第四章　　维度

4.1　半导体低维电子系统

1.维度

三维自由电子气体，沿z方向对体系的尺寸限制：

$$\varepsilon_n(k) = \varepsilon_n + \frac{\hbar^2 k^2}{2m}$$

k是波矢在 xy平面上的分量。

如限制势为方势阱：

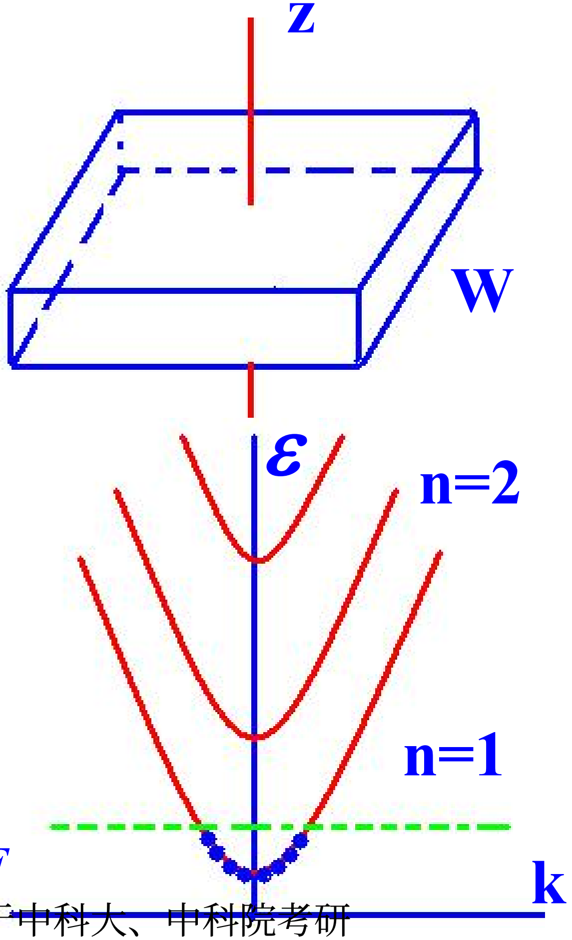
$$\varepsilon_n = \frac{(n\pi\hbar)^2}{2mW^2}, \quad W = \frac{n\lambda}{2}, \lambda\text{为电子的波长}$$

对于抛物线型的限制势 $\left(V(z) = \frac{1}{2} m\omega_0^2 z^2\right)$：

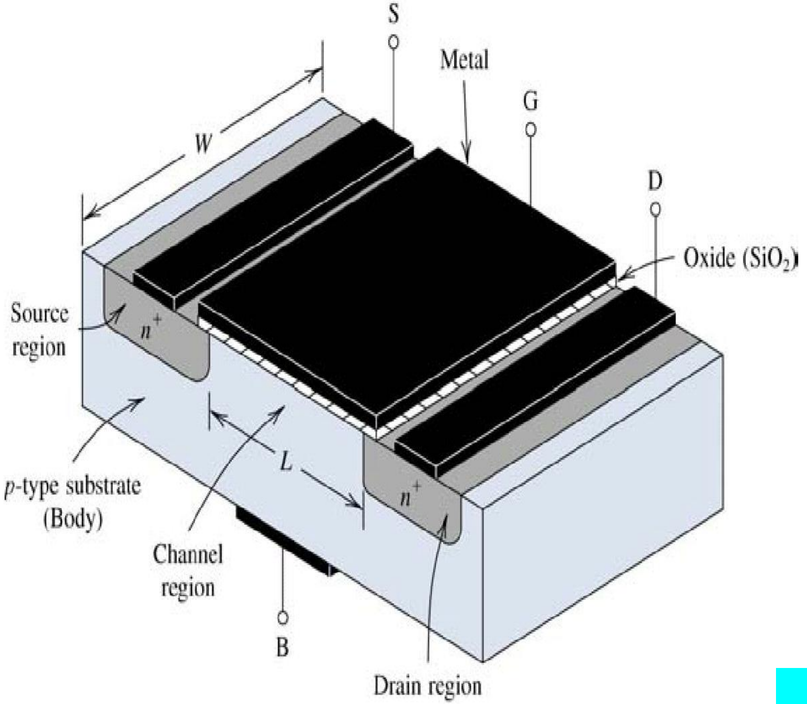
$$\varepsilon_n = \left(n - \frac{1}{2}\right)\hbar\omega_0$$

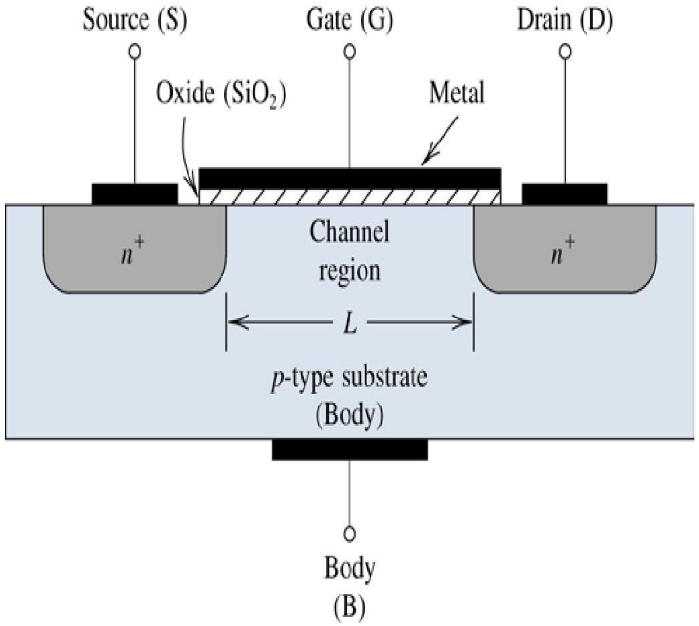
电子只占据n=1的子带，二维体系

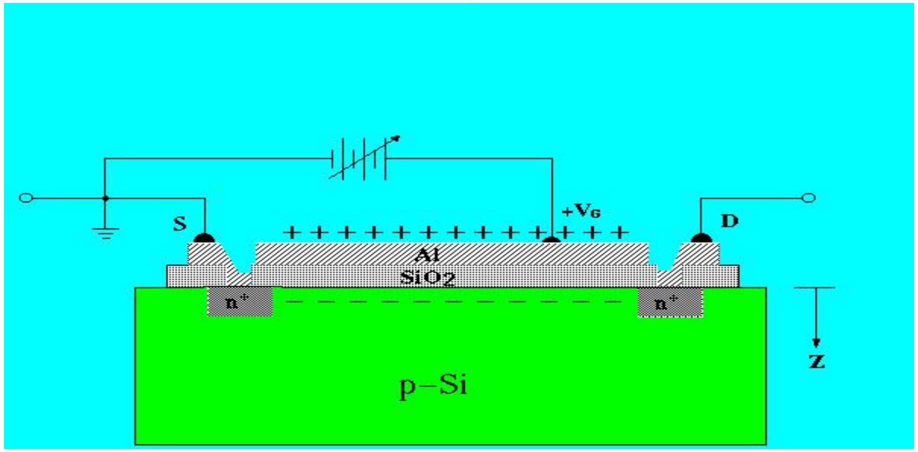
n>1也占据，准二维体系



2. Si反型层及GaAs-AlGaAs异质结

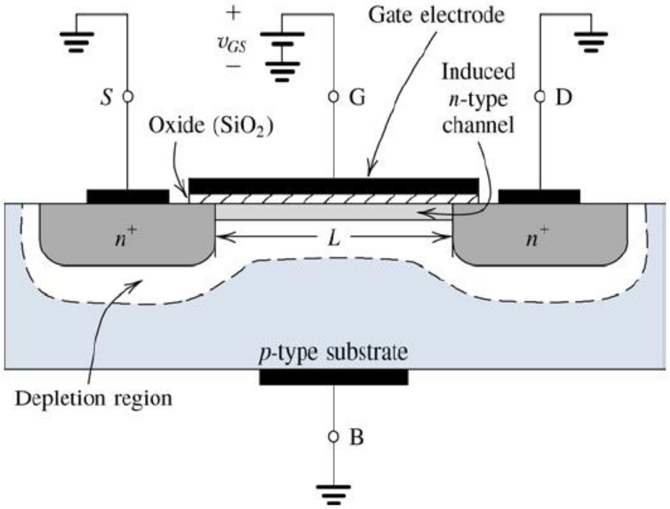


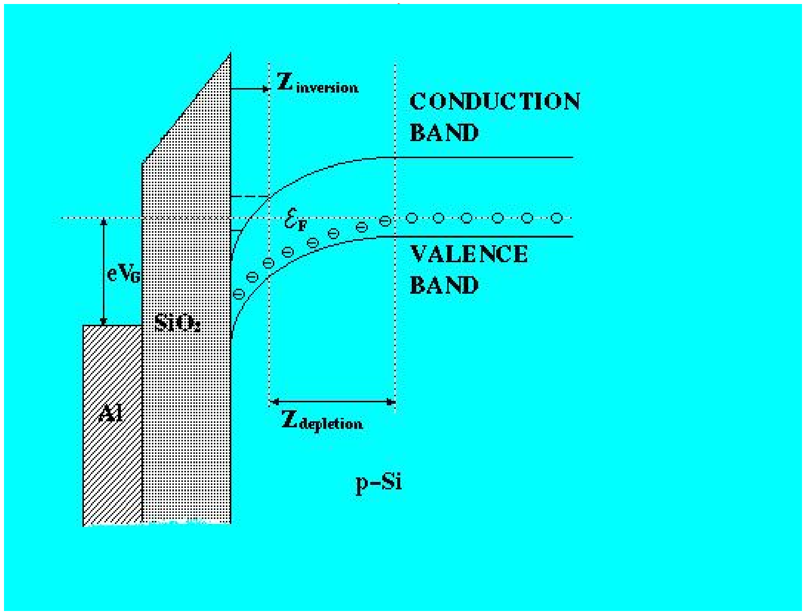




Device Operation

- No gate voltage ($v_{GS} = 0$)
  - Two back to back diodes both in reverse bias
  - no current flow between source and drain when voltage between source and drain is applied ($v_{DS} > 0$)
  - There is a depletion region between the p (substrate) and n^+ source and drain regions
- Apply a voltage on $v_{GS} > 0$
  - Positive potential on gate node pushes free holes away from the region underneath the gate and leave behind a negatively charged carrier depletion region
    - transistor in depletion mode
  - As v_{GS} increases, electrons start to gather at the surface underneath the gate (onset of inversion)
  - When v_{GS} is high enough, a n-type channel is induced underneath the gate oxide with electrons supplied by the n^+ source and drain regions
    - This induced region is called an inversion layer (or channel) and forms when v_{GS} > some **threshold voltage** V_t and current can flow between S & D
    - Transistor is in inversion mode
    - When $V_{DS} = 0$, no current flows between source and drain





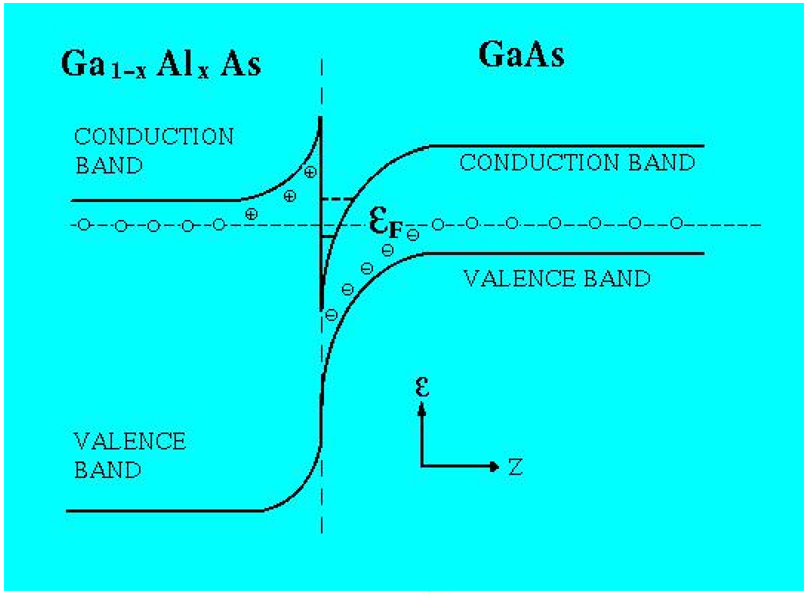
$Si(100)$表面电子的有效质量： $0.2m_e$

$\varepsilon_2-\varepsilon_1\approx 20meV$

$n_s \propto V_g \sim (1\sim 10)\times 10^{11}cm^{-2}$

迁移率：$10^4 cm^2/V\cdot s$

弹性散射平均自由程 $l:40\sim 120nm$



$x\approx 0.3$,导带底能量差～ $0.3eV$

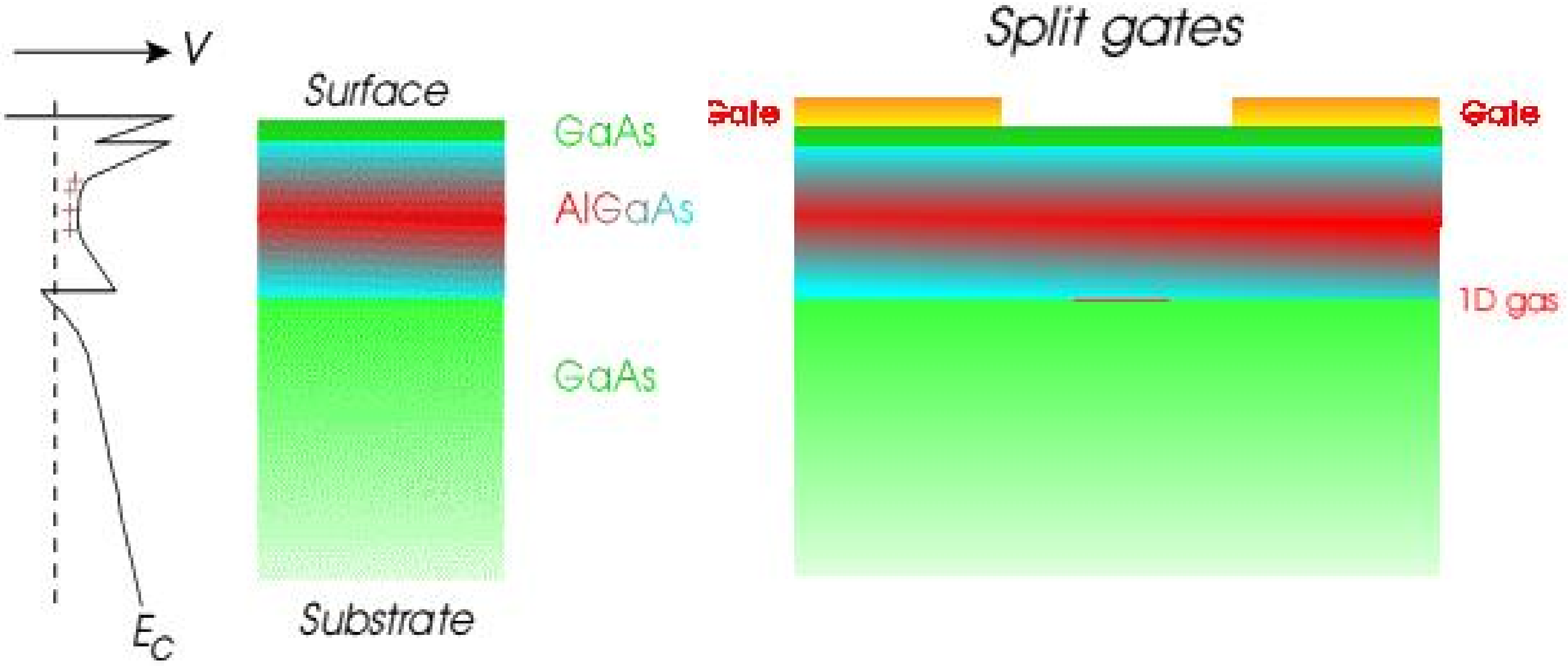
电子有效质量 $0.067m_e, n\sim 2$

$n_s\approx 4\times 10^{11}cm^{-2}$

高迁移率：10^4～$10^6 cm^2/V\cdot s$

长的弹性散射平均自由程$l=10^2\sim 10^4 nm$

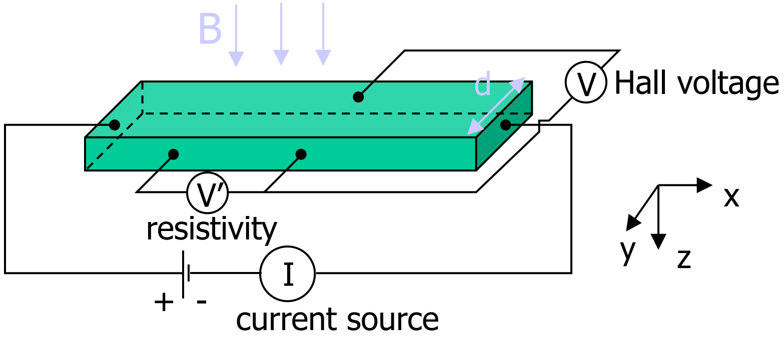
Split gates and one-dimensional electron gases

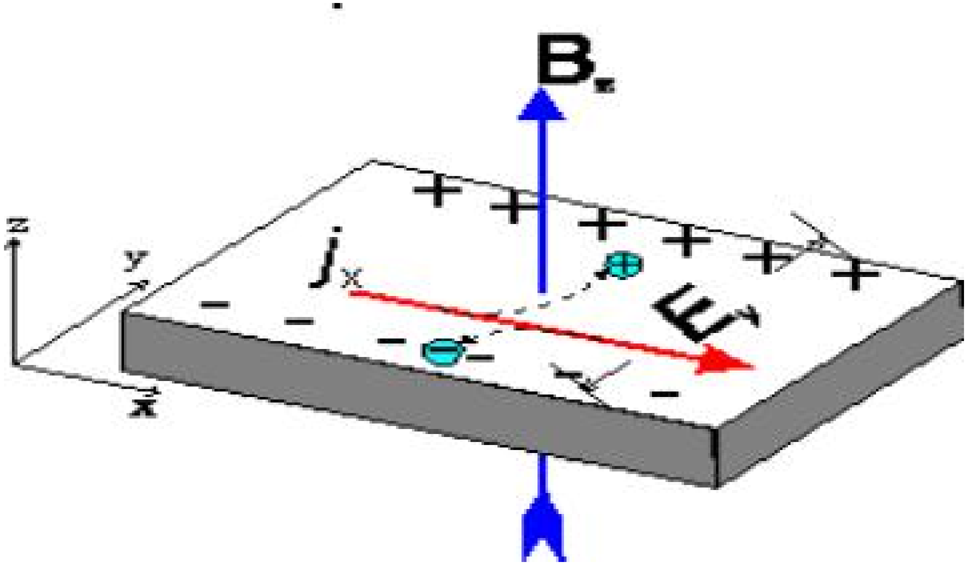


This "split-gate technique" was pioneered by the Semiconductor Physics Group at the Cavendish Laboratory of the University of Cambridge, in England, in 1986, by Trevor Thornton and Professor Michael Pepper.

3.量子化霍尔效应（Quantum Hall Effects (QHE))

(1)霍尔效应基础





E. Hall, Am. J. Math. 2, 287 (1879)
=> Hall effect

根据德鲁特电导理论, 金属中的电子在被杂质散射前的一段时间τ内在电场下加速, 散射后速度为零. τ称为弛豫时间. 电子的平均迁移速度为:

$$v_d = -eE\tau / m$$

电流密度为:

$$j = -nev_d = \sigma_0 E \qquad \sigma_0 = ne^2\tau / m$$

若存在外加静磁场, 则电导率和电阻率都变为张量

$$\sigma = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{bmatrix}, \quad \rho = \begin{bmatrix} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{bmatrix}$$

此处 $j = \sigma \cdot E, \quad E = \rho \cdot j$ 仍成立

有磁场时, 加入罗仑兹力, 电子迁移速度为

$$v_d = -e(E + \frac{v_d \times B}{c})\frac{\tau}{m}$$

稳态时， $j=-nev_d$ ，假定磁场沿z方向，在xy 平面内

$$\sigma_0 E_x = \omega_c \tau j_y + j_x \qquad \omega_c = \frac{eB}{mc}$$

$$\sigma_0 E_y = \omega_c \tau j_x + j_y$$

易得

$$\rho_{xx} = \rho_{yy} = \frac{1}{\sigma_0}, \quad \rho_{xy} = -\rho_{yx} = \frac{\omega_c \tau}{\sigma_0}$$

$$\sigma_{xx} = \sigma_{yy} = \frac{\sigma_0}{1+(\omega_c\tau)^2}, \sigma_{xy} = -\sigma_{yx} = \frac{-\sigma_0\omega_c\tau}{1+(\omega_c\tau)^2}$$

➡ $$\sigma_{xx} = \frac{\rho_{xx}}{\rho_{xx}^2+\rho_{xy}^2}, \quad \sigma_{xy} = -\frac{\rho_{xy}}{\rho_{xx}^2+\rho_{xy}^2}$$

如果 $\rho_{xy} \neq 0$ ，则当 ρ_{xx} 为0时 σ_{xx} 也为0.

另一方面 $$\sigma_{xy}=-\frac{nec}{B}+\frac{\sigma_{xx}}{\omega_c\tau}$$

由此，当 $\sigma_{xx}=0$ 时， $j_x=\sigma_{xy}E_y$ ， σ_{xy} 为霍尔电导

$$\sigma_H=\sigma_{xy}=-\frac{nec}{B}\qquad j_y=\sigma_{yx}E_x=-\sigma_{xy}E_x$$

在量子力学下（E沿x方向）

$$H=\frac{1}{2m}(P+\frac{eA}{c})^2+eEx$$

选择矢量势 $A=(0,Bx,0)$

波函数为 $\psi(x,y)=e^{-ik_y y}\phi(x)$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega_c^2(x-l_c^2k_y)^2+eEx\right]\phi(x)=\varepsilon\phi(x)$$

$$l_c=\left(\frac{\hbar c}{eB}\right)^{\frac{1}{2}}$$ 经典回旋半径

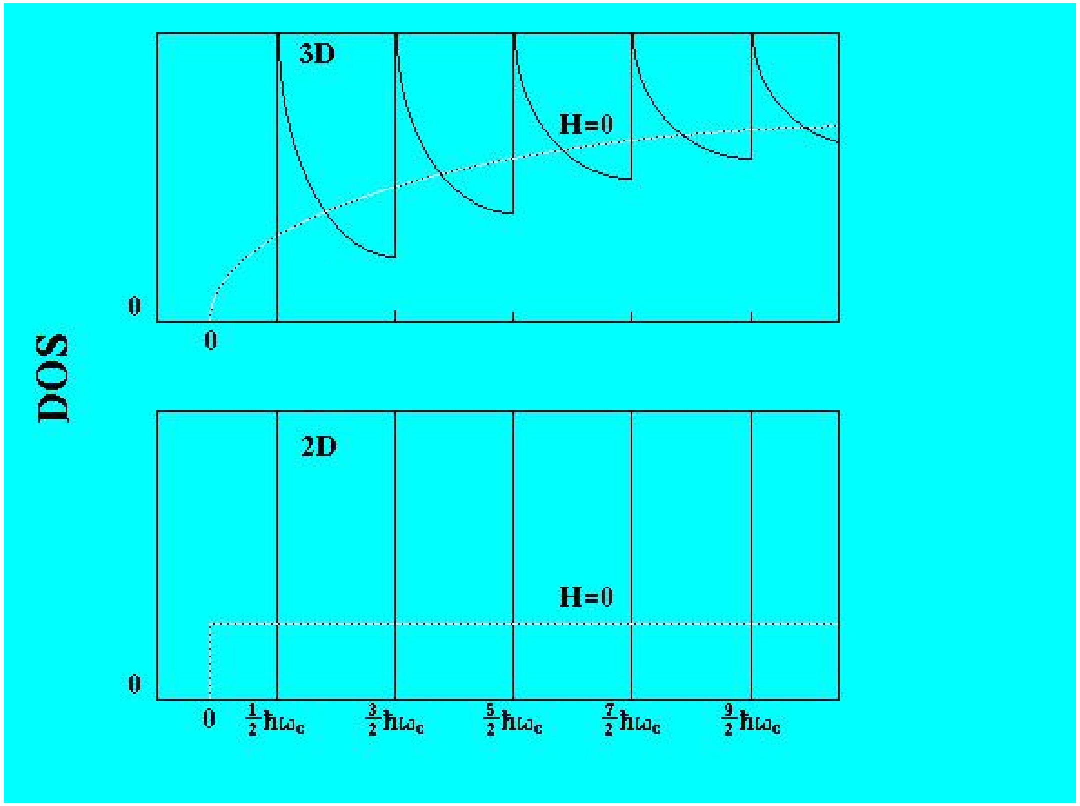
解为:

$$\varepsilon_i(E) = (i+\frac{1}{2})\hbar\omega_c + eE\,(l_c^2 k_y - \frac{eE}{2m\omega_c^2})$$

Landau 能级

$$\psi_i(x,y) = e^{(-ik_y y)} e^{[-\frac{(x-x_0)^2}{2l_c^2}]} H_i[\frac{(x-x_0)}{l_c}]$$

$$x_0 = l_c^2 k_y - \frac{eE}{m\omega_c^2}, \quad i = 0,1,2,3,\ldots$$



In two-dimensional systems, the Landau energy levels are completely seperate while in three-dimensional systems the spectrum is continuous due to the free movement of electrons in the direction of the magnetic field.

计算平均速度

$$< v_y >= \frac{1}{m}\int \psi_i^*\left(\frac{\hbar}{i}\frac{\partial}{\partial y}+\frac{eBx}{c}\right)\psi_i dr = -\frac{Ec}{B}$$

$$< v_x >= \frac{1}{m}\int \psi_i^*\frac{\hbar}{i}\frac{\partial}{\partial x}\psi_i dr = 0$$

➡ $$j_y = \frac{-neEc}{B}$$ 与经典结果相同.

在Landau能级上，纵向电流为0.

(2)整数量子霍尔效应

1975年S.Kawaji等首次测量了反型层的霍尔电导，1978年 Klaus von Klitzing 和Th. Englert 发现霍尔平台，但直到1980年, 才注意到霍尔平台的量子化单位 $\frac{h}{e^2}$ ，

K. von Klitzing, G. Dorda, and M. Pepper,
Phys. Rev. Lett. 45, 495 (1980)
for a sufficiently pure interface (Si-MOSFET)
=> integer quantum Hall effect

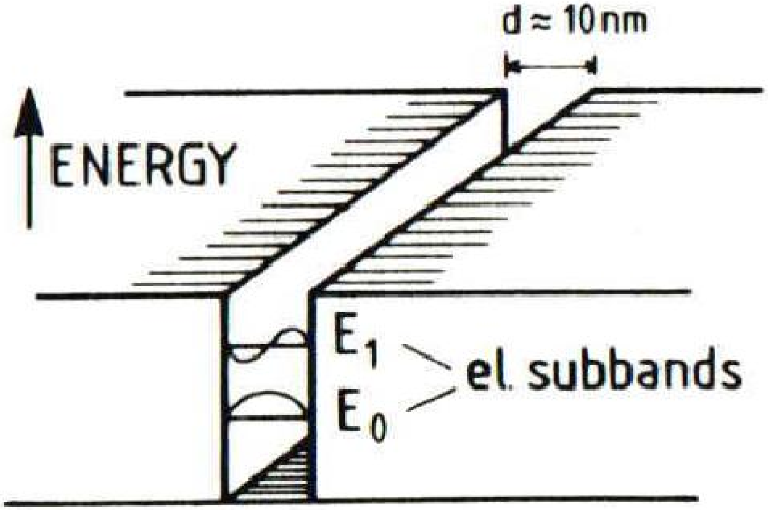
The Nobel Prize in Physics 1985

K. von Klitzing（1943~）

for the discovery of the quantized Hall effect.

Quantum Hall effect requires

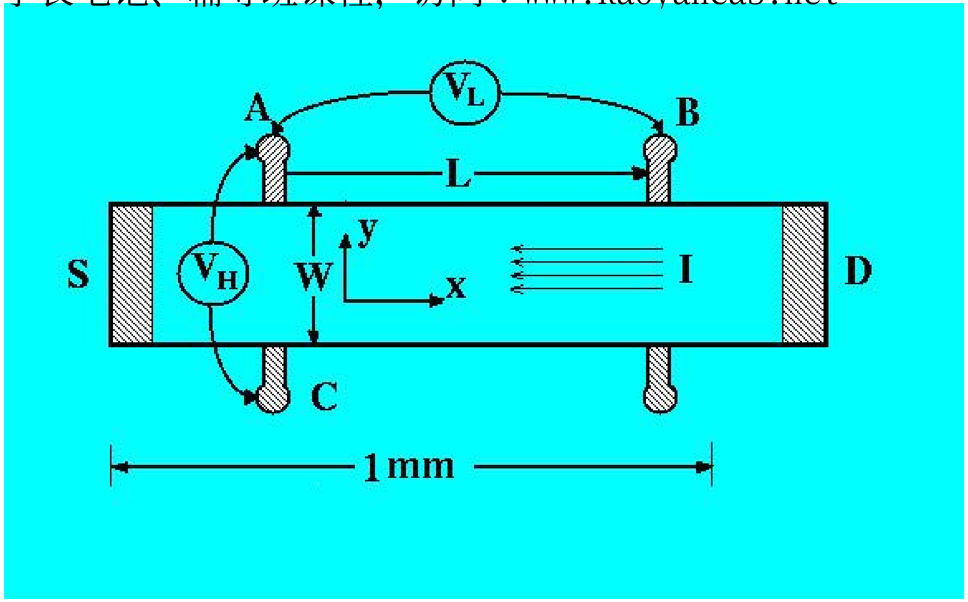
1. Two-dimensional electron gas
2. Very low temperature (< 4 K)
3. Very strong magnetic field (~ 10 Tesla)



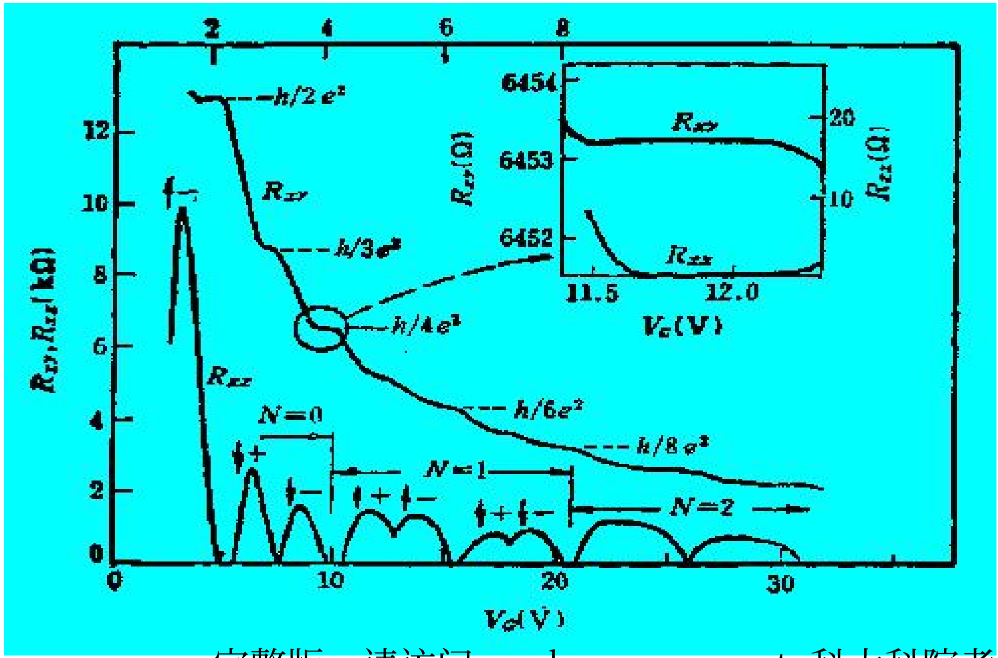
$$E = E_i + \frac{h^2 k_{\parallel}^2}{2m} \; ; \; k_{\parallel}^2 = k_x^2 + k_y^2$$

$$E_1 - E_0 > kT, \Gamma, E_F \rightarrow 2\,\mathrm{DEG}$$

实验设置示意图



实验观测到的霍尔电阻

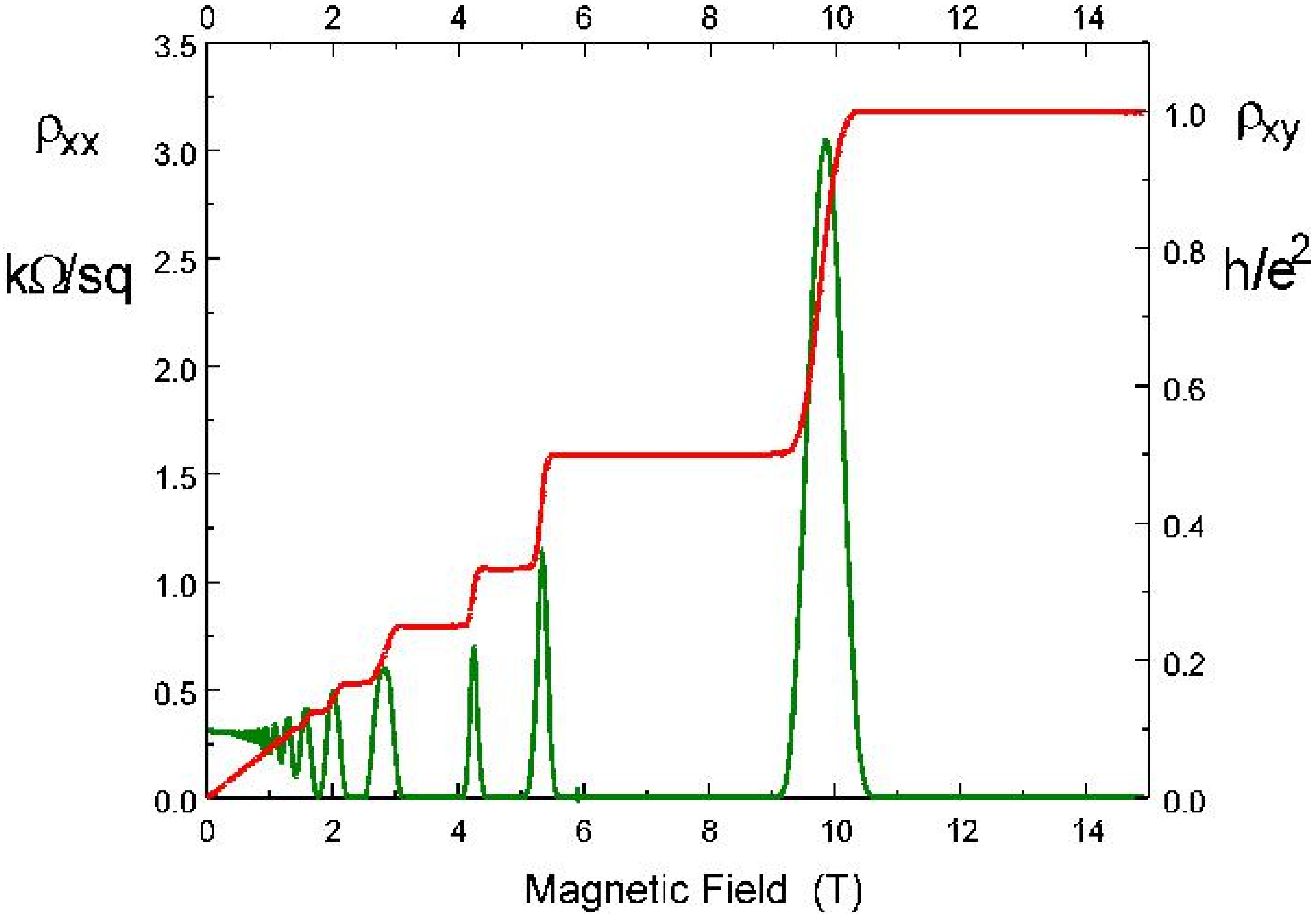


1, 霍尔电阻有台阶,

2, 台阶高度为 $\frac{h}{ie^2}$, i 为整数, 对应于占满第 i 个Landau能级,

精度大约为5ppm.

3, 台阶处纵向电阻为零.

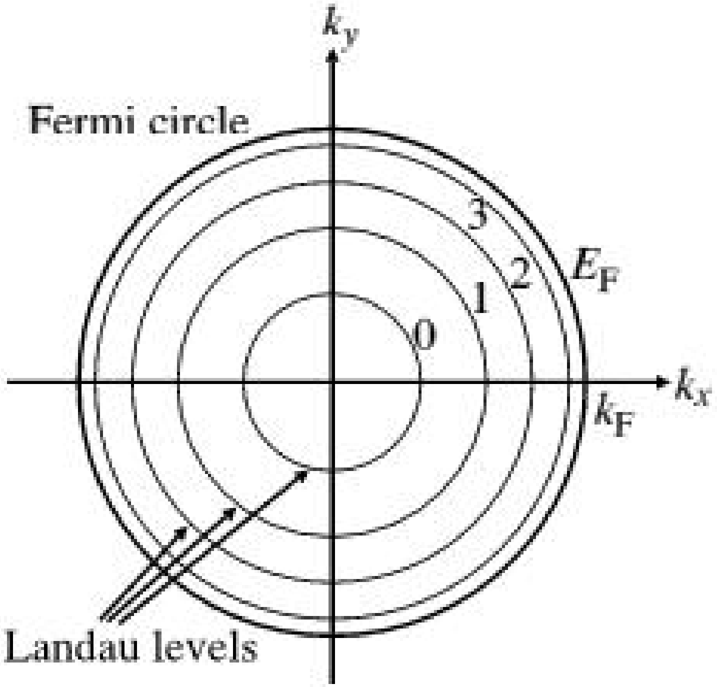

ρ_{xx}
kΩ/sq
ρ_{xy}
h/e^2
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0.0
0.2
0.4
0.6
0.8
1.0
0
2
4
6
8
10
12
14
Magnetic Field (T)

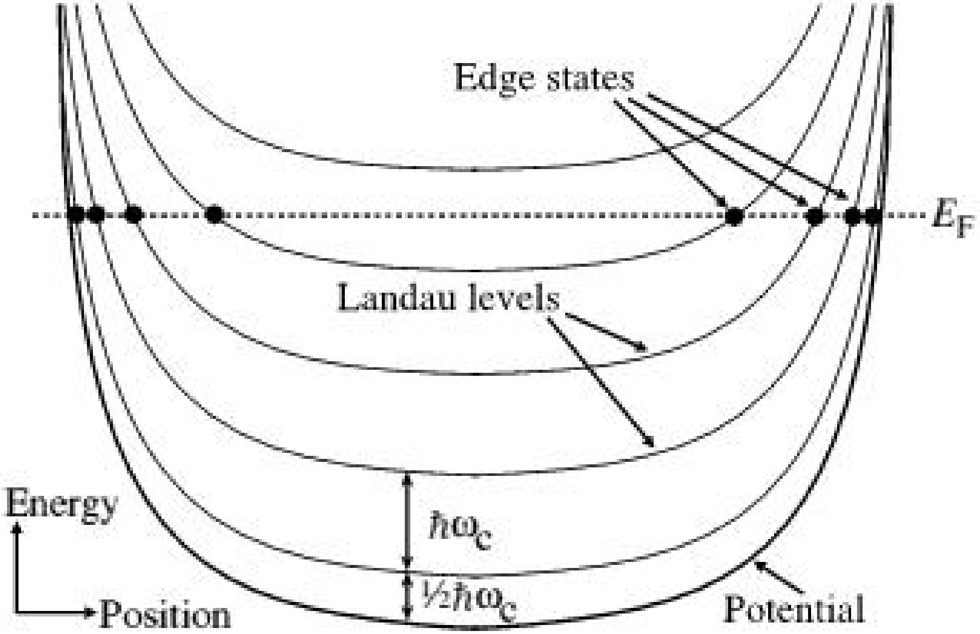
Why R_H has to be exactly $(h/e^2)/n$?

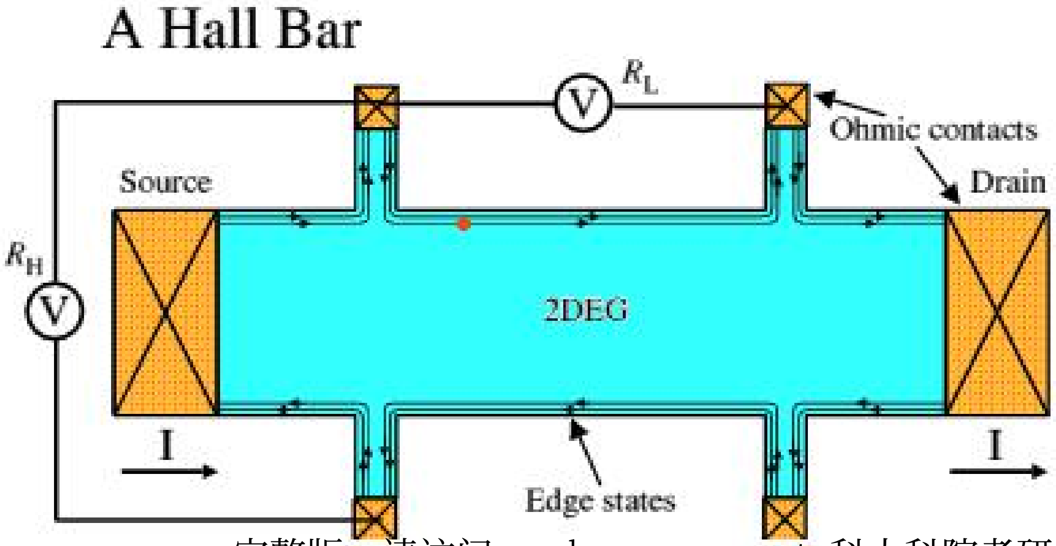
The importance of

1. Landau level (→ discrete levels)
2. Disorder and localization (→ plateaus)
3. Hidden gauge symmetry (→ quantization of R_H)

   (Laughlin, Phys. Rev. 23, 5632 (81))







When these levels are well resolved, if a voltage is applied between the ends of a sample, the voltage drop between voltage probes along the edge of a sample can go to zero in particular ranges of B, and the Hall resistance becomes extremely accurately quantised

由于杂质的作用，Landau能级的态密度将展宽(如下图).

两种状态：扩展态 和 局域态

只有扩展态可以传导霍尔电流(0度下)，因此若扩展态的占据数不变，则霍尔电流不变. 当Fermi能级位于能隙中时，出现霍尔平台.

Laughlin(1981) 和 Halperin(1982)基于规范变换证明：

如 *Fermi* 能级处于能隙中 $G_H = ec\dfrac{\partial n(\varepsilon_F)}{\partial B}$

无外磁场， $g(E) = \dfrac{m}{2\pi\hbar^2}$

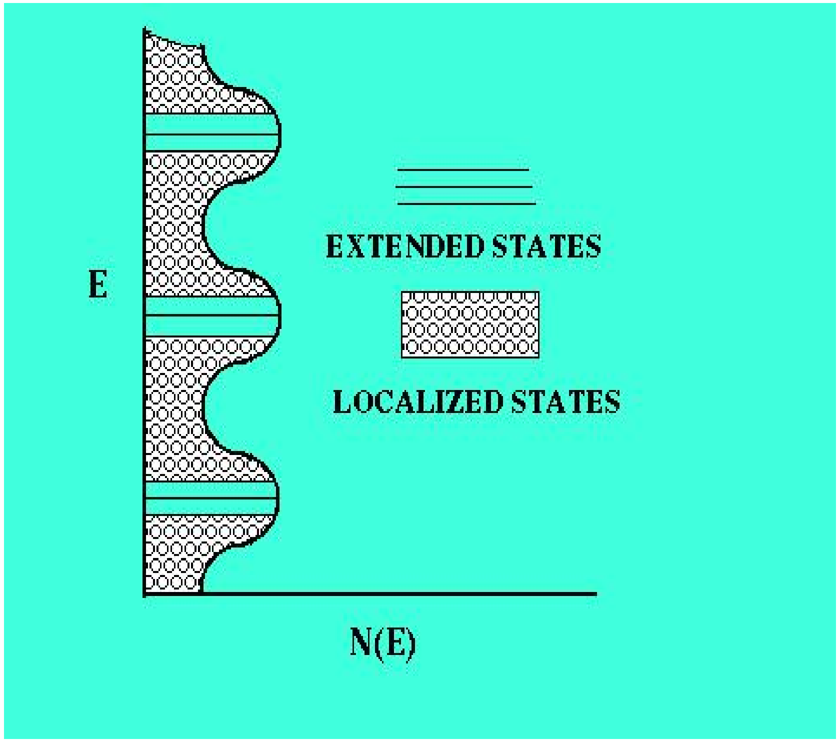
加磁场 → *Landau* 能级

→ 简并度 $\hbar\omega_c g(E) = \dfrac{eB}{hc}$

如电子占据 *i*个 *Landau* 能级：

$$n = \frac{ieB}{hc}$$

$$\Rightarrow R_H(i) = \frac{1}{G_H} = \frac{h}{e^2 i}$$



应用： (a) 电阻标准

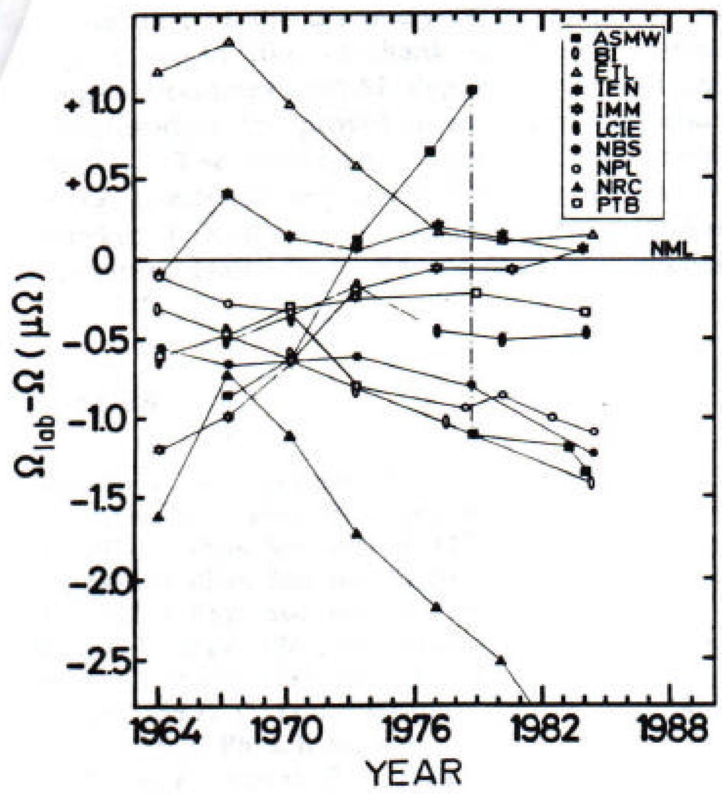


FIG. 26. Time dependence of the 1-Ω standard resistors maintained at the different national laboratories.

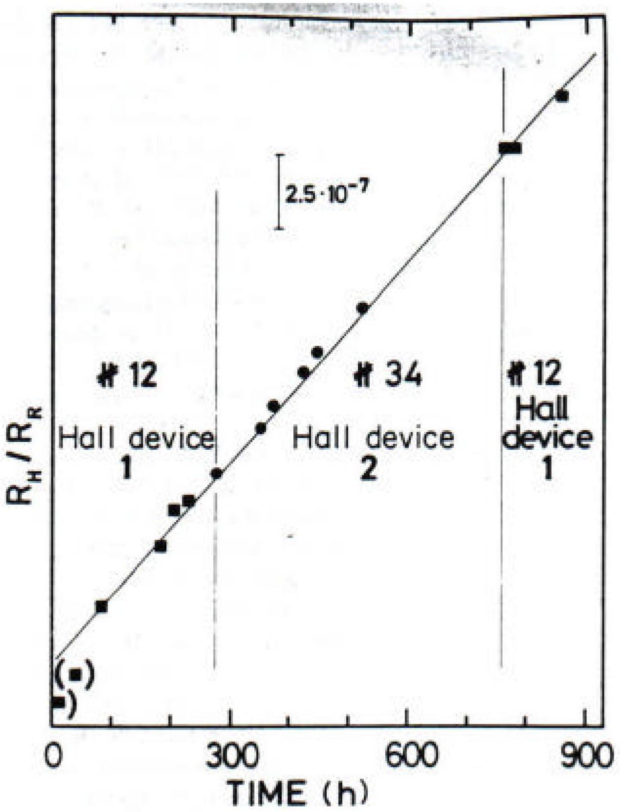
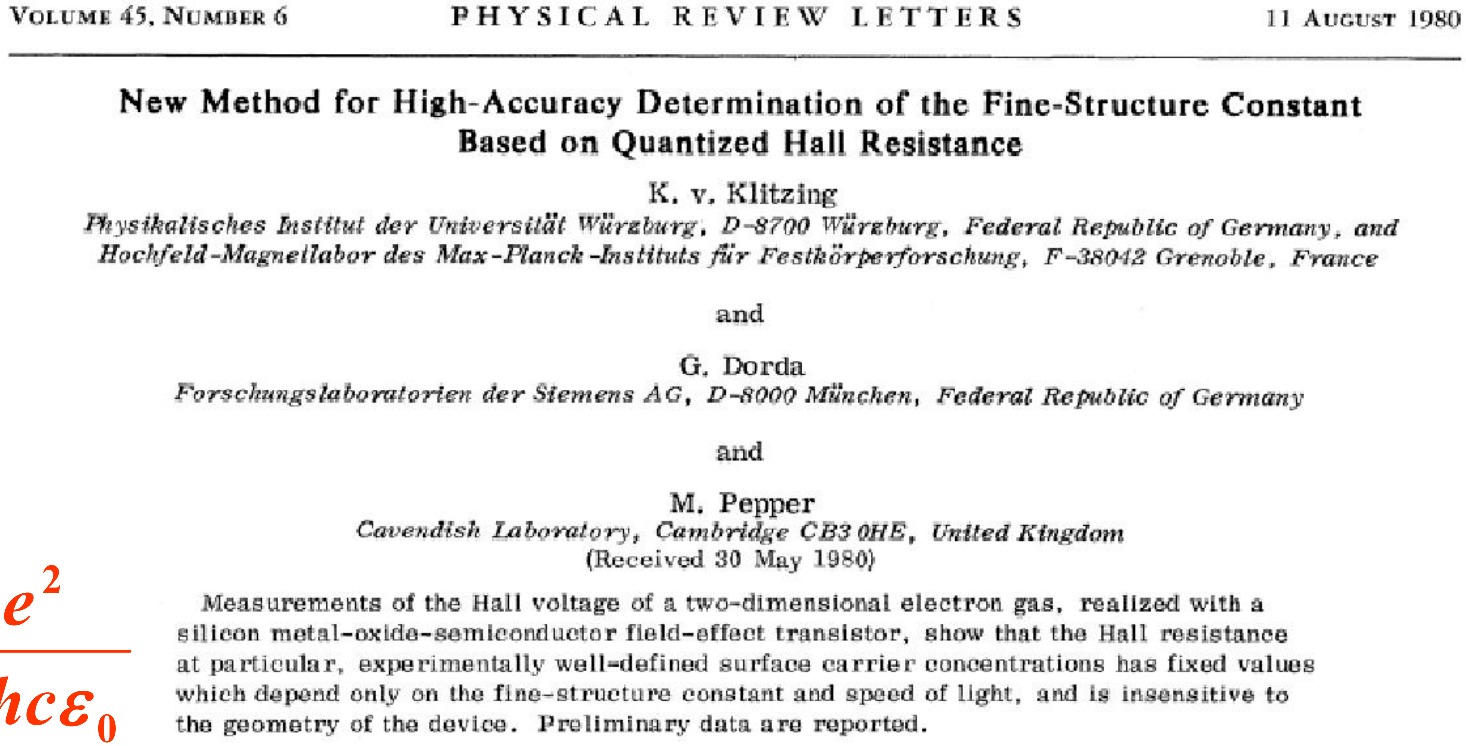


FIG. 27. Ratio R_H/R_R between the quantized Hall resistance R_H and a wire resistor R_R as a function of time. The result is time dependent but independent of the Hall device used in the experiment.

自1990年起，电阻标准：$\frac{h}{e^2} = 25812.806\,\Omega$ (精度～ 2×10^{-8})

应用：　(b)精细结构常数的测量



Volume 45, Number 6　　PHYSICAL REVIEW LETTERS　　11 August 1980

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
Forschungslaboratorien der Siemens AG, D-8000 München, Federal Republic of Germany

and

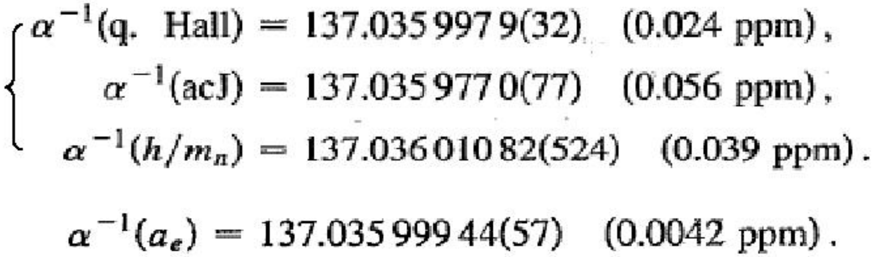
M. Pepper
Cavendish Laboratory, Cambridge CB3 0HE, United Kingdom

(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.

$$\alpha = \frac{e^2}{2hc\varepsilon_0}$$

experiment



$$\begin{cases} \alpha^{-1}(\text{q. Hall}) = 137.035\,997\,9(32) \quad (0.024\ \text{ppm}), \\ \alpha^{-1}(\text{acJ}) = 137.035\,977\,0(77) \quad (0.056\ \text{ppm}), \\ \alpha^{-1}(h/m_n) = 137.036\,010\,82(524) \quad (0.039\ \text{ppm}). \end{cases}$$

theory

$$\alpha^{-1}(a_e) = 137.035\,999\,44(57) \quad (0.0042\ \text{ppm}).$$

(Kinoshita, Phys. Rev. Lett. 1995)

(3)分数量子霍尔效应

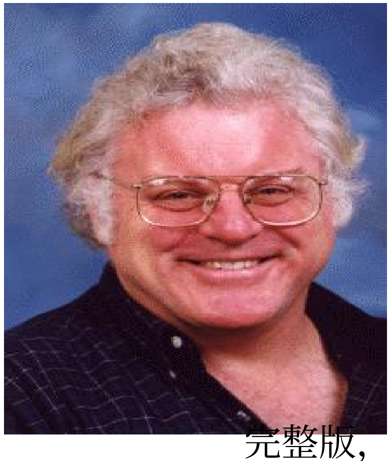
1982年, 崔琦, H.L. Stomer 等发现具有分数量子数的霍尔平台, 一年后, R.B.Laughlin写下了一个波函数, 对分数量子霍尔效应给出了很好的解释.

D. C. Tsui, H. L. Stormer, and A. G. Gossard, Phys. Rev. Lett. 48, 1559 (1982)
for an extremely pure interface (GaAs/AlGaAs heterojunction) where electrons could move ballistically => fractional quantum Hall effect
R.B.Laughlin, Phys. Rev. Lett. 50, No.18 (1983)

The Nobel Prize in Physics 1998

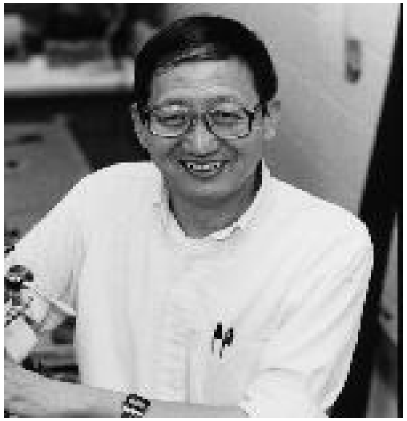
for their discovery of a new form of quantum fluid with fractionally charged excitations.

Robert B. Laughlin(1950)



Horst L. Stormer(1949)

DANIEL C. TSUI(1939)

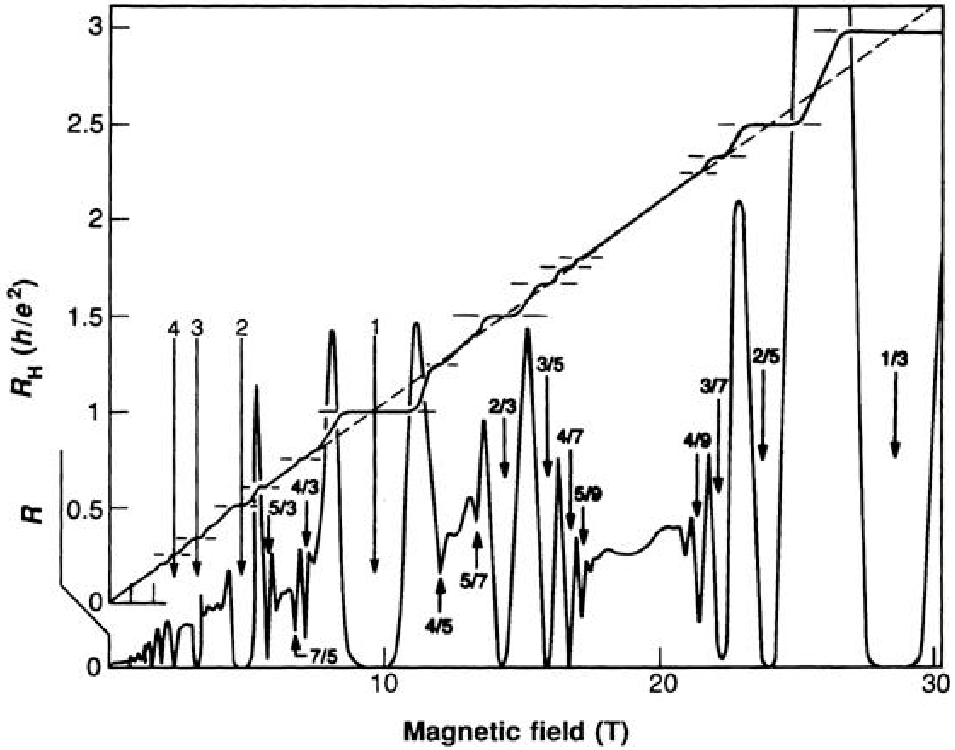


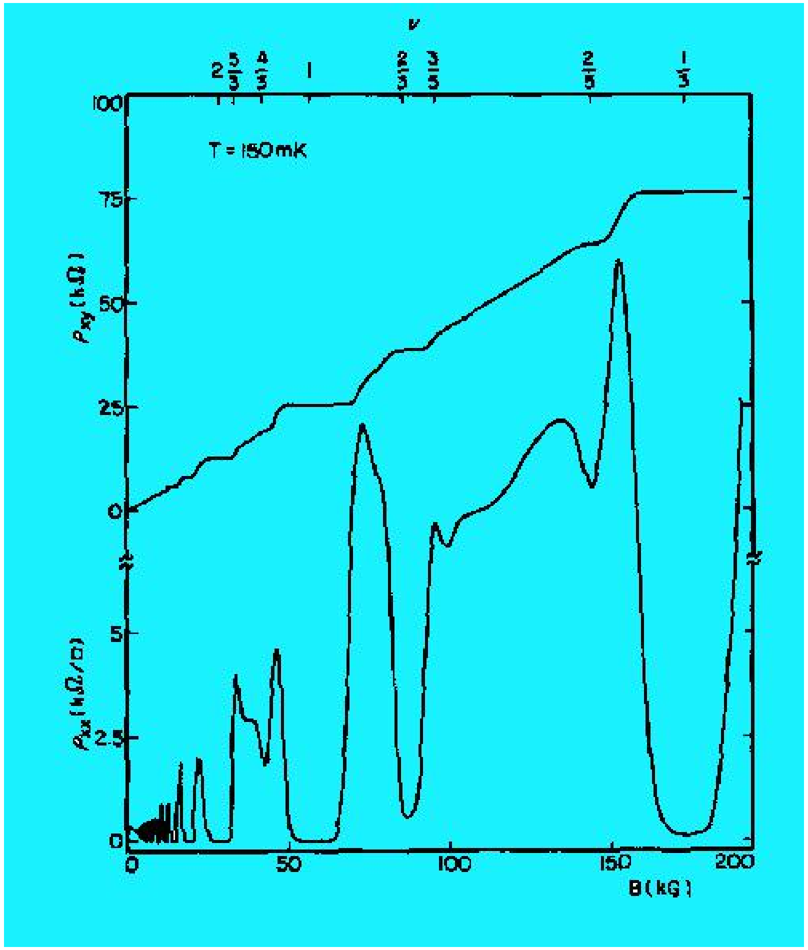
分数量子霍尔效应:

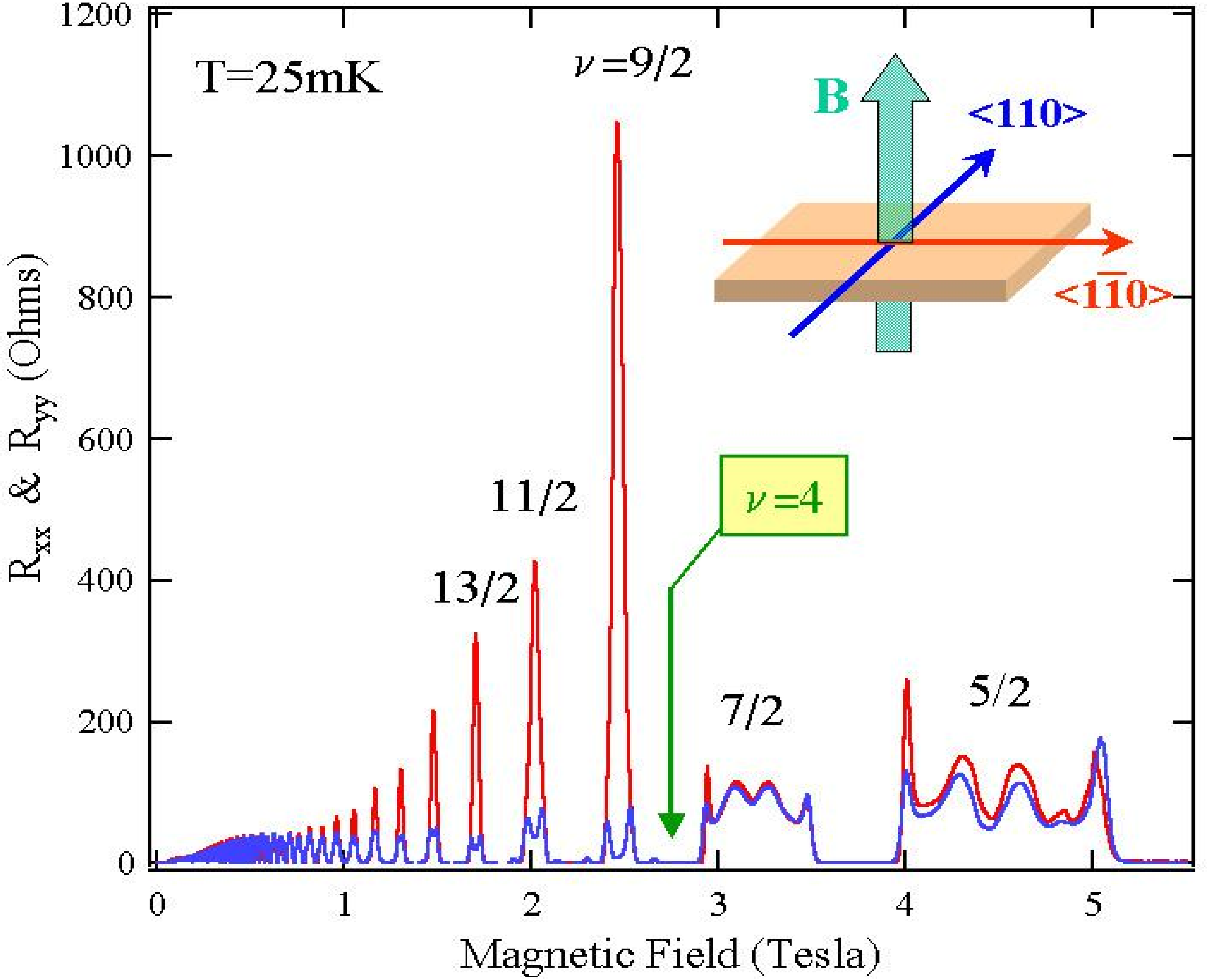
崔琦， Stomer 等发现， 当Landau能级的占据数

$$\nu = \frac{n}{h\omega_c g(E)} = \frac{p}{m}, \quad p,m为整数$$

有霍尔平台







first $\nu = n$ later $\nu = \frac{1}{2n+1}$ finally $\nu = \frac{p}{2np\pm 1}$ $n, p \in N$

分数量子霍尔效应不可能在单粒子图象下解释，引入相互作用

$$H=\sum_i\left[\frac{1}{2m}\left|p_i+\frac{eA_i}{c}\right|^2+V(r_i)\right]+\sum_{i>j}\frac{e^2}{|r_i-r_j|}$$

在超强磁场下，电子位于第一Landau能级．其单粒子波函数为

$$\psi_m=\frac{z^{*m}\exp(-|z|^2/4l_c^2)}{\sqrt{2^{m+1}m!\pi}},z=x+iy$$

这一状态对应于电子在一由下式给出的面积内运动

$$\pi<m||z|^2|m>=2\pi l_c^2(m+1)$$

Laughlin 建议了如下形式的波函数

$$\psi(z)=\prod_{i<j}(z_i-z_j)^m\exp(-\sum_k|z_k|^2/4l_c^2)$$

这一状态的占据数为 $\nu=\dfrac{1}{m}$

Laughlin 计算了m=3, m=5时这一波函数的能量，发现比对应密度下CDW的能量要低. 这一状态称为分数量子霍尔态，或Laughlin态，当密度改变从而偏离占据数1/3, 1/5时，对应于准粒子激发，激发谱具有能隙，准粒子的电荷为分数(1/3, 1/5). 因此Laughlin态是一个不可压缩的量子液体状态.

$\nu = 1/3$ **FQHE 态. 绿球代表被暂时冻结的电子，蓝色为代表性电子的电荷密度，黑色箭头代表磁通线.**

同 IQHE一样, Fermi 能级处于能隙位置时, 出现FQHE平台. 不同之处在于IHQE的能隙来源于单粒子态在强磁场中的量子化, 而FQHE的能隙来源于多体关联效应.

Haldane 和 Halperin, 利用级联模型, 指出Laughlin 态的准粒子和准空穴激发将凝聚为高阶分数态, 如从 1/3 态出发, 加入准粒子导致 2/5态, 加入空穴导致2/7态. 准粒子由这些态激发出来并凝聚为下一级的态 .

P 为偶数,

$$\nu = \frac{p}{mp+\alpha}$$

$$\alpha = 1$$

对应于粒子型元激发

$$\alpha = -1$$

对应于空穴型元激发

级联模型的特点：

1. 无法解释那一个子态是较强的态.
2. 几次级联后，准粒子的数目将超过电子的数目.
3. 系统在分数占据数之间没有定义.
4. 准粒子具有分数电荷.

复合费米子模型（CF）

一个复合费米子由一个电子和偶数个磁通线构成. 复合费米子包含了所有的多体相互作用.

FQHE是CF在一个有效磁场下的IQHE.

CF 具有整数电荷.

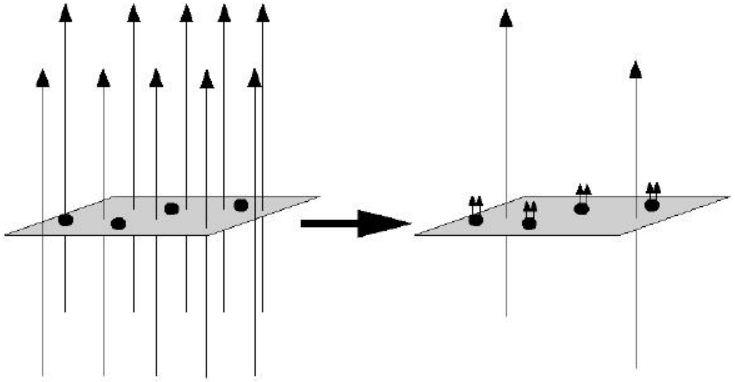
CF 模型可以给出所有观察到的分数态，包括这些态的相对强度及当减小温度，提高样品质量时出现的次序.

CF 指出： $v=1/2$ 态，对应的有效磁场为0，是具有金属特征的特殊状态.

Composite Particles

Consider $\vec{B}$ to be quantized in units of Φ_0

It is energetically favorable to place a Φ_0 onto an electron

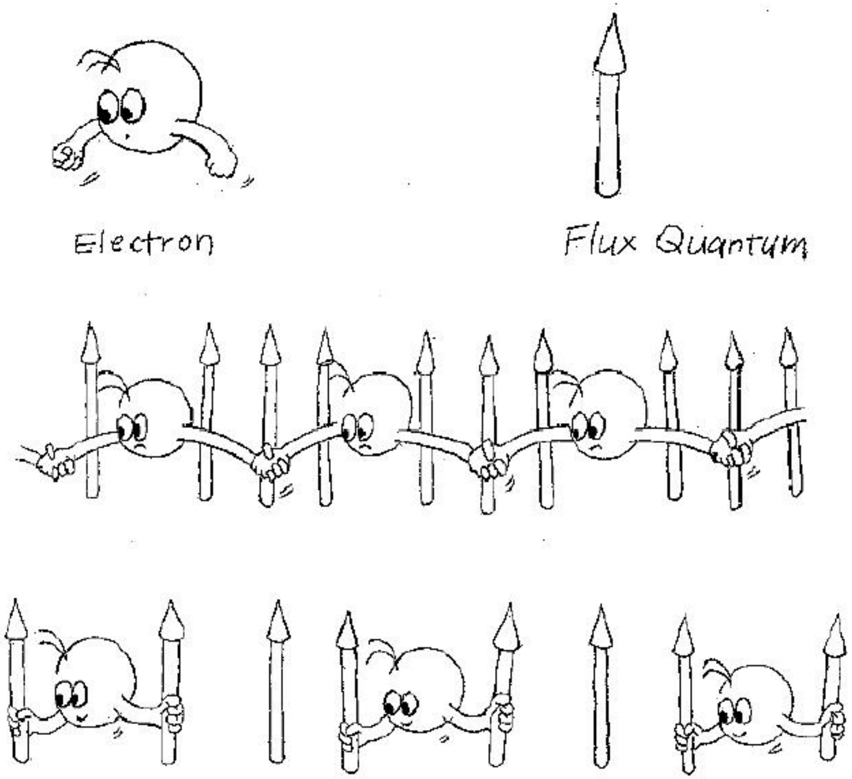


because it reduces the (Coulomb) interaction between electrons

(due to the increase of correlation)

New particles become weakly interacting

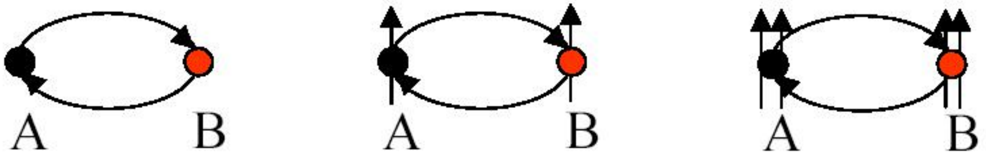
Metamorphosis



METAMORPHOSIS OF INTERACTING ELECTRONS INTO FREE COMPOSITE FERMIONS

Jainendra k. Jain

Statistics of these new particles



$\Psi \rightarrow -\Psi$ $\Psi \rightarrow \Psi$ $\Psi \rightarrow -\Psi$

Statistics depends on the number of Φ_0

If one attaches 2 p Φ_0 we have a fermi statistic.

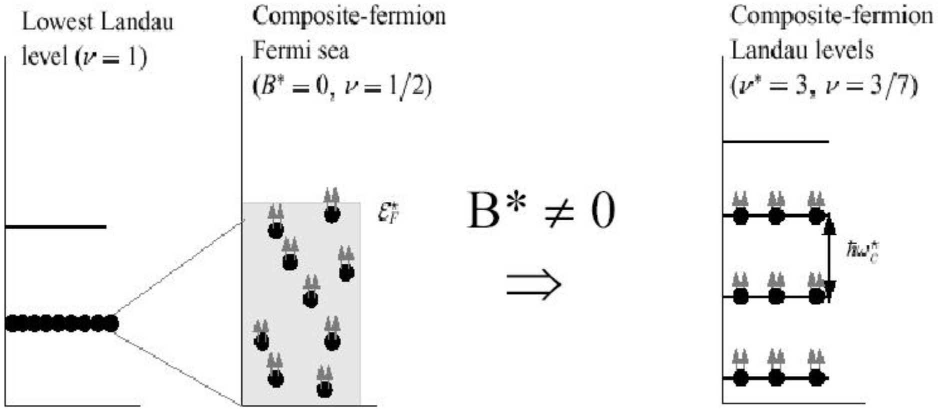
$\Rightarrow$ Composite Fermions

The FQHE becomes an IQHE

CFs experience the reduced magnetic field

$$B^* = B - p\Phi_0(N_e/L^2).$$

e - LL



Lowest Landau level ($\nu = 1$)

Composite-fermion Fermi sea ($B^* = 0$, $\nu = 1/2$)

ε_F^*

$B^* \neq 0$

$\Rightarrow$

Composite-fermion Landau levels ($\nu^* = 3$, $\nu = 3/7$)

$\hbar\omega_c^*$

CF - LL

$$\text{FQHE} \rightarrow \text{IQHE}$$

Finally

$$B^* = B - p\Phi_0 (N_e / L^2)$$

$$\nu_e = \frac{(N_e / L^2)}{B}\Phi_0 \quad \nu_{CF} = \frac{(N_e / L^2)}{|B^*|}\Phi_0 \Rightarrow \quad \nu_e = \frac{\nu_{CF}}{p\nu_{CF} \pm 1} \quad p, \nu_{CF} \in N$$

This explains everything.

Example: $p = 2,\ \nu_{CF} = 1 \Rightarrow \nu_e = \frac{1}{3}$

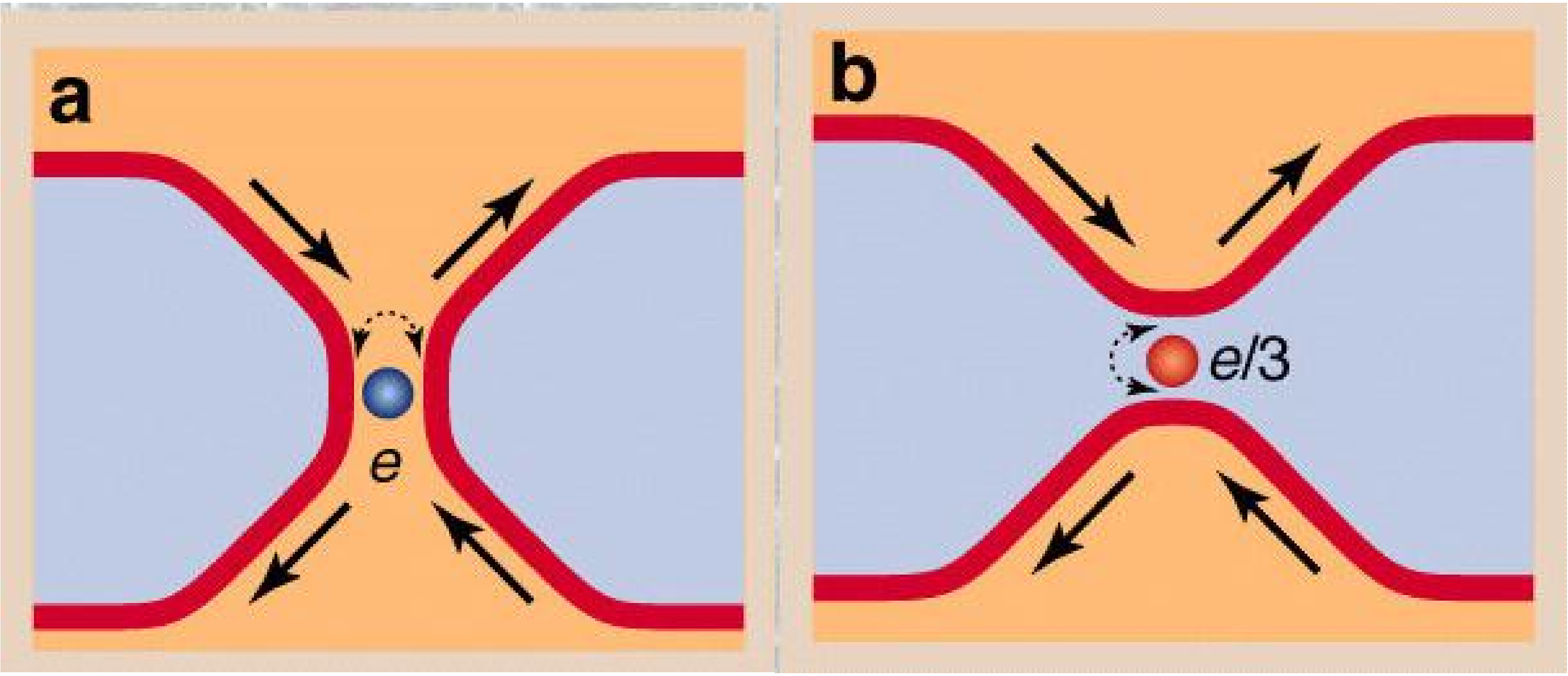
$p = 2,\ \nu_{CF} = 2 \Rightarrow \nu_e = \frac{2}{5}$

$p = 2,\ \nu_{CF} = 3 \Rightarrow \nu_e = \frac{3}{7}$

$p = 2,\ \nu_{CF} = 4 \Rightarrow \nu_e = \frac{4}{9}$

新进展

- 观察到分数电荷涨落.
- FQHE 的Ginsburg Landau 理论.
- 费米， 玻色 和分数统计.
- 边缘态和共形场论.



利用一维结观察分数电荷 **C.L. Kane and M.P.A. Fisher, Shot in the Arm for Fractional Charge, Nature 389, 119 (1997).**

Room-Temperature Quantum Hall Effect in Graphene

PI: Philip Kim, Department of Physics, Columbia Universty

Supported by NSF (No. DMR-03-52738 and No. CHE-0117752), NYSTAR
DOE (No. DE-AIO2-04ER46133 and No. DE-FG02-05ER46215), and Keck Foundation

The Quantum Hall effect (QHE) is one example of a quantum phenomenon that occurs on a truly macroscopic scale. The signature of QHE is the quantization plateaus in the Hall resistance (R_{xy}) and vanishing magnetoresistance (R_{xx}) in a magnetic field. The QHE, exclusive to two-dimensional metals, has led to the establishment of a new metrological standard, the resistance quantum, h/e^2, that contains only fundamental constant. As with many other quantum phenomena, the observation of the QHE usually requires low temperatures (previously reported highest temperature was 30 K). In graphene, a single atomic layer of graphite, however, we have observed a well-defined QHE at room temperature owing to the unusual electronic band structure and the *relativistic* nature of the charge carriers of graphene.

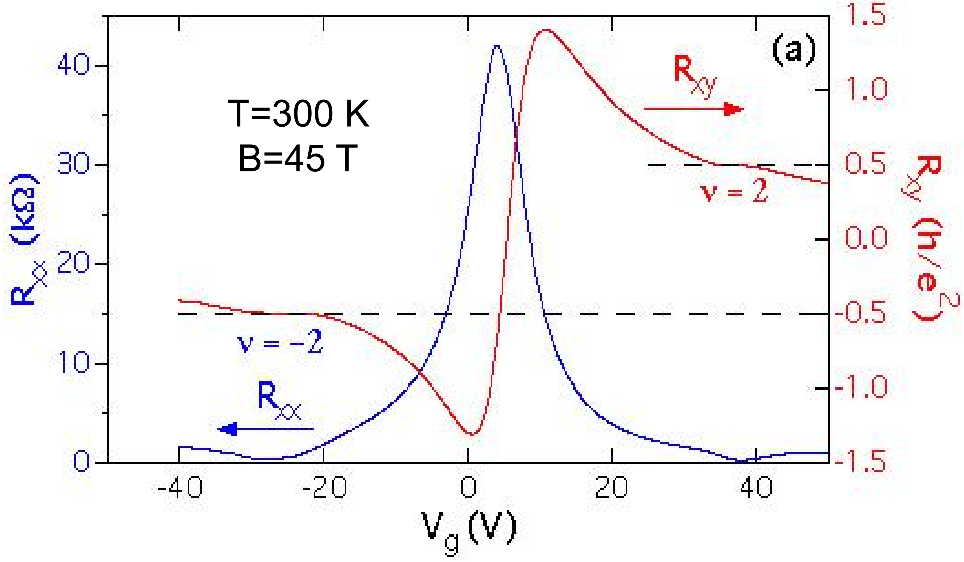


Figure: Magnetoresistance (R_{xx}) and Hall resistance (R_{xy}) of graphene as a function of the back gate voltage (V_g) in a magnetic field of B=45 T at room temperature.

Novoselov, K.S.; Jiang, Z.; Zhang, Y.; Morozov, S.V.; Stormer, H.L.; Zeitler, U.; Maan, J.C.; Boebinger, G.S.; Kim, P. and Geim, A.K., **Science**, **315** (5817), 1379 (2007).

COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK

NHMFL

4.2　二维体系中的相变

连续相变的描述：序参量　　非零→零
维度对相变、临界行为有重要影响
一维体系，T>0时，体系总是无序，不存在长程序，无相变

二维体系？

相变取决于序参量的自由度数

$$G(r) \sim \begin{cases} e^{-\frac{r}{\xi(T)}} \text{(一维)} \\ r^{-\eta(T)} \text{(二维)} \\ c(T) \text{ (三维)} \end{cases}$$

N=1, 有相变，如二维Ising模型
N=3, 无相变，如二维Heisenberg模型

N=2：序参量为零，但可有准长程序，
　　Kosterlitz-Thouless(K-T)相变　　相变概念的拓宽

序参量自由度n=2的二维系统：

自旋X-Y模型，二维超流体、二维超导体及二维晶体等

低温下，自旋的关联随距离作代数式的衰减。对有限尺寸的样品，二维X-Y模型的低温相就呈现出表观的长程序（准长程序），到高温，则为没有长程序的无序相所取代，期间有无相变？

1970年：Brezinskii提出涡旋对松解所对应的连续相变思想 (Z.Eksp.Tev.Fiz.,59,907(1970))

1973年：Kosterlitz和Thouless讨论二维超流相变，独立提出类似想法并发展为较完整理论（J.Phys.C,6,1181(1973))

基本思想：拓扑缺陷(如涡旋（Vortex))介入的相变

拓扑激发：

二维点阵格点：格点i上的自旋与X轴夹角为 ϕ_i
通过任意一些格点，划一闭合回路L，沿此回路逆时针方向绕行一周，相邻两格点的方向角之差：

$$\Delta\phi_i = \phi_{i+1} - \phi_i \qquad -\pi < \Delta\phi_i \le \pi$$

$$\Phi_L = \sum_L \Delta\phi_i$$

(1)$\Phi_L = 0$：每个格点上自旋的方向角是确定的，单值的，非拓扑性激发

(2)$\Phi_L \neq 0, \Phi_L = n\cdot 2\pi \quad (n = \pm1,\pm2,\ldots)$ n决定了涡旋的强度，称为拓扑荷

每个格点上自旋的方向角将是多值的，拓扑性的，拓扑性激发

将$\phi(r)$看成流体中的速度势，定义速度场：

$\vec{v}(r) = \nabla\phi(r)$

将速度场$\vec{v}$分为无旋场$\vec{v}_s$和无源场$\vec{v}_v$

$$\vec{v} = \vec{v}_s + \vec{v}_v \qquad \begin{cases}\nabla\cdot\vec{v}_s = 4\pi D(r)\\ \nabla\times\vec{v}_s = 0\end{cases} \qquad \begin{cases}\nabla\times\vec{v}_v = 2\pi\Omega(r)\vec{e}_z\\ \nabla\cdot\vec{v}_v = 0\end{cases}$$

可以证明：$\vec{v}_s$和$\vec{v}_v$之间没有相互作用：$\int(\vec{v}_s\cdot\vec{v}_v)d\vec{r} = 0$

拓扑激发和非拓扑激发可分开来讨论

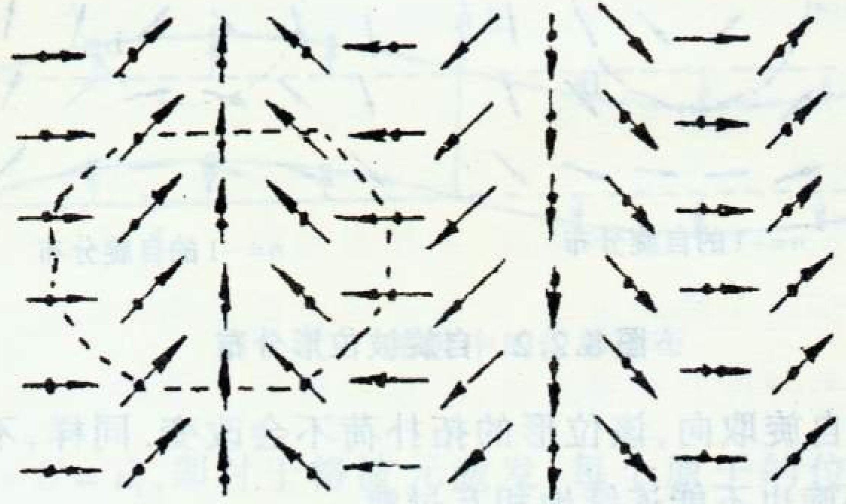
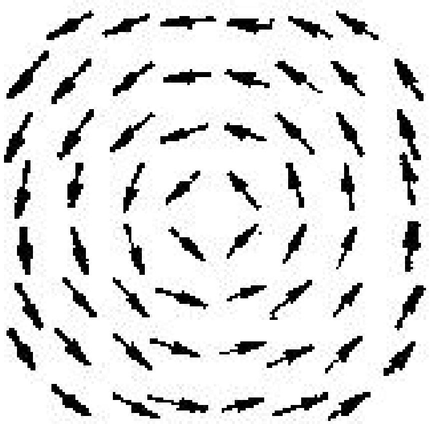
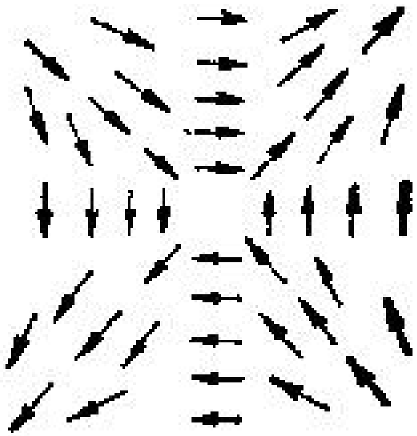


图 8.2.1　自旋波位形分布

自旋涡旋



正涡旋 (a)



负涡旋 (b)

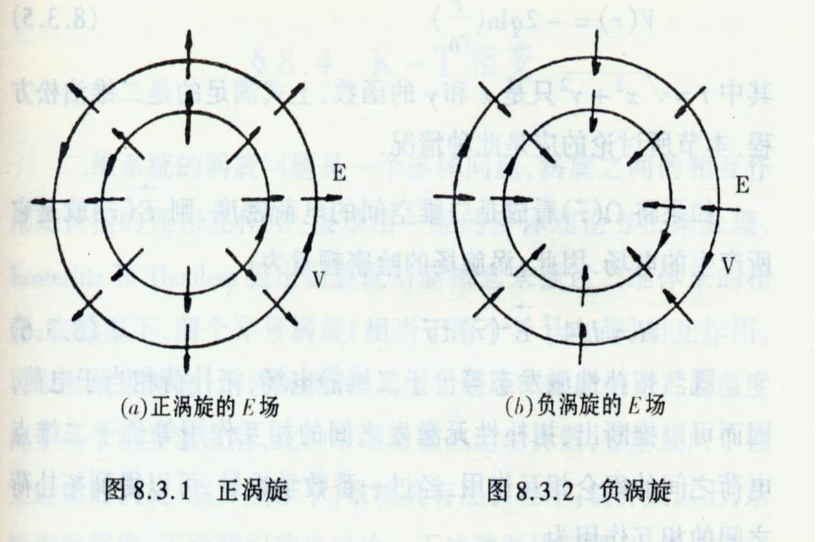
拓扑性元激发之间的相互作用

拓扑性元激发的相互作用在形式上等同于二维点电荷之间的相互作用。这些二维点电荷位于拓扑性元激发的位置上，其电荷量正比于该拓扑性元激发的拓扑荷。

拓扑性元激发所对应的无源场 $\vec{v}_v$是xy平面上的二维矢量

定义新的二维矢量场： $\vec{E}(r) = -2\vec{e}_z \times \vec{v}(r)$

$$\begin{cases} \nabla \times \vec{E} = 0 \\ \nabla \cdot \vec{E} = 4\pi\Omega(r) \end{cases} \Longrightarrow \text{二维静电场}$$



(a)正涡旋的 E 场　　(b)负涡旋的 E 场

图 8.3.1　正涡旋　　图 8.3.2　负涡旋

二维点电荷：

(1)分布在二维平面里，满足三维泊松方程

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)V(\vec{r}) = -4\pi q\delta(\vec{r}) \Rightarrow V(\vec{r}) = \frac{q}{r}$$

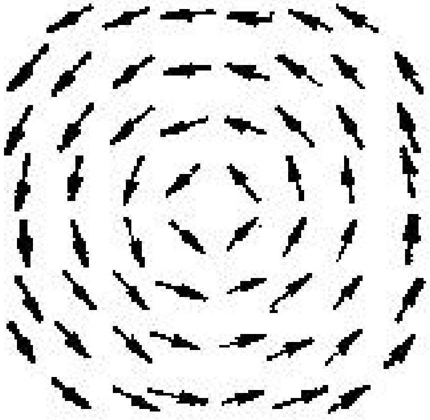
(2)均匀带电的直线电荷，在垂直于直线的任何二维平面内：

$$V(r) = -2q\ln\left(\frac{r}{r_0}\right) \qquad r = \sqrt{x^2 + y^2}$$

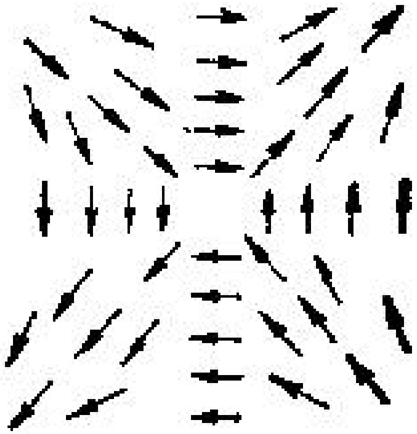
$$U(\vec{r}_i, \vec{r}_j) = -2q_i q_j \ln\left(\frac{\left|\vec{r}_i - \vec{r}_j\right|}{a}\right)$$

二维泊松方程

K-T相变

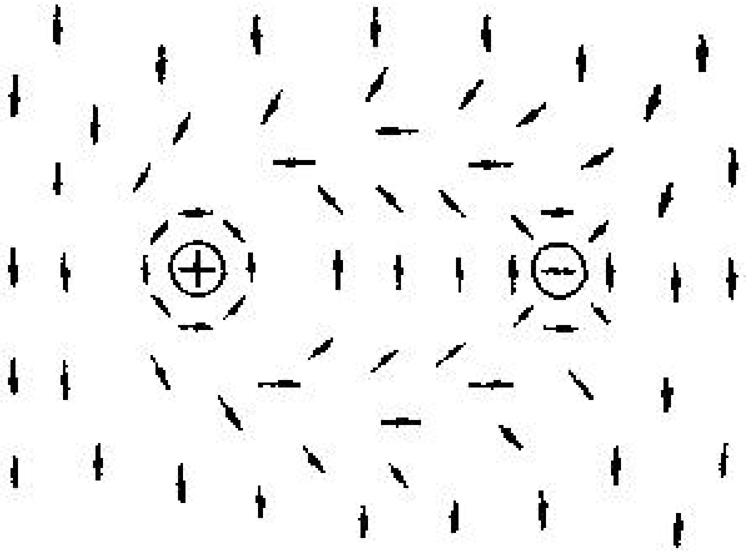


正涡旋 (a)



负涡旋 (b)

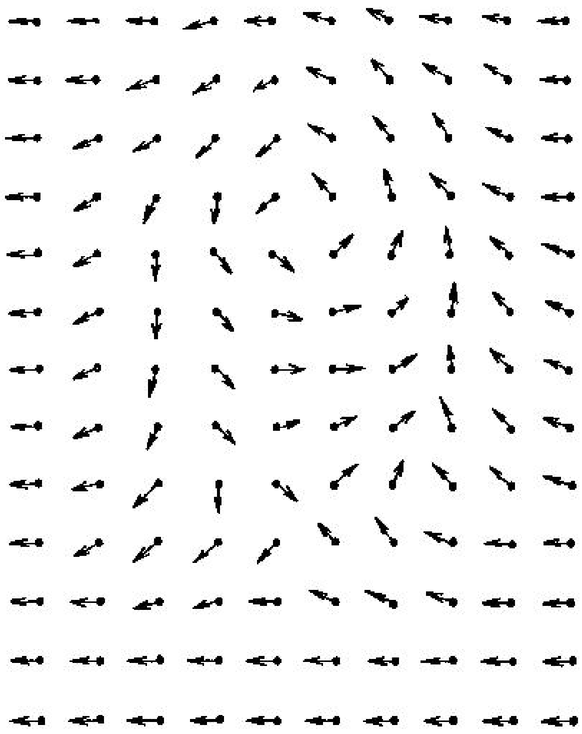
涡旋对



低温下，正负涡旋构成束缚对，对长程的自旋排列影响不大，系统具有拓扑长程序。

高于某临界温度，系统中产生大量的单个涡旋，导致拓扑长程序被破坏。

Heisenberg *Hamilton* 量：$H=-J\sum_{ij}s_i\cdot s_j$



$X-Y$模型 (只考虑最近邻相互作用)：

$$H=-J\sum_{ij}\cos(\phi_i-\phi_j)$$

作简谐近似：$H=\frac{J}{2}\sum_{ij}(\phi_i-\phi_j)^2$

与涡旋中心距离 r处的自旋对能量的贡献：

$$\frac{J}{2}\cdot\left(\frac{2\pi}{2\pi r}\right)^2\cdot(2\pi r)$$

一个涡旋的能量：$E_v=\frac{J}{2}\int_0^L\frac{2\pi dr}{r}=J\pi\ln\left(\frac{L}{a}\right)$

a：点阵间距。相应的熵 $k_BT\ln\left(\frac{L}{a}\right)^2$，自由能：

$$F_v=J\pi\ln\left(\frac{L}{a}\right)-k_BT\ln\left(\frac{L}{a}\right)^2$$

自由能等于零 → 相变：$T_c=\frac{\pi J}{2k_B}$

T_c以上涡旋自由能为负 → 大量涡旋自发产生，破坏准长程序

考虑低温下存在具有有限能量的束缚涡旋对（可由热激发，不破坏长程的自旋序）

涡旋系统的约化 *Hamilton* 量

$$H_v = -\pi K \sum_{|r-r'|>a} s(r)s(r')\ln\left[\frac{|r-r'|}{a}\right] + E_c \sum_r s^2(r)$$

$s(r)$为涡旋度 (n)， E_c表示涡旋的核心区域的 能量，

温度已包含在 K及核心能中。

涡旋对类似于屏蔽正负电荷相互作用的电介质的作用

K-T理论是对屏蔽效应的重正化群的处理。

自由能的第n级微商在相变点出现突变就称为第n级相变

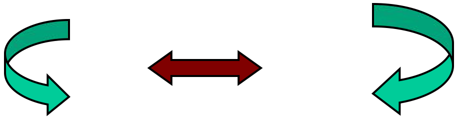
K-T相变是无穷级

Two dimensional helium

- Since helium is attracted to almost anything* , it will form a 2D film.

*except for Cs

- Most long-range order is forbidden in 2D (Mermin-Wagner theorem), e.g. BEC not allowed for T>0 because the system is susceptible to long-range phase decoherence.
- <u>However, it does become a superfluid.</u>
- The transition is called the Kosterlitz-Thouless transition.
- Superfluid-normal fluid transition is caused by vortex-anti-vortex unbinding.



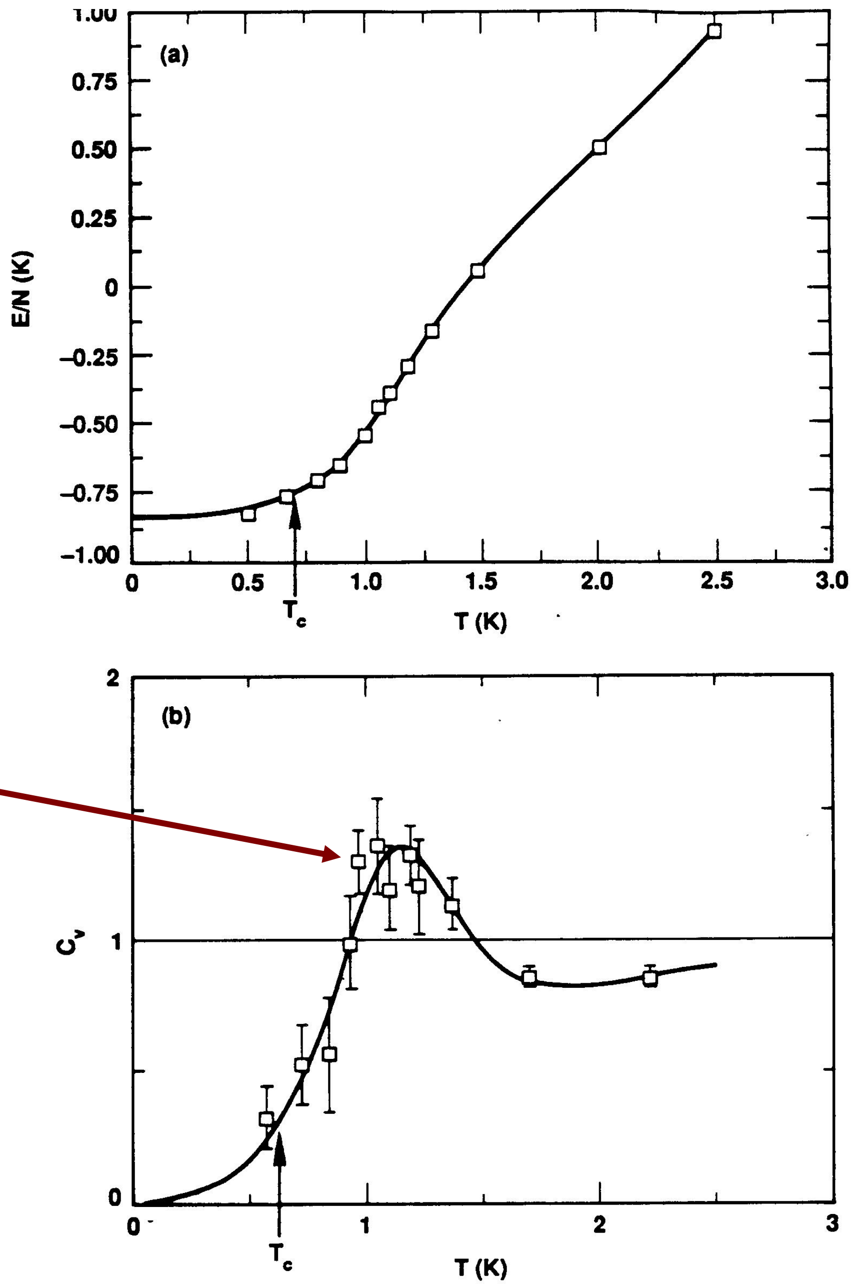
- KT predicts algebraic decay of single particle density matrix

$$n(r) \rightarrow n_0 \left(\frac{a}{r}\right)^{\frac{T}{\rho_s}}$$

2d helium energetics

- In contrast to 3D the energy is a smooth function of temperature.

- Bump in C_v above the transition.
- No feature at the transition (only an essential singularity)



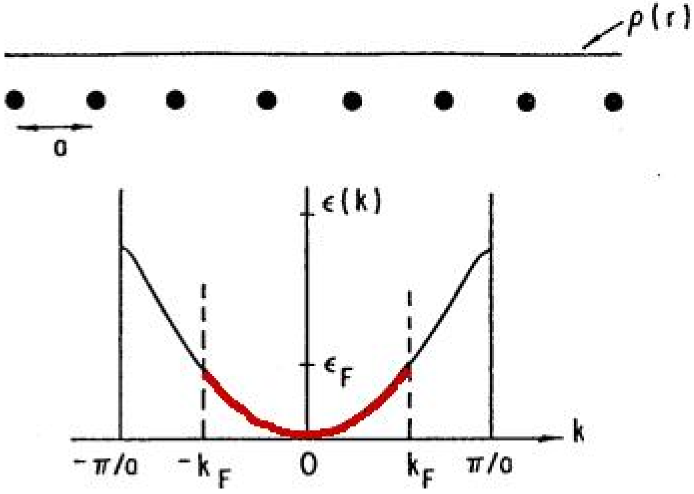
4.3 准一维体系的Peierls不稳定性和电荷密度波

1. 一维体系

导电聚合物、金属卤化物、KCP晶体、过渡金属三硫化合物、电荷转移有机复合物、有机超导体Bechgaard盐(TMTSF)$_2$X，有机铁磁体m-PDPC，半导体纳米线或量子线...

2. 一维晶格的能带和布里渊区

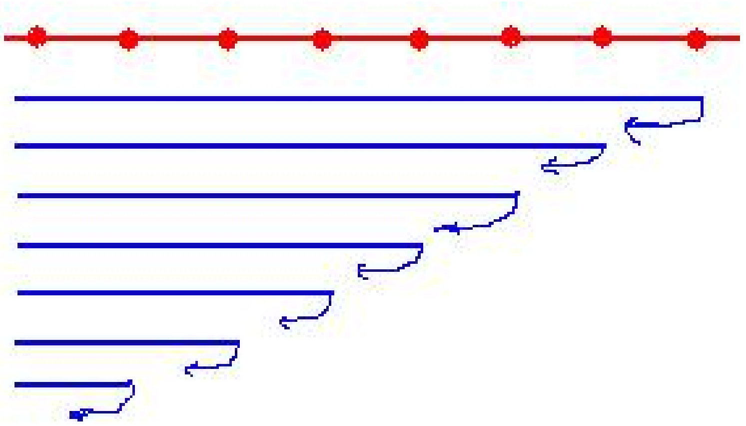
- •constant charge distribution
- •parabolic energy bands
- •filled up to the Fermi wavevector
- •metallic conductivity



$$E_0(\vec{k}) = \frac{\hbar^2}{2m}k^2 \qquad k_F = \frac{n}{4} = \frac{1}{4a}$$

格点原子对电子的散射（电一声相互作用）：

波长为$\lambda=\frac{1}{k}$的电子在一维晶格中传播，受格点反射，相邻两格点反射波位相差为：



$$\Delta\varphi=\frac{\Delta l}{\lambda}\cdot 2\pi=\frac{2a}{\lambda}\cdot 2\pi$$

如$\lambda >> 2a$(长波),$\Delta\varphi$很小，原入射电子波基本不因晶格原子的反射而衰减

→能谱接近自由电子能谱

动量增加，$\Delta\varphi$不断增加，各反射波之间不能完全抵消，晶格原子对电子波传播产生影响，$E(\vec{k})$偏离$E_0(\vec{k})$

$\lambda=2a,\Delta\varphi=2\pi\rightarrow$波长为$\lambda=2a$的电子波不能继续传播，

对应动量：$k_B=\frac{1}{\lambda}=\frac{1}{2a}$

电子的能谱$E(k)$在k_B上发生跳跃，出现能隙

同理，$\Delta\varphi=2n\pi,k_B^{(n)}=\frac{n}{2a}\quad(n=\pm1,\pm2,\pm3...)$ 也有能隙

费米动量k_F与晶格常数a无关，由电子密度决定。

$k_B^{(n)}$由晶格常数决定。

3. Peierls不稳定性

对于半满能带的一维晶格，等距离的原子排列是不稳定的，要发生二聚化，晶格周期变为2a. 此时布里渊区边界与费米面重合，电子能量降低，系统更稳定。

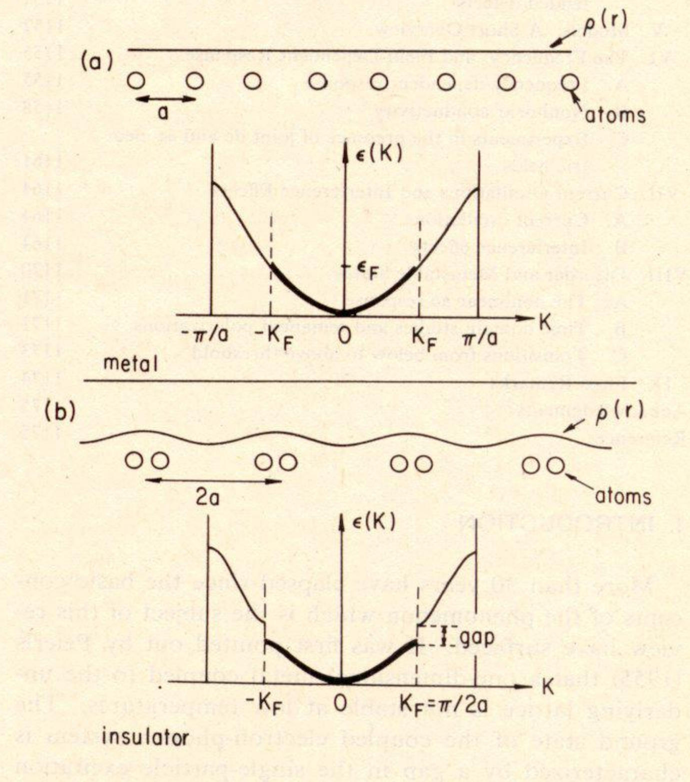
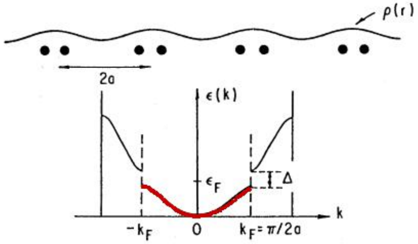


FIG. 1. Peierls distortion in a one-dimensional metal with a half-filled band: (a) undistorted metal; (b) Peierls insulator.

低温下，一维体系处于二聚化的半导体或绝缘体状态，不导电。温度升高，电子获得热能，费米面上的能隙消失，一维体系变成导体，Peierls相变。

4. 电荷密度波(CDW)

一维体系发生Peierls相变后，晶格周期由a变为a’，形变后周期为a’的晶格称之为超晶格。电子密度在这一新的周期场中重新分布，称为CDW，波长＝a’．



$$\rho(x) = n + n_c \cos(2\pi \frac{x}{\lambda} + \varphi)$$

n_c为密度起伏的幅度，φ是初位相。新的布里渊区边界为：

$$k_B^{'} = \frac{1}{2a^{'}}$$

Peierls 不稳定性要求：$k_B^{'} = k_F$

$$a^{'} = \frac{1}{2k_F} = \frac{2}{n} \text{或} \lambda = \frac{2}{n}$$

λ(或$a^{'}$)与a无关，只决定于电子的费米动量或电子密度。

(1). $\frac{a^{'}}{a}$ = 有理数，相变后的晶格在整体上仍具有周期性，叫可公度相变

(2). $\frac{a^{'}}{a}$ = 无理数，相变后的晶格无周期性，叫非公度相变

CDW state

spatially modulated charge density
energy gap at the Fermi energy

semiconducting conductivity

考虑电子之间的相互作用，需计入电子的自旋，正负自旋电子的CDW位形可以不同， $\varphi_\uparrow \neq \varphi_\downarrow$ 。此时将会导致体系中出现自旋密度的起伏，即自旋密度波(SDW).

$$\rho_\uparrow(x) = \frac{n}{2} + \frac{n_c}{2}\cos(2\pi\frac{x}{\lambda} + \varphi_\uparrow)$$

$$\rho_\downarrow(x) = \frac{n}{2} + \frac{n_c}{2}\cos(2\pi\frac{x}{\lambda} + \varphi_\downarrow)$$

总的CDW和SDW：

$$\rho(x) = \rho_\uparrow(x) + \rho_\downarrow(x) = n + n_c\cos(\frac{\varphi_\uparrow - \varphi_\downarrow}{2})\cos(2\pi\frac{x}{\lambda} + \frac{\varphi_\uparrow + \varphi_\downarrow}{2})$$

$$S(x) = \rho_\uparrow(x) - \rho_\downarrow(x) = \frac{n_c}{2}\sin(\frac{\varphi_\uparrow - \varphi_\downarrow}{2})\cos(2\pi\frac{x}{\lambda} + \frac{\varphi_\uparrow + \varphi_\downarrow - \pi}{2})$$

如$\varphi_\uparrow = \varphi_\downarrow$，体系只有$CDW$而无$SDW$

如$\varphi_\uparrow = \varphi_\downarrow + \pi$，体系只有$SDW$而无$CDW$

不仅一维电子－晶格相互作用体系会出现CDW,其他体系也会存在