5$ K in magnetotransport of high-mobility, two-dimensional electrons, when the lowest-energy, spin-polarized Landau level is $\frac{1}{2}$ filled. The formation of a Wigner solid or charge-density-wave state with triangular symmetry is suggested as a possible explanation.

$$\rho_{xy} = \frac{h}{2e^2} \quad v = \frac{1}{3}, \frac{2}{3}, \dots$$

Lægsta Landau-stig

$$\rightarrow E_{kin} = \frac{\hbar \omega_c}{2} : \text{fasti}$$

\rightarrow áhrif virkunarar!
 ekki DOS

EKKI til litill stiki fyrir truflauarð!

(6)

VOLUME 50, NUMBER 18

PHYSICAL REVIEW LETTERS

2 MAY 1983

Anomalous Quantum Hall Effect: An Incompressible Quantum Fluid with Fractionally Charged Excitations

R. B. Laughlin
Lawrence Livermore National Laboratory, University of California, Livermore, California 94550
 (Received 22 February 1983)

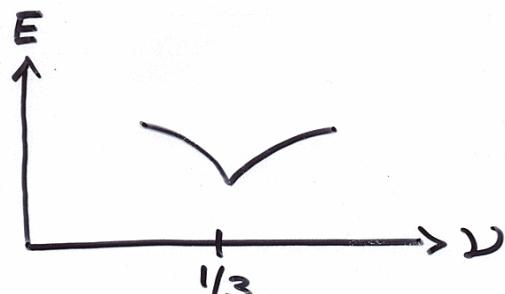
This Letter presents variational ground-state and excited-state wave functions which describe the condensation of a two-dimensional electron gas into a new state of matter.

Tilgata um bylgjufall (margeindu)

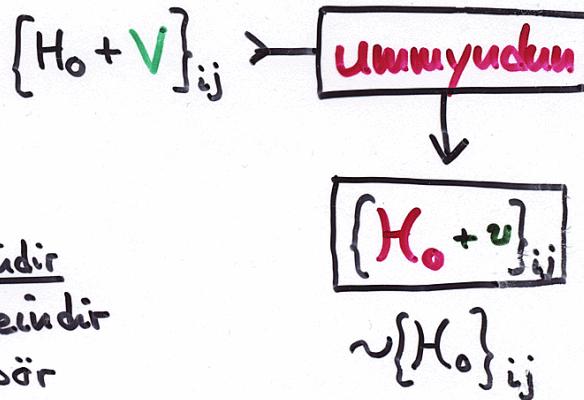
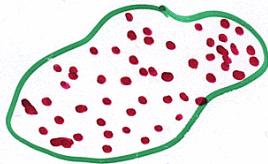
Vörpun á OCP (Bernstein)

Lægst ortha fyrir $v = \frac{1}{3}, \frac{1}{5}, \dots$

Lægri en fyrir CDW, reytu m. HCA

Búist v. kristóllur f. Lægri $v (< \frac{1}{3})$ Örvauir með hleðslu ve !!Ósamþjappanlegur vöku

Sýndareindir



Kerti
Rofeindir Sýndareindir
plasmaeindir
Cooper pör

⋮

Nöbelsverðlaun 1985 Klitzing

Athverju einu?

Nákvæmir neiku fyrir fóar eindir, rétt H

$$\left\{ H_0 + V \right\}_{ij}$$
 stift + tett á homalinnu-form

stofusta hugmyndir Laughlin

(7)

Margar hugmyndir

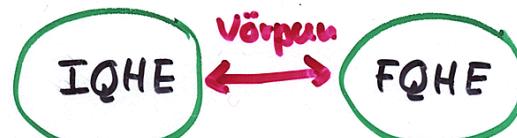
Samsettar fermíeindir (CF)

samhverfa ρ_{xx} i filraun beudir á

sýndareind

$$e^- + 2m\frac{\Phi}{\phi_0} \quad \text{segulfl. sk.}$$

$m = 1, 2, \dots$



Bein umaling brot hleðslu!

Hlustað á suð i malingum, einstater eindir

$$q = \frac{e}{3}, \dots$$

De-Picciotto, R. Reznikov, M. Heiblum,
Nature 11. Sept. 1997 389 bls. 162

L. Samuel, D.C. Glattli,

PRL 29. Sept. 1997 79 bls. 2526

(8)

Nöbelsverðlaun 1998

Mitse rafeinda kerti

Störse kerti (málmar, hálflíðarar)

Ófjádrandi árekstrar rafeinda við veilur og hljóðeindir (mjög tictir)

brengla \downarrow unþyrdis fosa rafeinda

medal vegar milli árekstra li

klassist sveim
alger fosa breuglum

Lögum skiptir ekki vali
'Öll sýni eins'

Smása kerti

$$L \ll l_i$$

engar veilur
samfassq flutningar
leidni hæð Lögum

Hítse kerti

$$L \approx l_i$$

Hreinleiki 2DEG
i GaAs
 $l_i \sim \mu_m, m_m$

Órfáar veilur
lítill fara brengun
leidni hæð Lögum
og staðsett. veitna

Eigin tuö kerfi eins

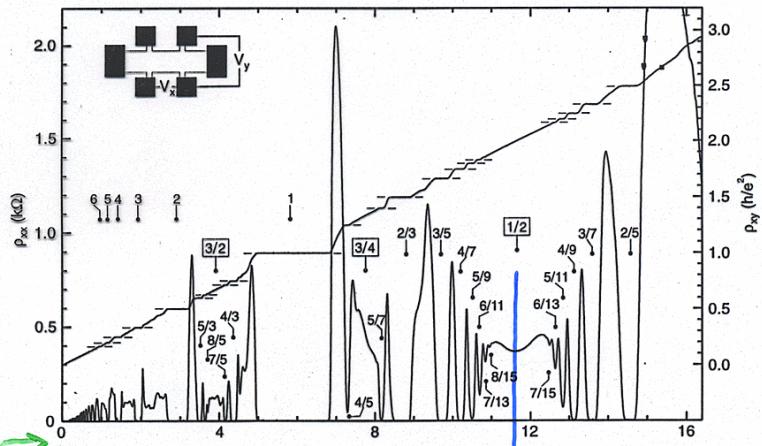
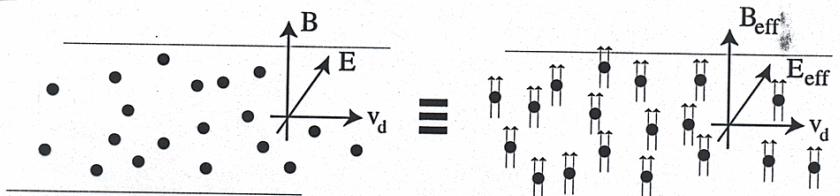


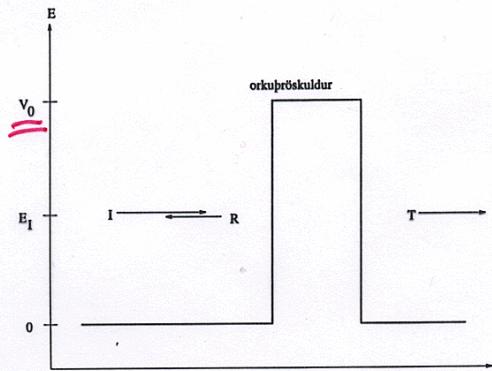
Fig. 15.1: Hall and magneto-resistance of a homogeneous two-dimensional electron system. Numbers indicate the filling factor $\nu = 2\pi e^2 n_s$ (n_s : electron sheet density). Courtesy of J. H. SMET.



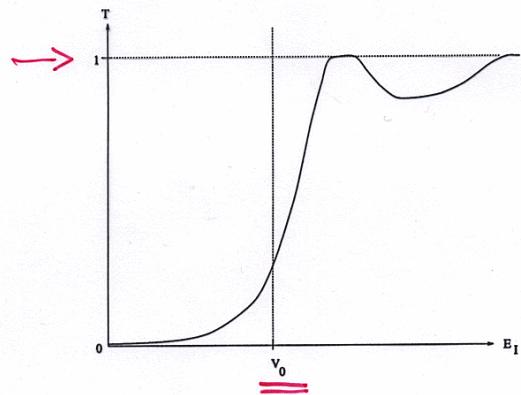
samsettar fermíeindir
við $\nu = 1/2$
tveir segulflo distamuntar
á sind = Sjúdereind
 $\rightarrow B_{eff} = 0$

Orkuþrökuldur - smug

Rafeindir geta „smogið gegnum“ þrökuld!

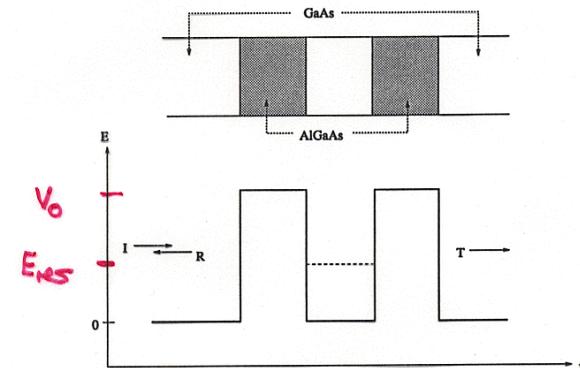


Mynd 2: Smug um orkuþrökuld.

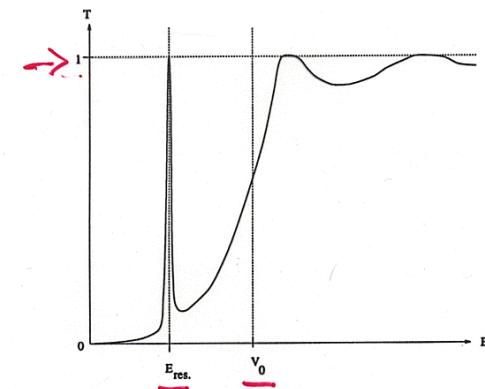


Mynd 3: Líkur þess að rafeind smjúgi gegnum þrökuldana.

Hermusmug

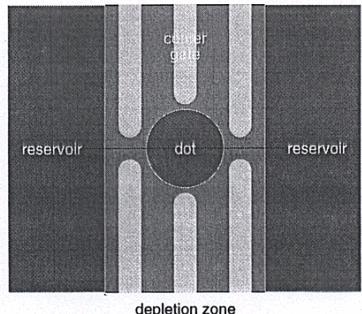


Mynd 7: Smug um two orkuþrökulda.

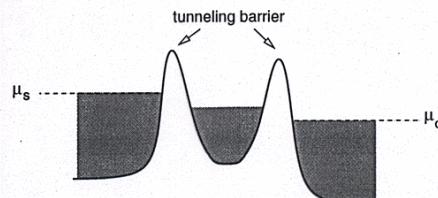


Mynd 8: Líkur þess að rafeind smjúgi gegnum þrökuldana.

Dæmi um smug um einn skamntapunkt



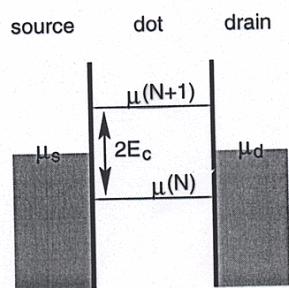
(a) top view



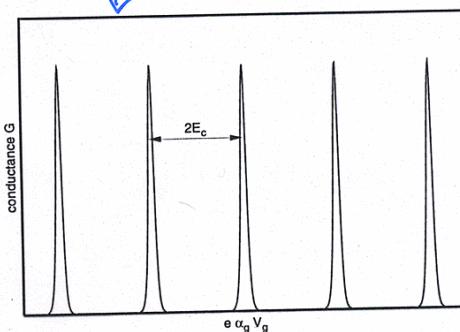
(b) Band edge profile. See also Fig 4.2(b)

Orkúrð af skamntapunkts kannad með smug meðlingu

tappar fyrir útbót rafeinda

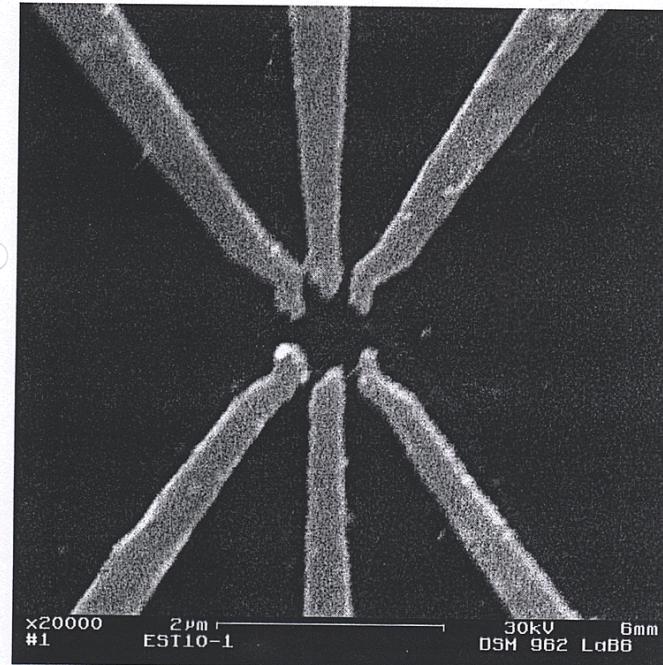


(a) Energy diagram depicting occupied single-particle states in the reservoirs and addition energies of the dot.



(b) Coulomb blockade oscillations (schematic).

N : fjöldi rafeinda innan punkts



Einstakur punktur
skilgreindur með
málu hliðum

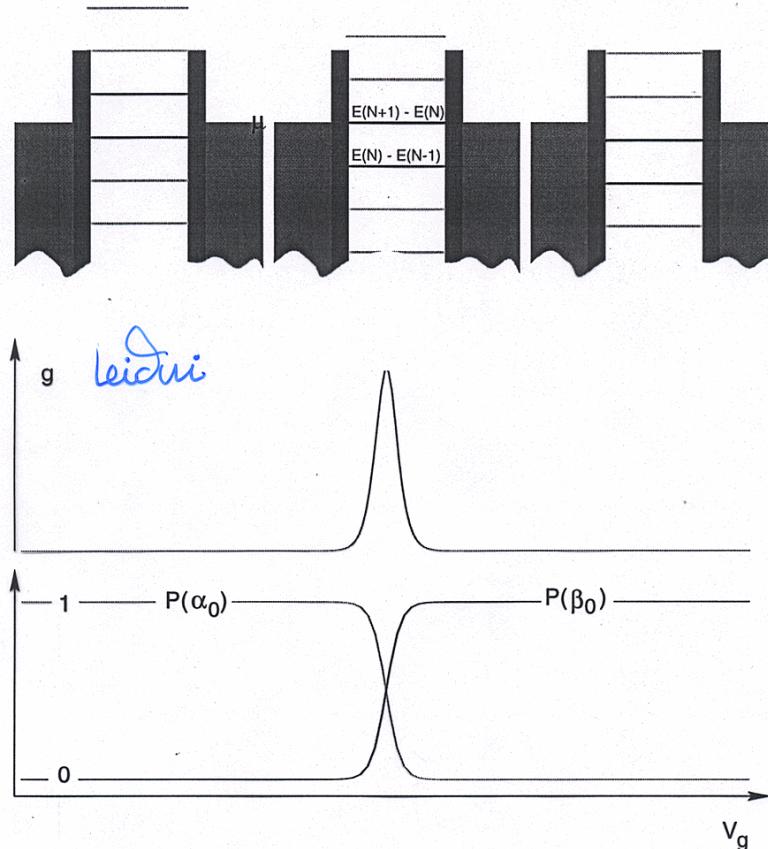
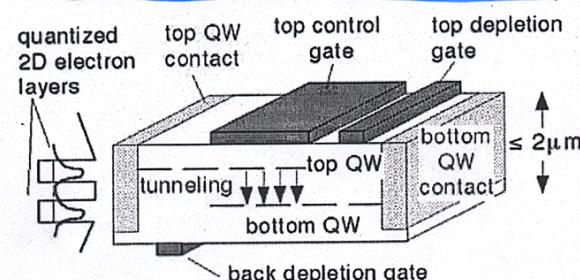


Fig. 11.6: Conductance (middle panel) and ground state occupation probability (lower panel) during the transition from N to $N + 1$ particles on the quantum dot induced by an increasing gate voltage V_g . Upper panel: Shift of the quasi-single particle levels $E(N + 1) - E(N)$.

astand Xo utan punkts
-||- βo utan -||-

Quantum Tunneling Transistor



Schematic diagram of a quantum tunneling transistor, an on-off switch that exploits an electron's ability to pass through normally impenetrable energy barriers. The various contacts and gates adjust the voltage between the upper quantum well (labelled "top QW") and the lower quantum well ("bottom QW"), both made of gallium arsenide and having thicknesses of just 150 Angstroms (where 1 Angstrom equals 10^{-10} meters). Adjusting the voltage in the right way allows the electrons in the top QW to "tunnel through" an ordinarily insurmountable barrier (made of aluminum gallium arsenide, depicted as a sawtoothed energy barrier in the leftmost diagram) to the bottom QW. Tunneling occurs when the top QW and bottom QW accept electrons with the same energy and momentum states. (Figure courtesy Sandia National Laboratories)

This research was described at the 1997 IEEE International Electron Device Meeting in Washington, DC, December 7-10, 1997.

Smug um tuo skamntapunkta

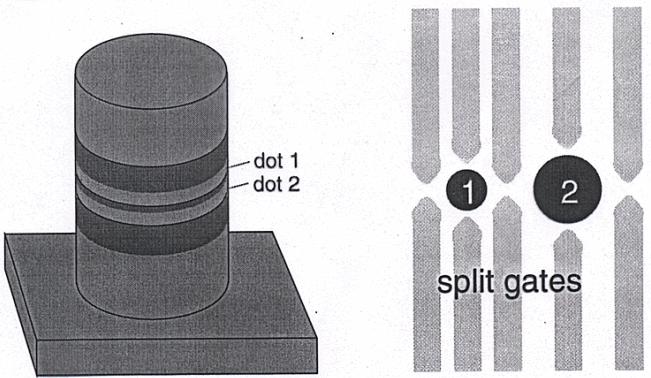


Fig. 12.1: Vertical and lateral double dot structures.

Löcher ↑
Smug ↗
Lattice

KAPITEL 4. DER DOPPEL-QUANTENPUNKT

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4.1. SIMULATION DER QUANTENPUNKTPOTENTIALE

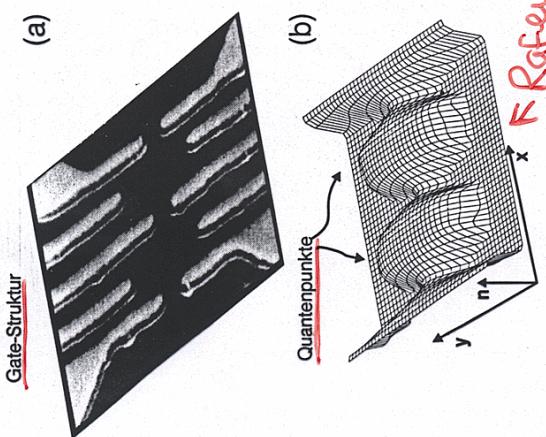


Abbildung 4.1.2:
 Ansicht der Gatesstruktur eines symmetrischen Doppelquantenpunktes: Rasterelektronenmikroskopische Aufnahme der Struktur (a). Im unteren Teil (b) ist die resultierende Ladungsträgerdichte entsprechend der Geometrie der Mikrostruktur aus (a) dargestellt. Rechts und links befinden sich die Reservoire (2DEG), die linsenförmigen Quantenpunkte liegen, über Tunnelbarrieren aufgelöst, dazwischen. Die Elektronenzahl liegt hier bei $N = 54 \pm 2$ je Quantenpunkt.

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4.1. SIMULATION DER QUANTENPUNKTPOTENTIALE

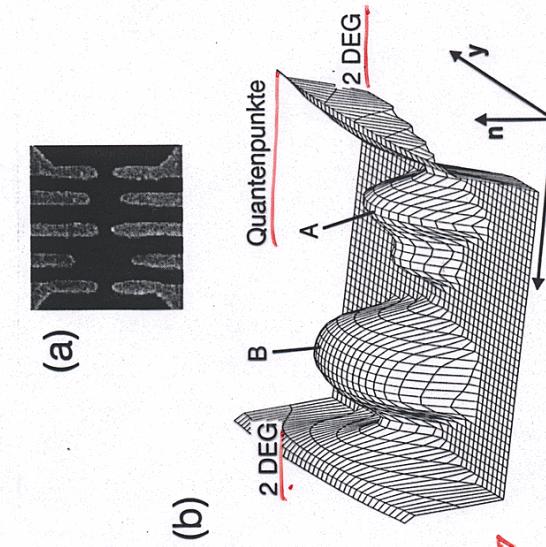


Abbildung 4.1.3:
 Darstellung des asymmetrischen Doppelquantenpunktes (a). Berechnete Elektronendichte in den Quantenpunkten (b). Der kleine Quantenpunkt zeigt Abweichungen von der gewöhnlichen hemisphärischen Gestalt, da die Steuergeräte dichter am Quantenpunkt liegen.

Smug um tvöpunktta

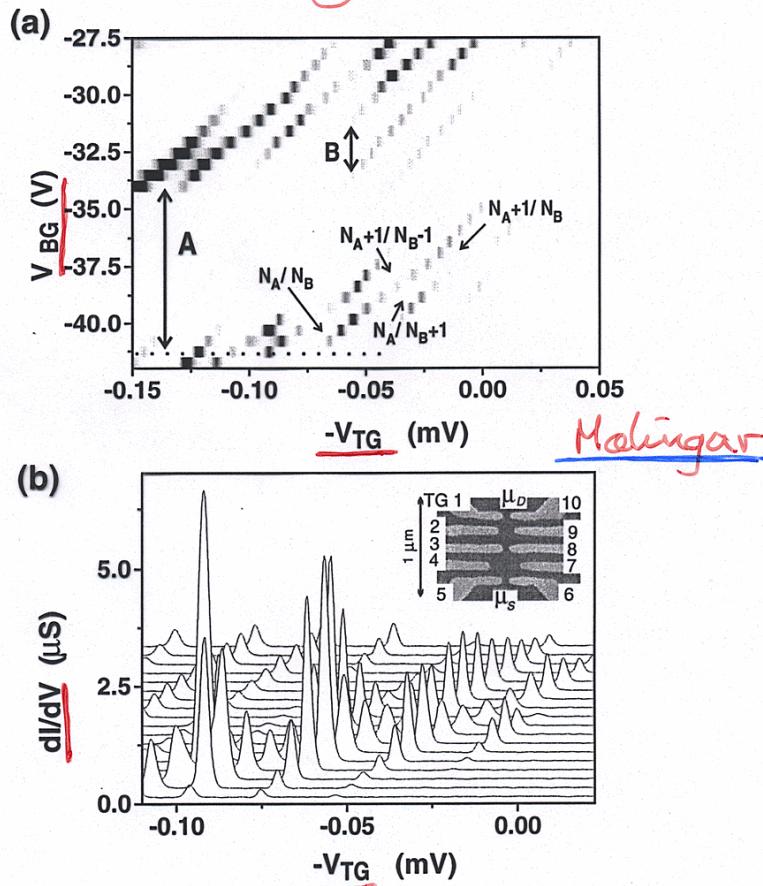
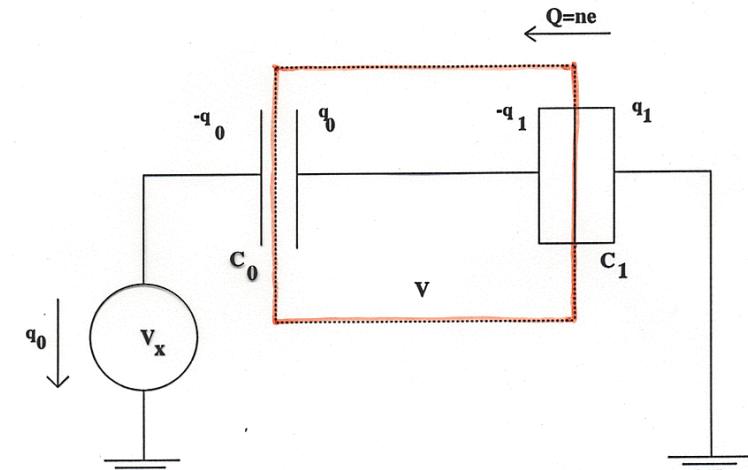


Fig. 12.6: Measured charging diagram of the double quantum dot depicted in the inset. a) The conductance is represented in a gray scale plot - white: $\sigma < 0.5 \mu S$, black: $\sigma > 2.5 \mu S$. b) Line plot corresponding to the lower part of a). Courtesy of R. H. BLICK.

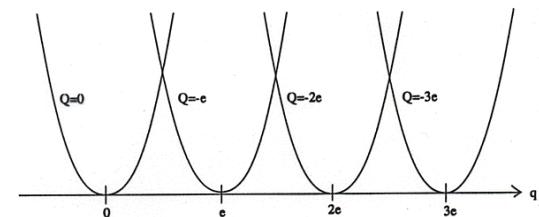
ground state, then, is a superposition of two different ground states with neighboring

Bloch-sveiflur - rafeindatalning



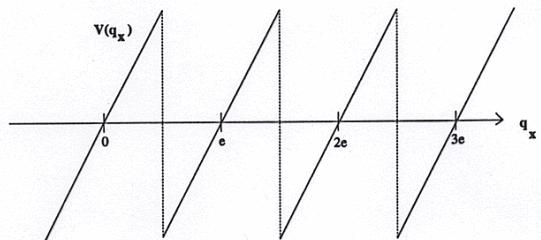
Mynd 4: Rás með örsmáum smugtvisti.

$$E_{ch} = \frac{1}{2C}(Q + q_x)^2.$$



Mynd 5: Stöðuorka rafeindanna í kassanum á mynd 1, sem fall af hleðslunni q_x sem tekin er út úr kassanum.

$$V = \frac{\partial E_{ch}(Q, q_x)}{\partial q_x}$$



Mynd 6: Spenna þess hlutar rásarinnar á mynd 1. sem er innan strikaða kassans, sem fall af hleðslunni q_x sem tekin er út úr rásinni.

Coulomb-lokun



miljarður skammtapunkta í einu kerfi
hver með nákvæmlega sama rafeindafjölda.

C verður að vera svo smá rýmd að hleðsluorkan fyrir
eina rafeind sé $>> k_B T$.

\sim attó farad $10^{-18} C$

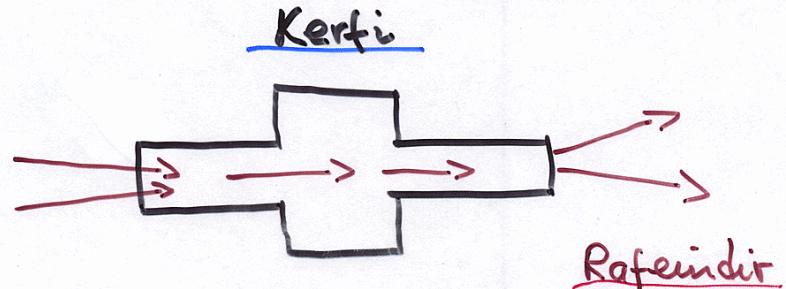
Hermuleiðni

Leiðni í miðsæjum kerfum er háð lögun kerfis og snertipunkta þess.

Leiðnin er ekki óhmsk, $I \neq \sigma V$.

Hermusmug, Coulomb-lokun.

Athugum líkan eftir K.F. Bergren, eðlisfræðideild Háskólans í Linköping.



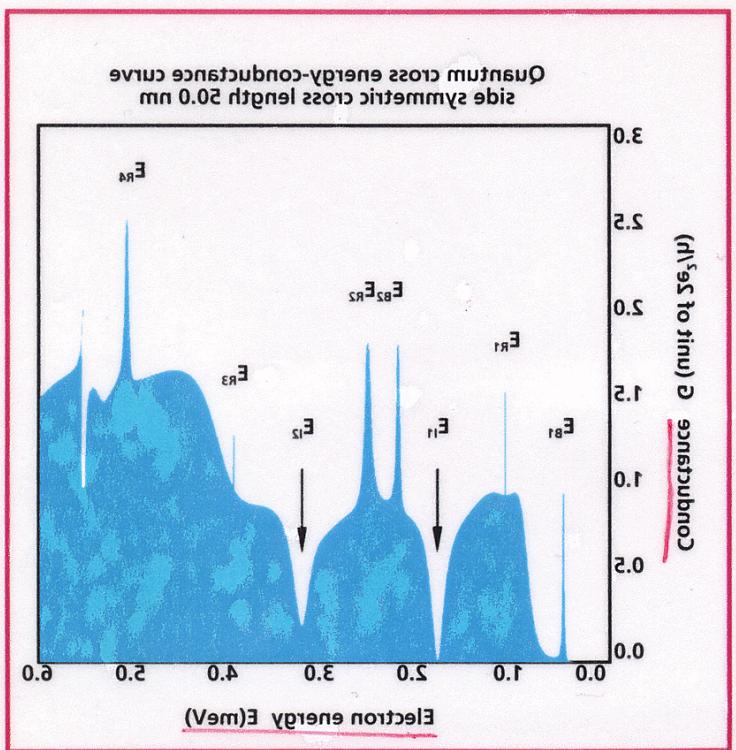
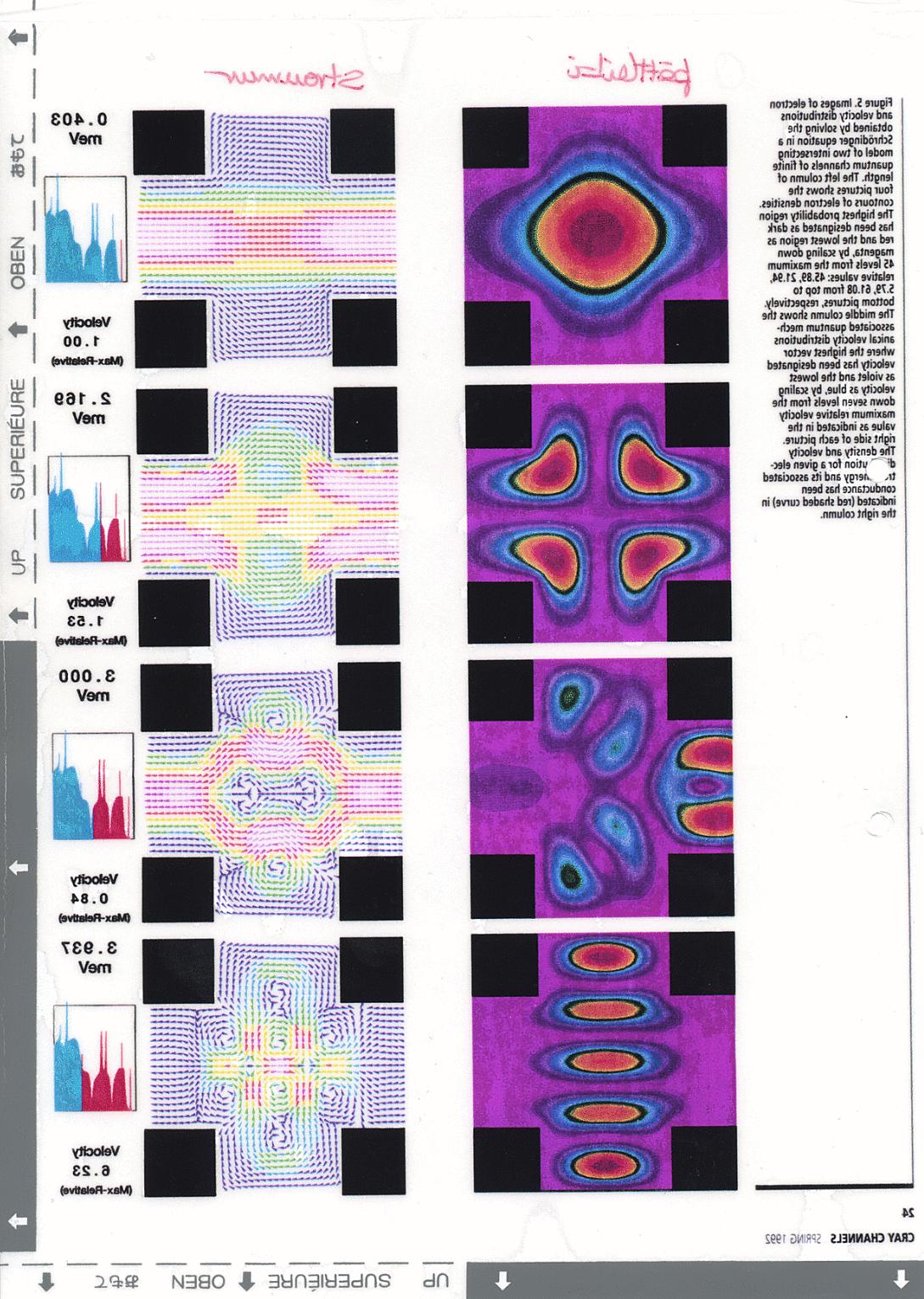
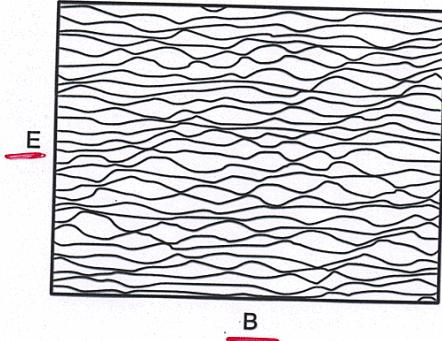


Figure 1. The conductance
as a function of the energy
of the electrons.

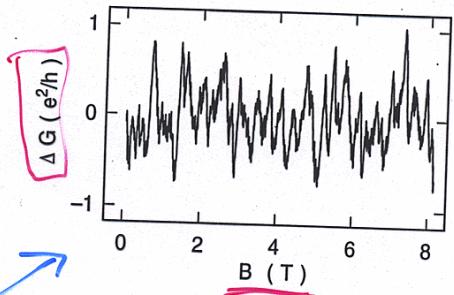


Algilt leidni flökkt i miðsæu kerfi

Segulsvid rúnglar rofeindir
i miðsæu kerfi



Orkuraf

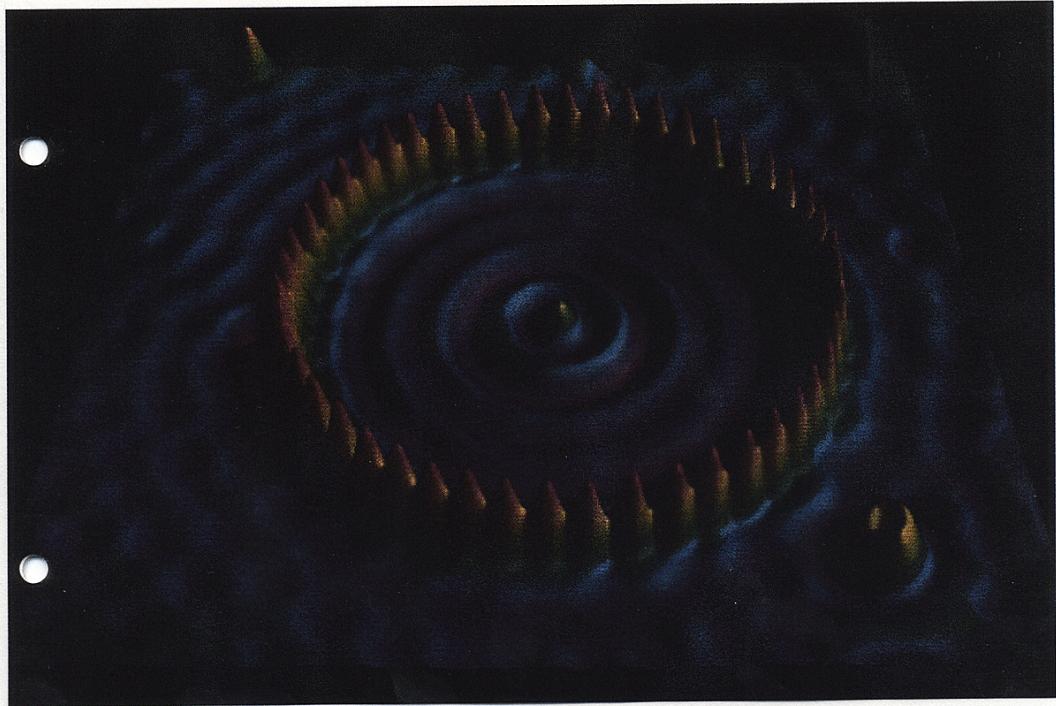


Leidni flökkt

háð kerfi
fungarfar

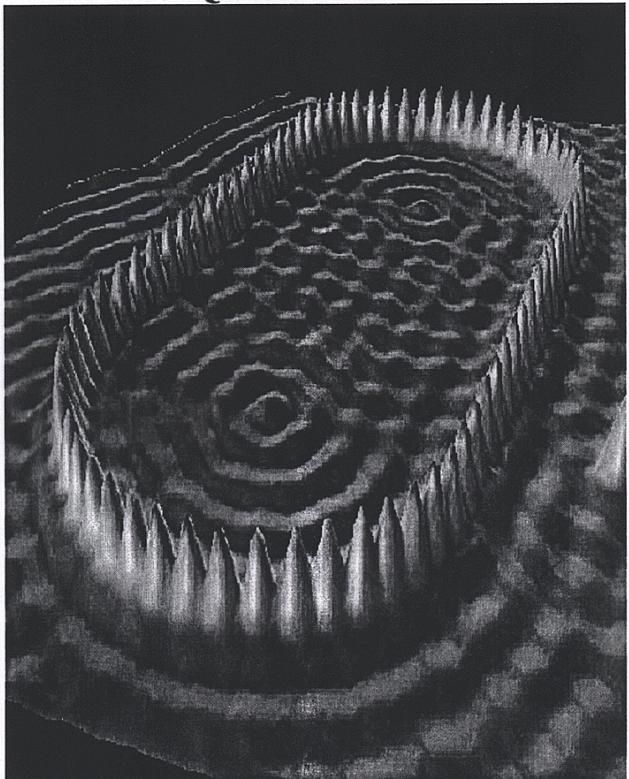
nákvæmlega endurtakarilegt
Stöðugt í tíma

Nanótekní



48 jörnatóm ráðad í hrung á
koparyfirborði með smugsjá

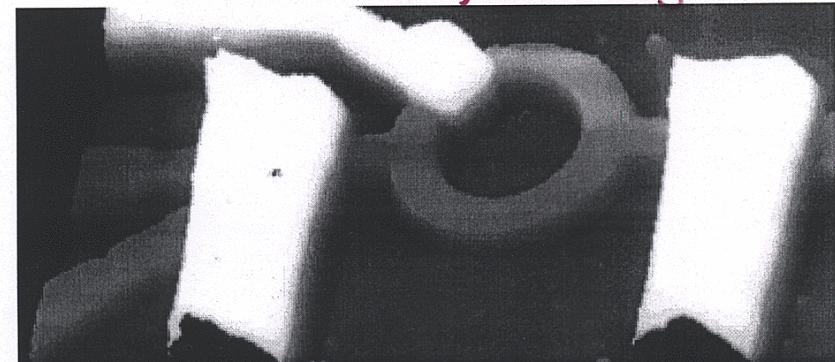
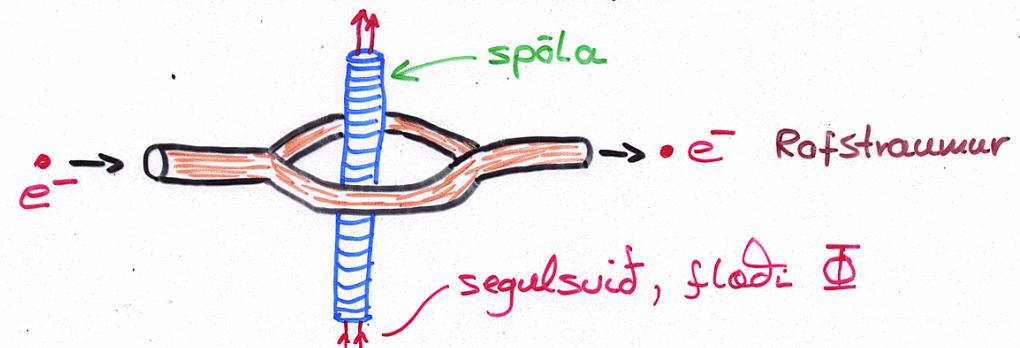
Quantum Corral



Scanning tunnelling microscope (STM) picture of a stadium-shaped "quantum corral" made by positioning iron atoms on a copper surface. This structure was designed for studying what happens when surface electron waves in a confined region. Courtesy, Don Eigler, IBM.

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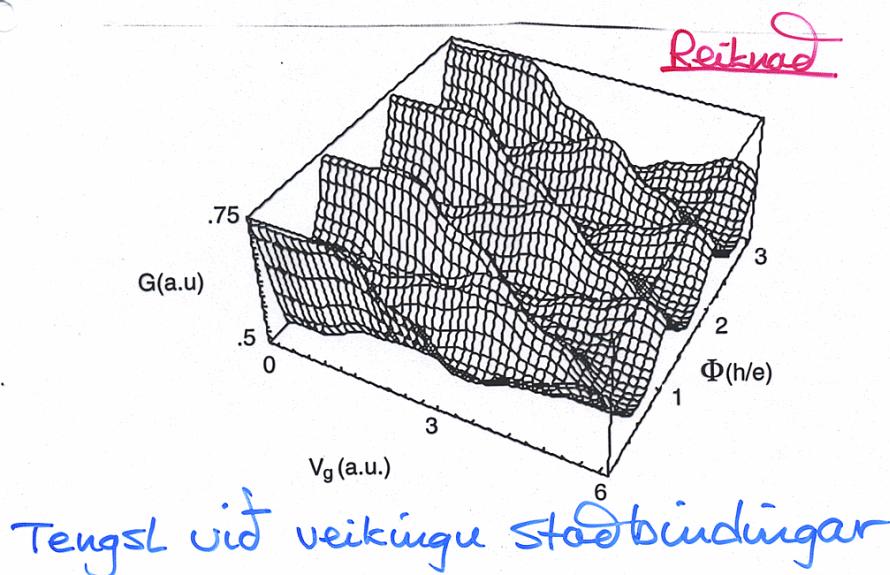
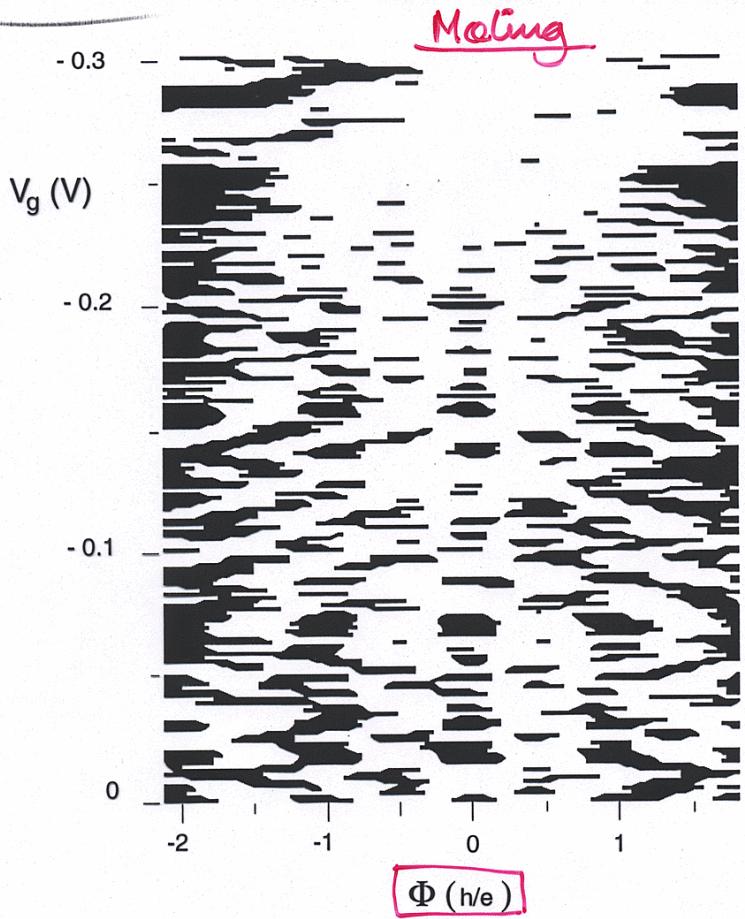
Aharanov - Bohm - hrif

Hreint kerti → fasi rofendu brauglasteki
 ↗ Sístadrir Straumar

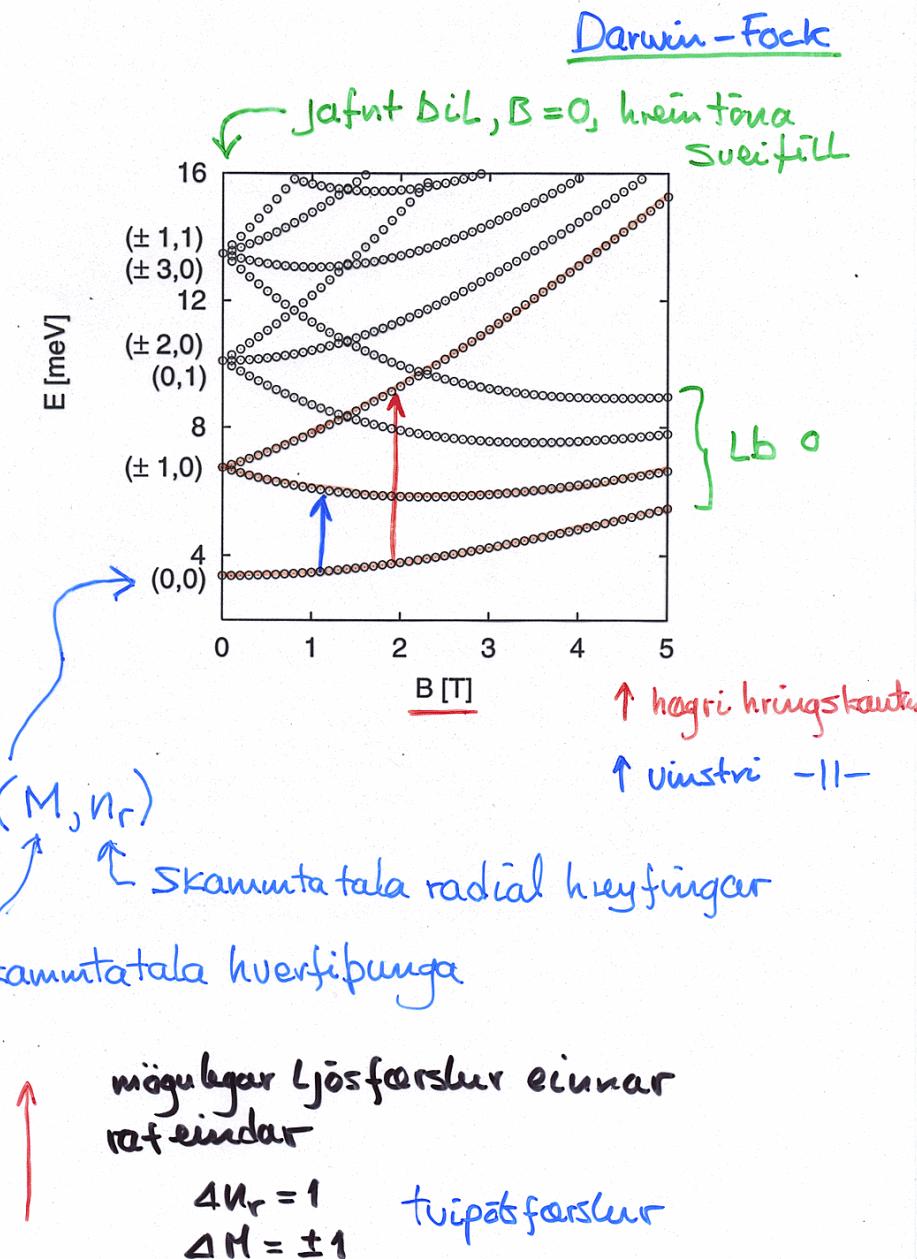
Breyting á Φ bæytir fosa

Stykjandi og eyðandi víxl

Leidni stýrt með segulsvidi, rofendi,
sjá ekki Φ!

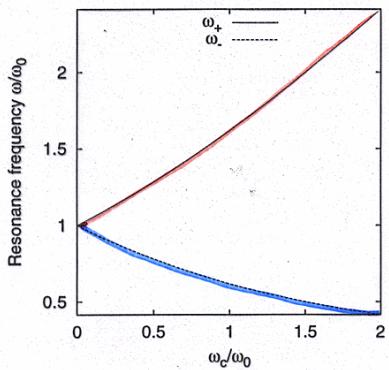


Orkuraf skamntapunkts kannad með fjar-innraðu ljósísgí



Ljós ísog punkts

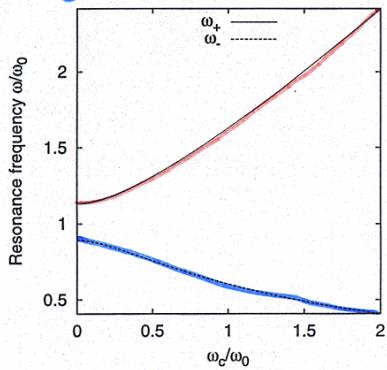
Hringlaga



(a) FIR resonances of a parabolically confined quantum dot.

Sporuölkulaga

tvisturgröf



(b) FIR resonances of an elliptic dot with $\omega_x/\omega_0 = 1.05$ and $\omega_y/\omega_0 = 0.95$ (eq. (2.8)).

Ísog óhæf N, fjölda rafeinda!

Kohns regla: Ef $\lambda \gg L$, fleyboga inni lokun

Ljósid örvar ódeins hreyfingar massamíðju

Engar innubyrdis hreyfingar

$$\text{ísogs tilnái } F\left(\frac{Q}{M} = -\frac{Ne}{Nm}\right)$$

eins og fyrir
eina sind

Heildarorka rafeinda i fleygboga skamnta punkti

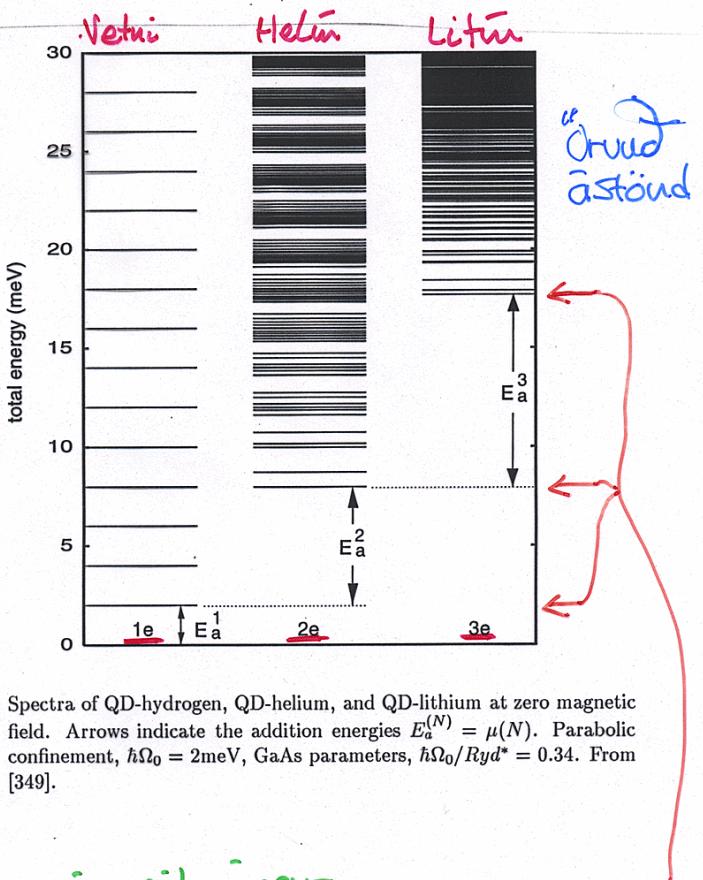
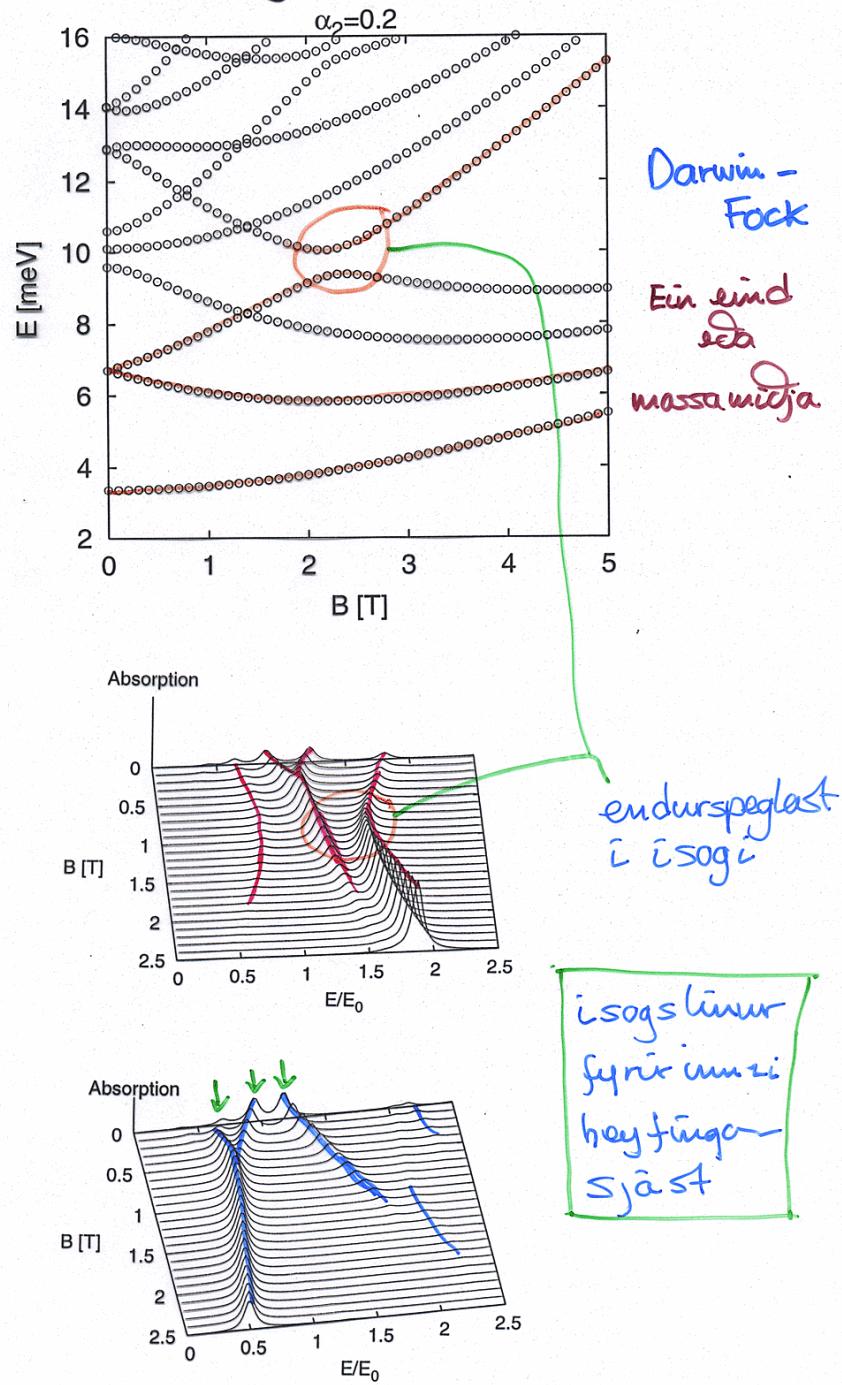


Fig. 11.4: Spectra of QD-hydrogen, QD-helium, and QD-lithium at zero magnetic field. Arrows indicate the addition energies $E_a^{(N)} = \mu(N)$. Parabolic confinement, $\hbar\Omega_0 = 2\text{meV}$, GaAs parameters, $\hbar\Omega_0/\text{Ryd}^* = 0.34$. From [349].

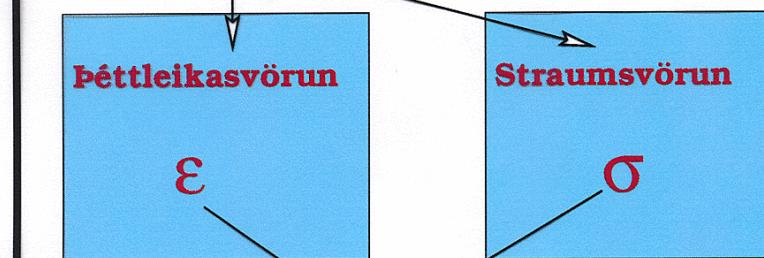
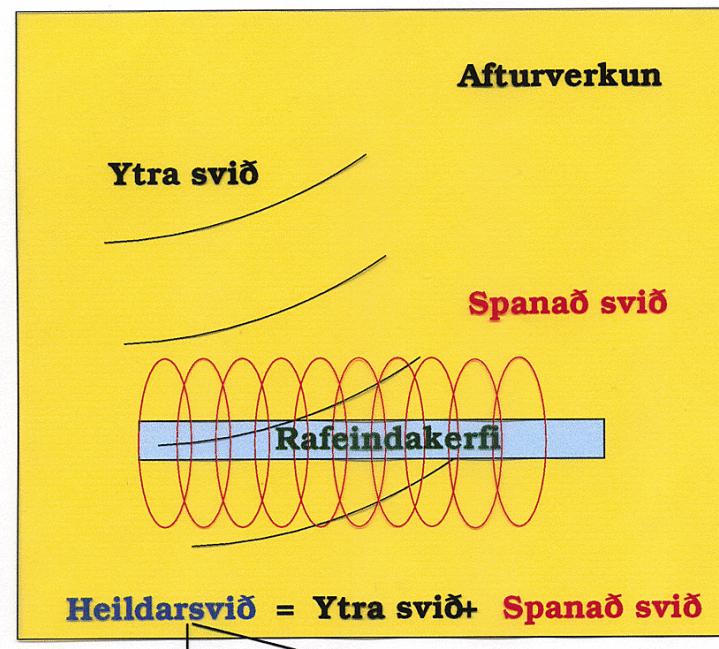
Nákvæmir reikningar

Grunnástand

Kassalaga innilokum



Ljósísog



pötkluiki rafeinda i kassalega punkti

32

Many electron quantum dots

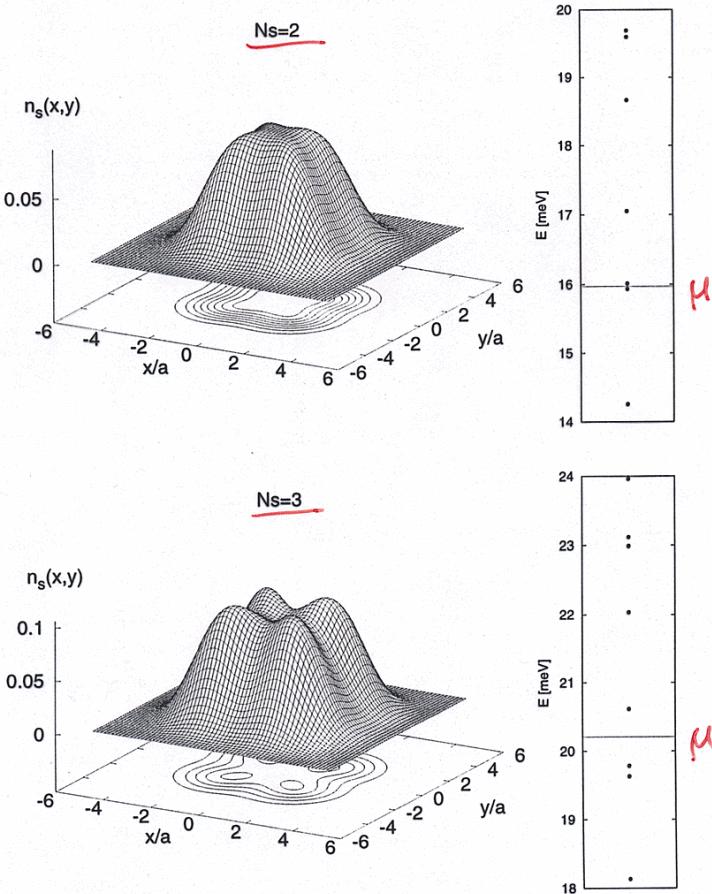


Figure 4.5: The density of two (above) and three (below) interacting electrons subject to a square symmetric confinement, $\alpha_1 = 0.0$ and $\alpha_2 = 0.4$. The magnetic length is $a = 13$ nm.

Spanadur pötkluiki vegna ísogs

7.2 Excitation spectra

51

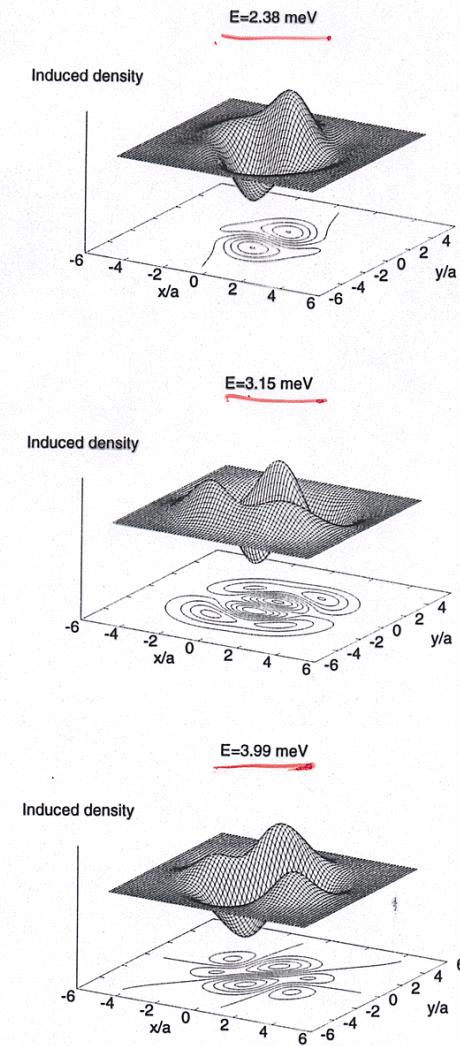
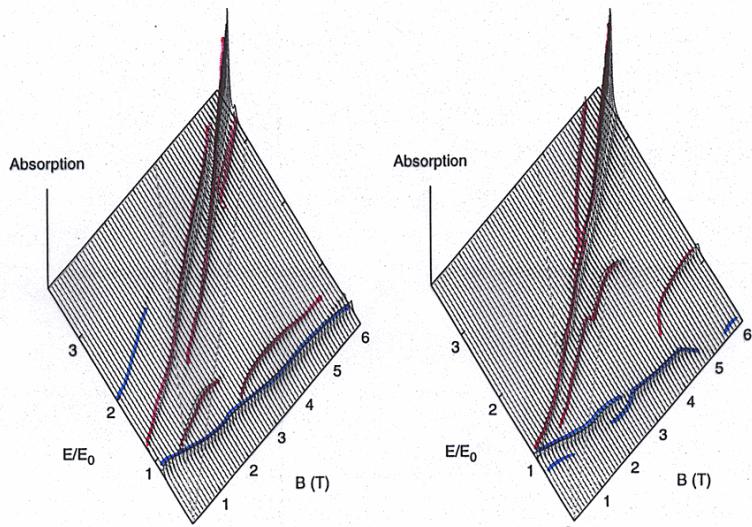
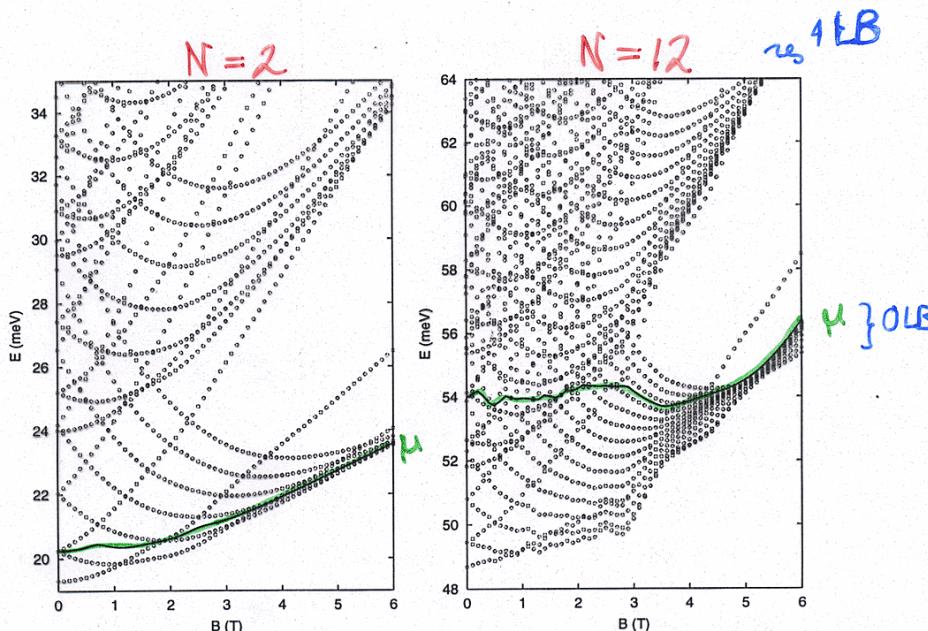


Figure 7.2: The induced density at the absorption peaks for $N_p = -1$. See discussion in text.

Inuri hreyfingar

Skamntapunkter med gati i midju



4.3 Deviations from the parabolic confinement potential: Quantum chaos

Klassisk huytning retainda borun saman við likindadætt. Þeirva samantr. stónum fátr.

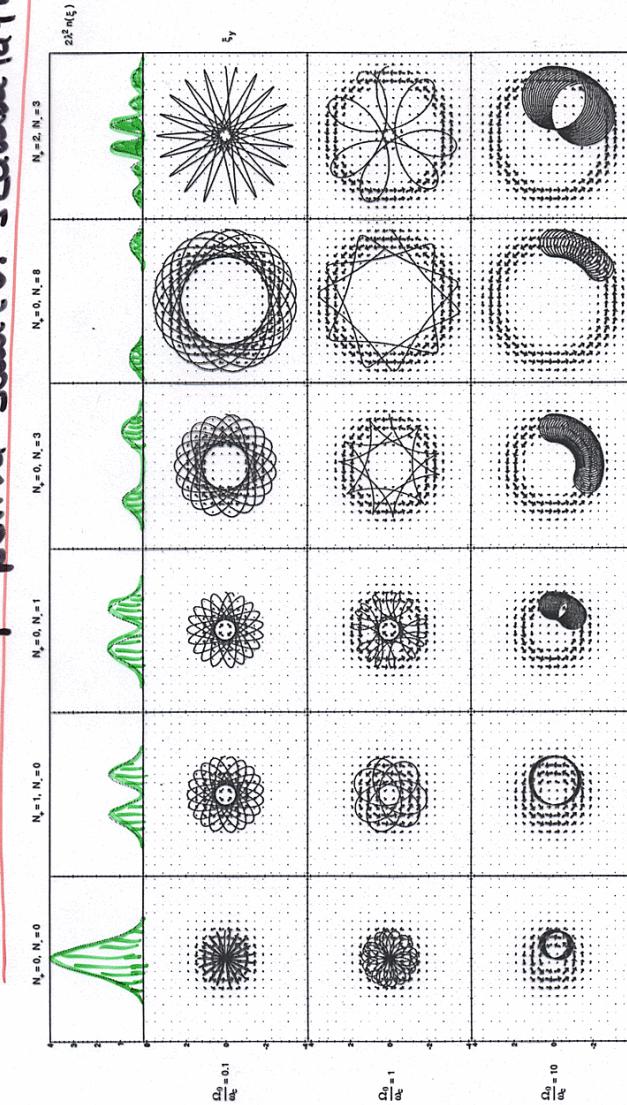
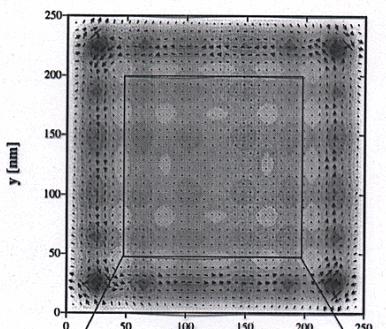


Fig. 4.4: Density (upper row) and current distribution (lower rows) in parabolic quantum dot states $|N_+, N_-\rangle$ at different ratio Ω_0/ω_c . Solid lines indicate corresponding classical orbits.

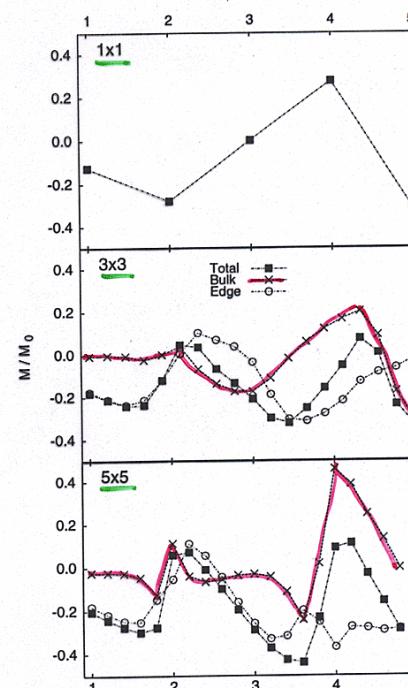
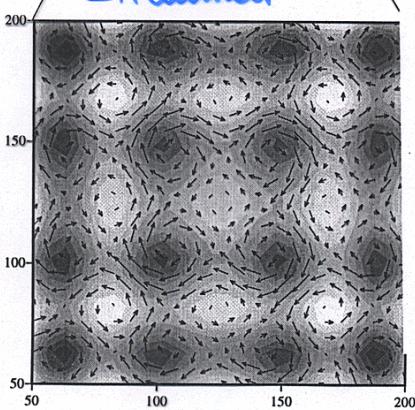
Rafeind i punti

Seglun i 2DEG

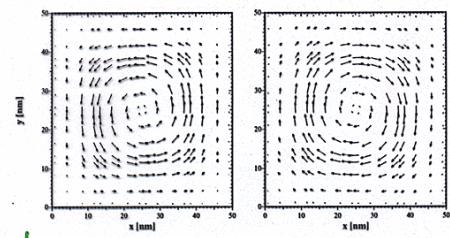
Micse kerti



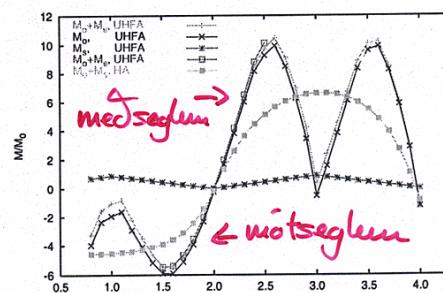
Jafnwegi
Straumar



Litit kerfi Stótted
Jadar



Viðböt rafeinda
suðr seglum og
straumum við

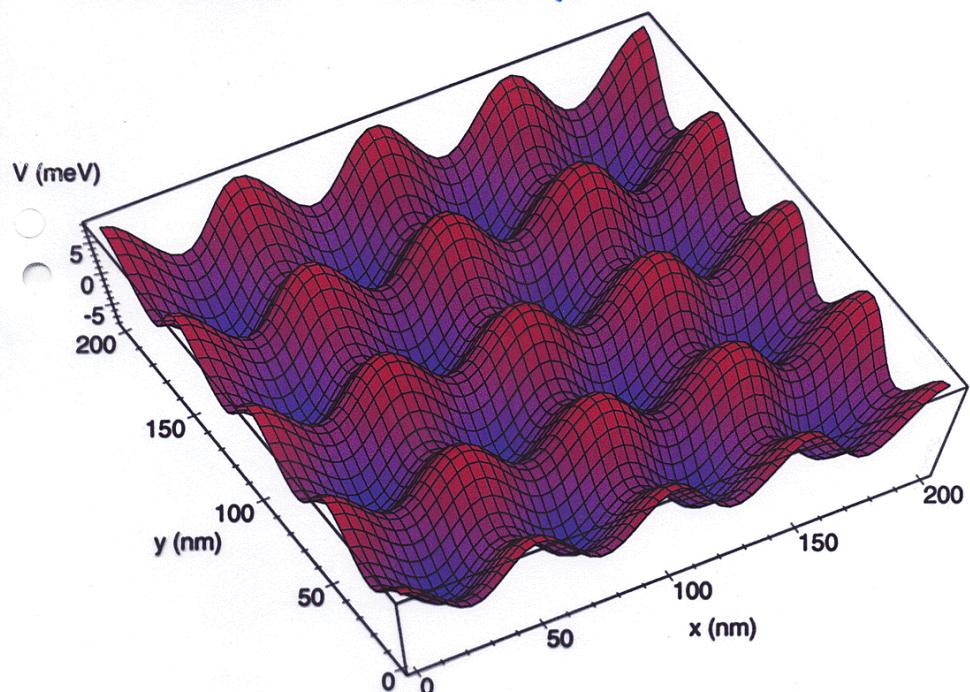


Ósendan lega stórt
lotubundin kerti

Rafeindir i lotubundnu tvívidu kerti

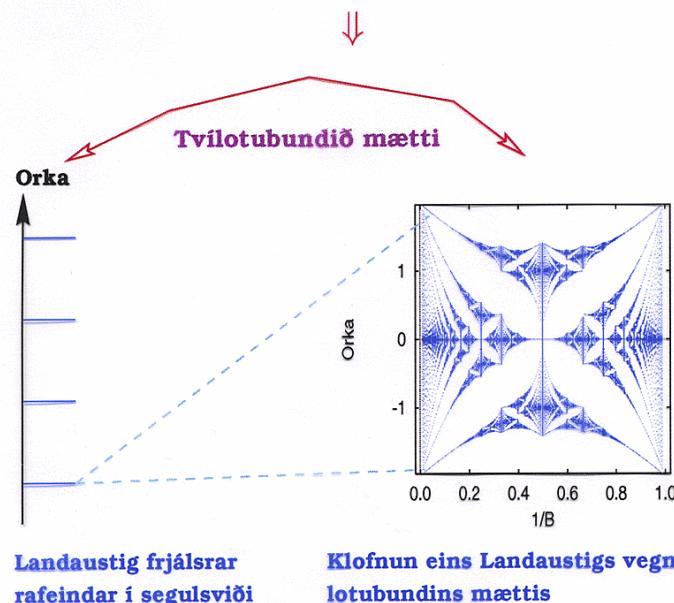
Kristallur
⋮
máluð kerfi

Cond-mat 9509064



[REDACTED]

Víxlverkandi rafeindir í tvilotubundnu ytra mætti og þverstæðu einsleitu segulsviði \vec{B}



Fiðrildi Hofstadters \leftrightarrow Grunnástand, ljósísog

Tilraunir í undirbúningi fyrir ljósísog

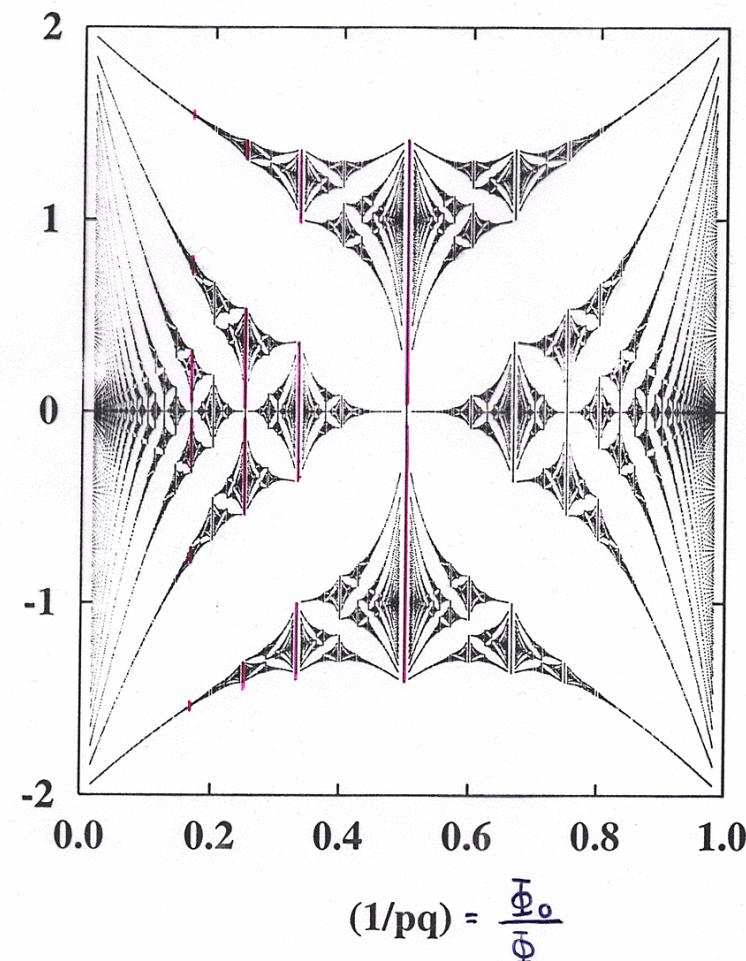
Energy levels and wave functions of Bloch electrons in rational and irrational magnetic fields*

Douglas R. Hofstadter[†]

Physics Department, University of Oregon, Eugene, Oregon 97403

(Received 9 February 1976)

An effective single-band Hamiltonian representing a crystal electron in a uniform magnetic field is constructed from the tight-binding form of a Bloch band by replacing $\hbar\vec{k}$ by the operator $\vec{p} - e\vec{A}/c$. The resultant Schrödinger equation becomes a finite-difference equation whose eigenvalues can be computed by a matrix method. The magnetic flux which passes through a lattice cell, divided by a flux quantum, yields a



$$\frac{1}{6}, \frac{1}{4}, \frac{1}{3}, \frac{1}{2}$$

Samanstekt \leftrightarrow notkun

- * Smakku \bar{n} , klassikt \rightarrow skamanta
- * Smárar fyrir einstakar í ofteindir, SET
- * Ljósnefur á fjöri um randa súðinu
- * Vélbúnaður fyrir "cellular automata"
- * Skamanta tölver
- * Grunnrannsóknir

$$E_{\text{tot}} = E_{\text{kin}} + E_{\text{direct}}^{(n)} + E_{\text{xc}} + E_{\text{corr.}}[[\bar{n}]]$$

PHYSICAL REVIEW

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9 NOVEMBER 1964

Inhomogeneous Electron Gas*

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This paper deals with the ground state of an interacting electron gas in an external potential $v(r)$. It is proved that there exists a universal functional of the density, $F[n(r)]$, independent of $v(r)$, such that the expression $E = \int v(r)n(r)dr + F[n(r)]$ has as its minimum value the correct ground-state energy associated with $v(r)$. The functional $F[n(r)]$ is then discussed for two situations: (1) $n(r) = n_0 + \pi(r)$, $n/n_0 < 1$, and (2) $n(r) = \varphi(r/r_0)$ with φ arbitrary and $r_0 \rightarrow \infty$. In both cases F can be expressed entirely in terms of the correlation energy and linear and higher order electronic polarizabilities of a uniform electron gas. This approach also sheds some light on generalized Thomas-Fermi methods and their limitations. Some new extensions of these methods are presented.

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Self-Consistent Equations Including Exchange and Correlation Effects*

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From a theory of Hohenberg and Kohn, approximation methods for treating an inhomogeneous system of interacting electrons are developed. These methods are exact for systems of slowly varying or high density. For the ground state, they lead to self-consistent equations analogous to the Hartree and Hartree-Fock equations, respectively. In these equations the exchange and correlation portions of the chemical potential of a uniform electron gas appear as additional effective potentials. (The exchange portion of our effective potential differs from that due to Slater by a factor of $\frac{1}{2}$.) Electronic systems at finite temperatures and in magnetic fields are also treated by similar methods. An appendix deals with a further correction for systems with short-wavelength density oscillations.

Sanna $E_{\text{tot}} = E_{\text{tot}}[n]$ DFT

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