Electronic states of two-dimensional systems around an impurity in a strong magnetic field

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§1. Experiment

Scanning tunneling spectroscopy (STS) of graphite surface

Localized bound states below each Landau levels

What do we see?

§2. Calculation of bound states

Systems with parabolic dispersion and linear dispersion

Bound states around an impurity

§3. LDOS

Calculate LDOS and compare with experiment

§1. Experiment

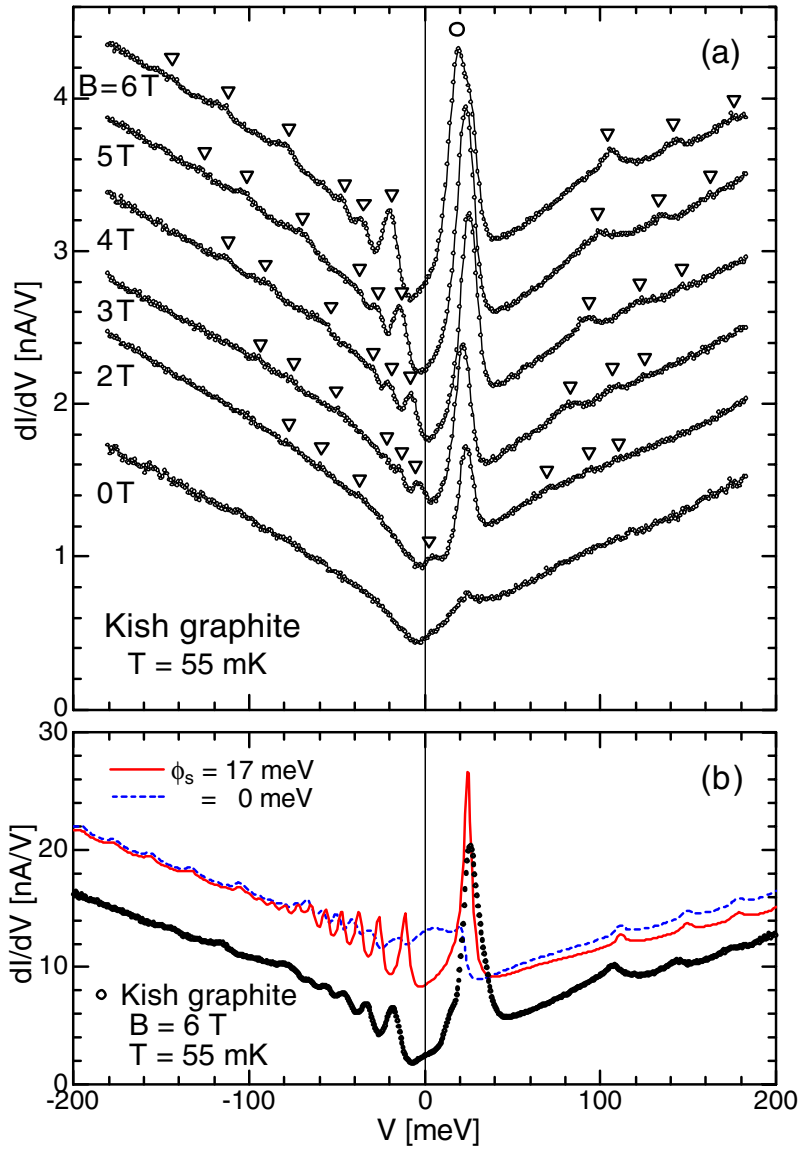
Experiments by Hiroshi Fukuyama's group at Univ. of Tokyo

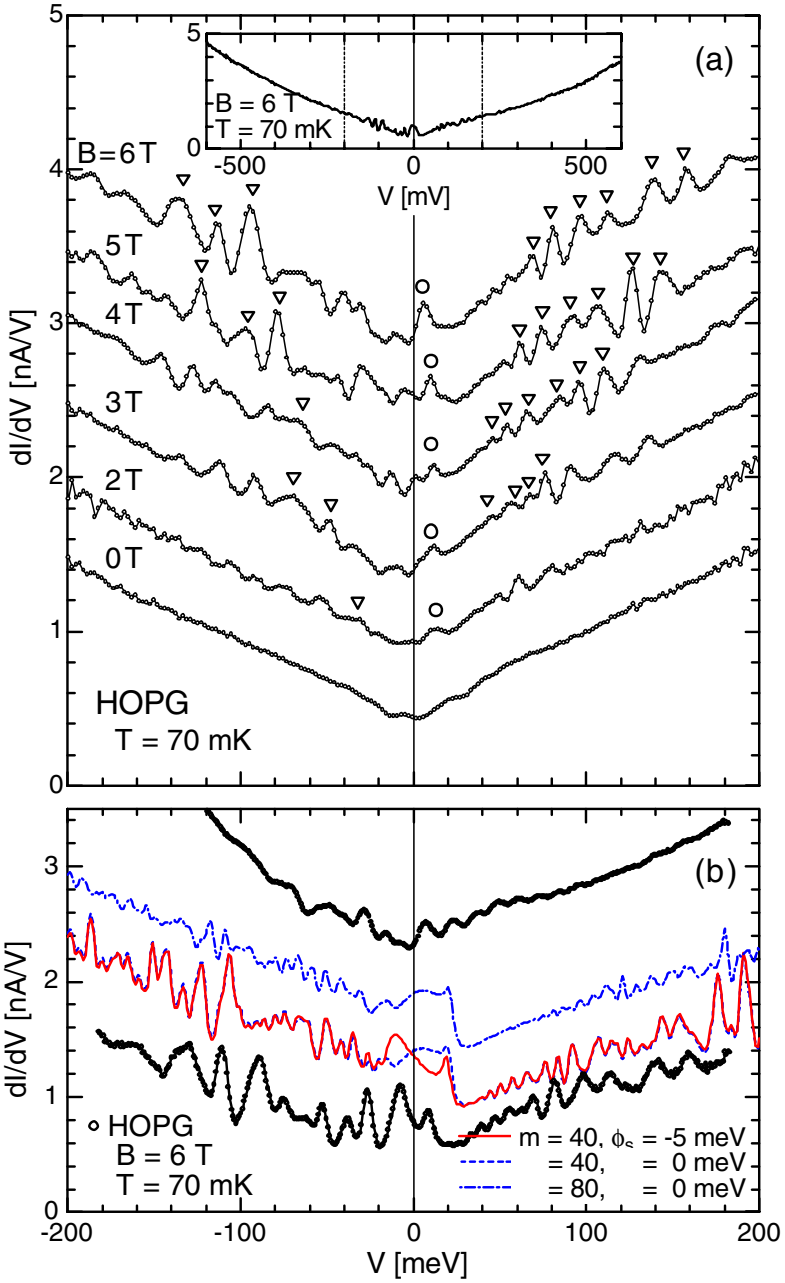
Material: HOPG graphite

Method: STS at low temperature in a strong magnetic field

T. Matsui et al., Phys. Rev Lett. 96 (2005) 226403

- **Observation of 2-d Landau levels for HOPG graphite**
- **3-d behavior for Kish graphite**
  - **HOPG has many stacking faults**
  - **Surface states of HOPG graphite is a 2-dimensional system**


(a)
B=6T
5T
4T
3T
2T
0T
Kish graphite
T = 55 mK
dI/dV [nA/V]
(b)
ϕ_s = 17 meV
= 0 meV
Kish graphite
B = 6 T
T = 55 mK
V [meV]


(a)
B = 6 T
T = 70 mK
V [mV]
B=6T
5T
4T
3T
2T
0T
HOPG
T = 70 mK
dI/dV [nA/V]
(b)
HOPG
B = 6 T
T = 70 mK
m = 40, ϕ_s = -5 meV
= 40, = 0 meV
= 80, = 0 meV
V [meV]

Y. Niimi et al., Phys. Rev. Lett. 97 (2006) 236804

Observation of localized states around impurities

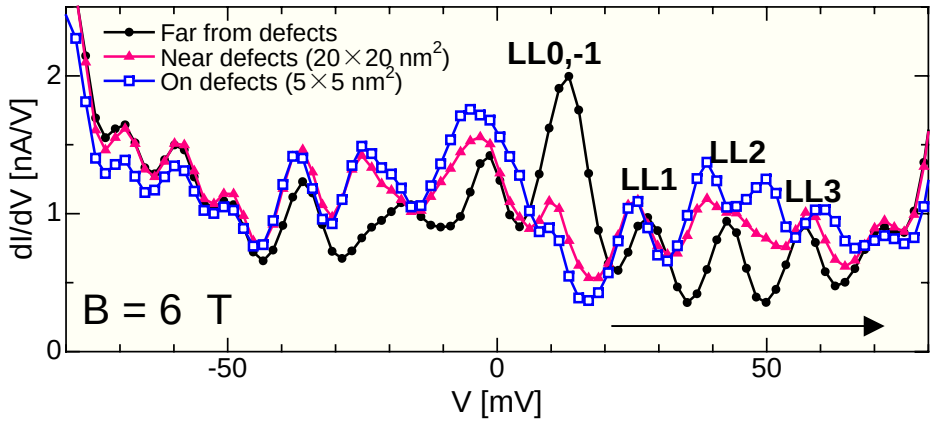
Bound states are formed below each Landau levels

They appear as bright spots at energy between Landau levels

How do we understand these spots?

What determines the shape of the spot, and what we learn from the shape?

欠陥付近におけるdI/dV像のエネルギー依存性 (6 T)

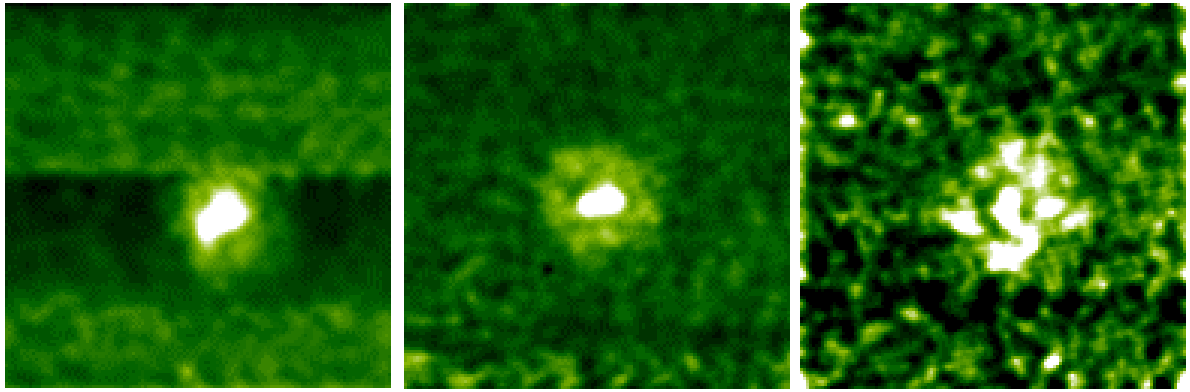


80 nm × 80 nm

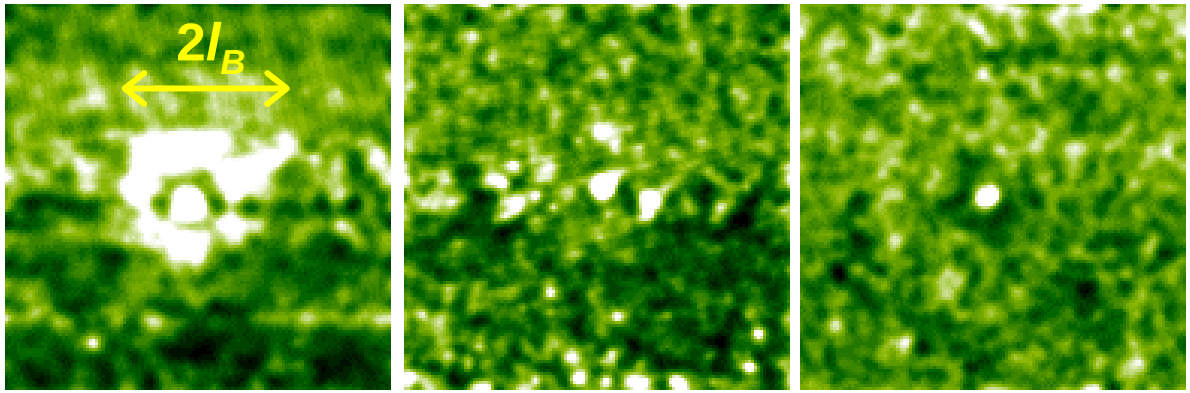
T = 30 mK

＊全てのdI/dV像に同じコントラストを適用

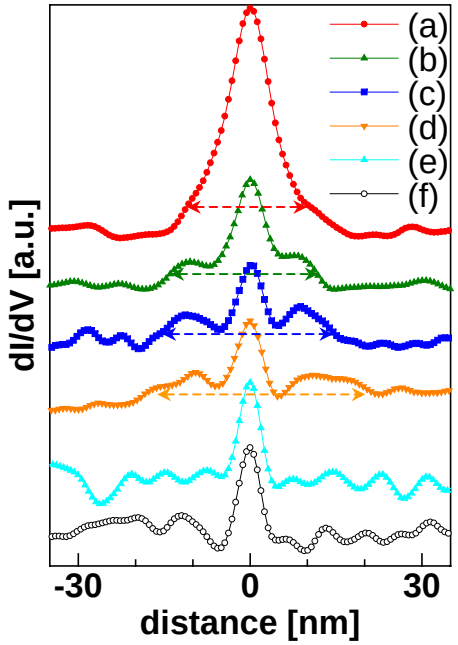
欠陥付近におけるdI/dV像の磁場依存性 (LL1-LL2)

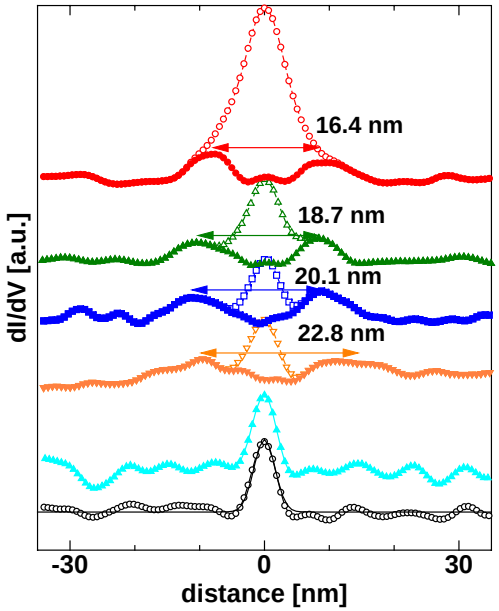


6 T 36 meV　4 T 32 meV　3 T 30 meV



2 T 28 meV　1 T 26 meV　0 T 25 meV

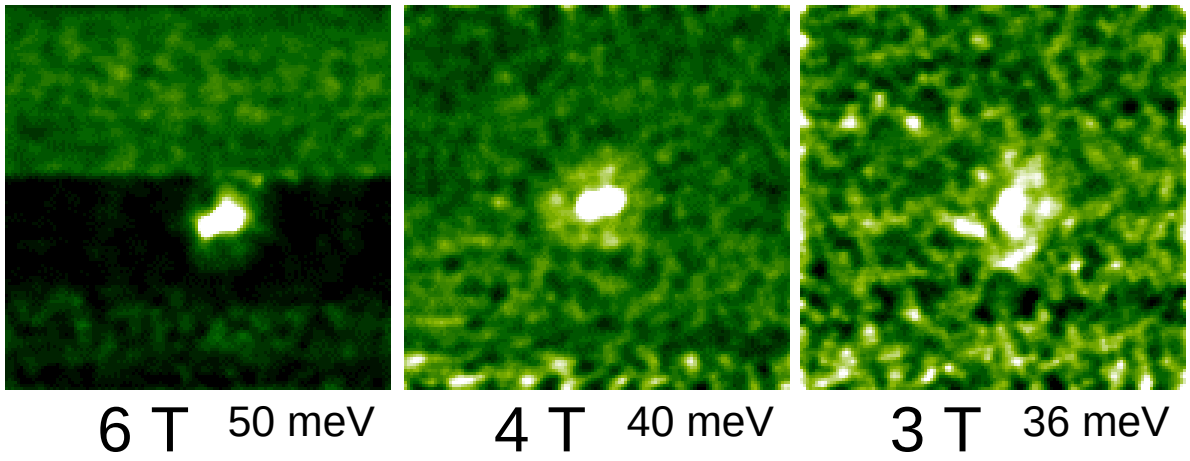




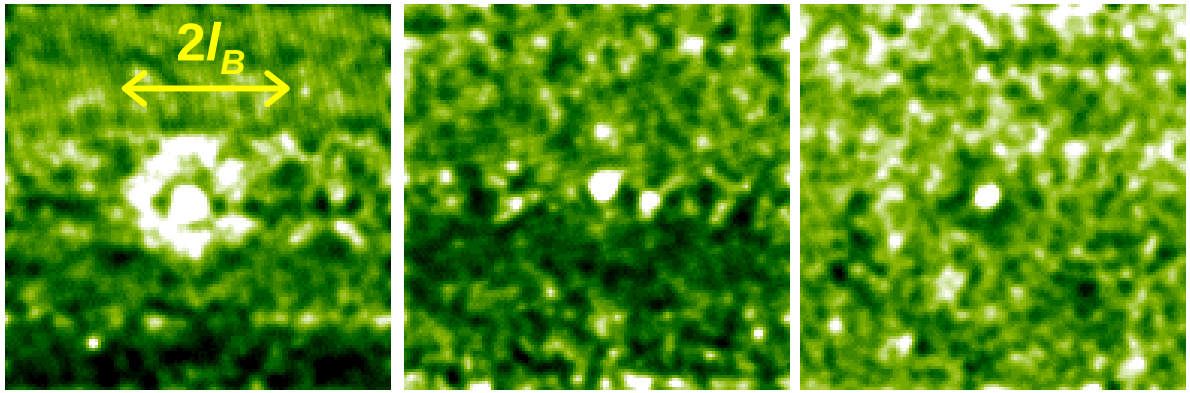
80 nm × 80 nm, T = 30 mK

16384 pts, V = 178 mV, I = 0.2 nA, V_{mod} = 1 mV

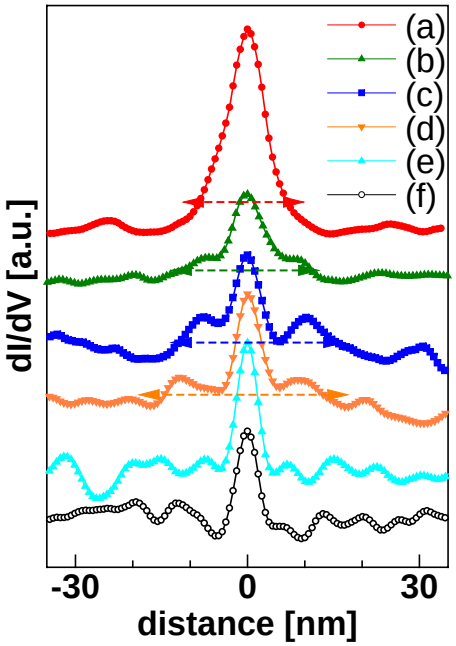
欠陥付近におけるdI/dV像の磁場依存性 (LL2-LL3)

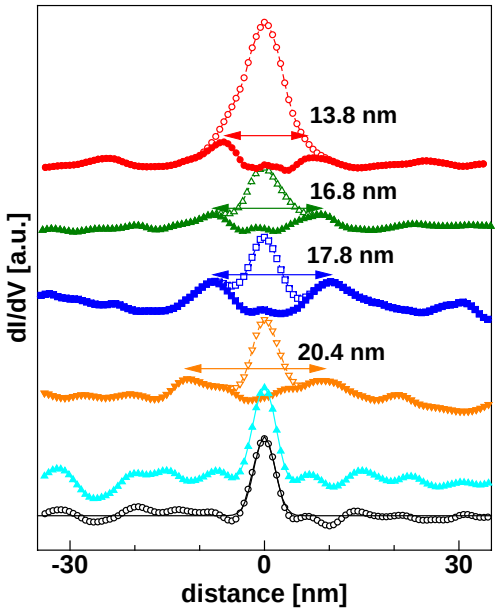


6 T 50 meV　4 T 40 meV　3 T 36 meV



2 T 33 meV　1 T 30 meV　0 T 27 meV





80 nm × 80 nm, *T* = 30 mK

16384 pts, V = 178 mV, I = 0.2 nA, V_{mod} = 1 mV

§2. Calculation of bound states

Calculate bound states around an impurity

in a strong magnetic field

2-d system with

$$\begin{cases} \text{parabolic dispersion} \\ \text{linear dispersion (graphene)} \end{cases}$$

for impurity potential of

$$\begin{cases} \propto 1/r \\ \propto 1/\sqrt{r^2+d^2} \\ \propto r^2 \end{cases}$$

§§2-1. 2-d system with parabolic dispersion

Bound state in an impurity potenital $V(r)$ at the origin

$$H = \frac{1}{2m_{\mathrm{e}}}\left(\pi_x^2 + \pi_y^2\right) + V(r)$$

ladder operator

$$a^\dagger = \frac{l_{\mathrm{B}}}{\sqrt{2}\hbar}\left(\pi_x + \mathrm{i}\pi_y\right) , \quad a = \frac{l_{\mathrm{B}}}{\sqrt{2}\hbar}\left(\pi_x - \mathrm{i}\pi_y\right)$$

$$b^\dagger = \frac{1}{\sqrt{2}l_{\mathrm{B}}}\left(X - \mathrm{i}Y\right) , \quad b = \frac{1}{\sqrt{2}l_{\mathrm{B}}}\left(X + \mathrm{i}Y\right)$$

Eigenstats $|n, m\rangle$:

$$a^\dagger a|n, m\rangle = n|n, m\rangle , \quad b^\dagger b|n, m\rangle = m|n, m\rangle$$

Diagonalize the Hamiltonian using these states as bases

(In these equations, $\boldsymbol{\pi} = \boldsymbol{p} - e\boldsymbol{A}$, $(X, Y) = \boldsymbol{r} + \frac{l_{\mathrm{B}}^2}{\hbar}(-\pi_y, \pi_x)$)

For isotropic potential such as $V(r) \propto 1/r$, $1/\sqrt{r^2+d^2}$, r^2

- **angular momentum $L_z = (n-m)\hbar$ is conserved**
- **degeneracy with respect to m is lifted**

L_z of the lowest energy state each Landau level n:

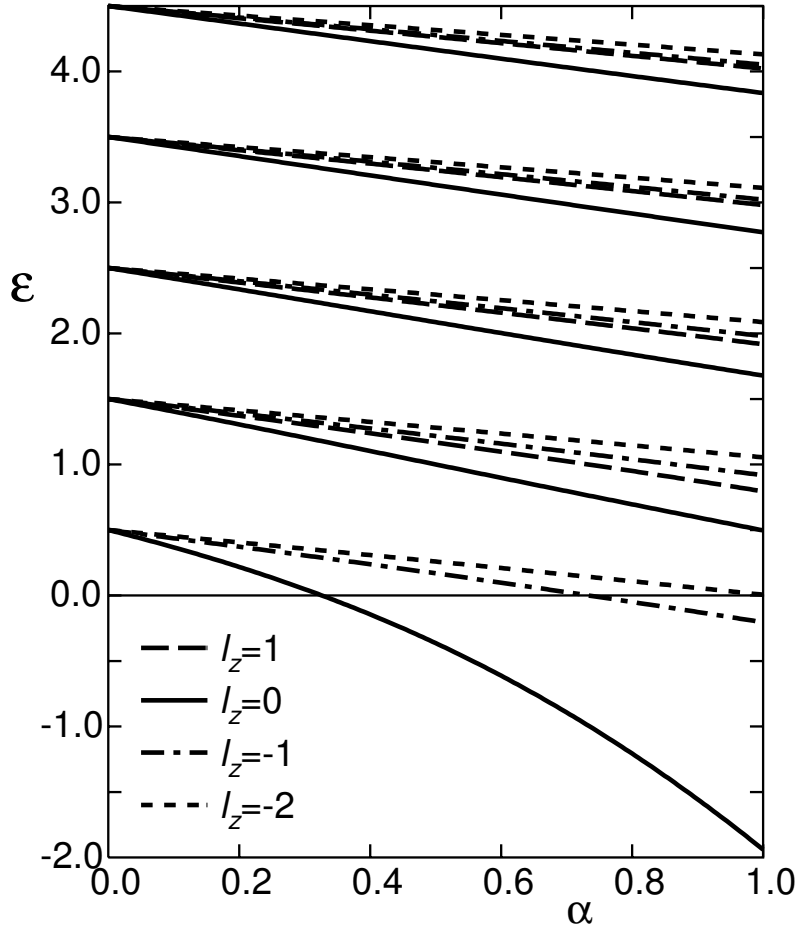
for $V(r) \propto 1/r$, $L_z = 0$, i.e. $n = m$ is the lowest energy state

for $V(r) \propto r^2$, $m = 0$, $L_z = n\hbar$ is the lowest energy state

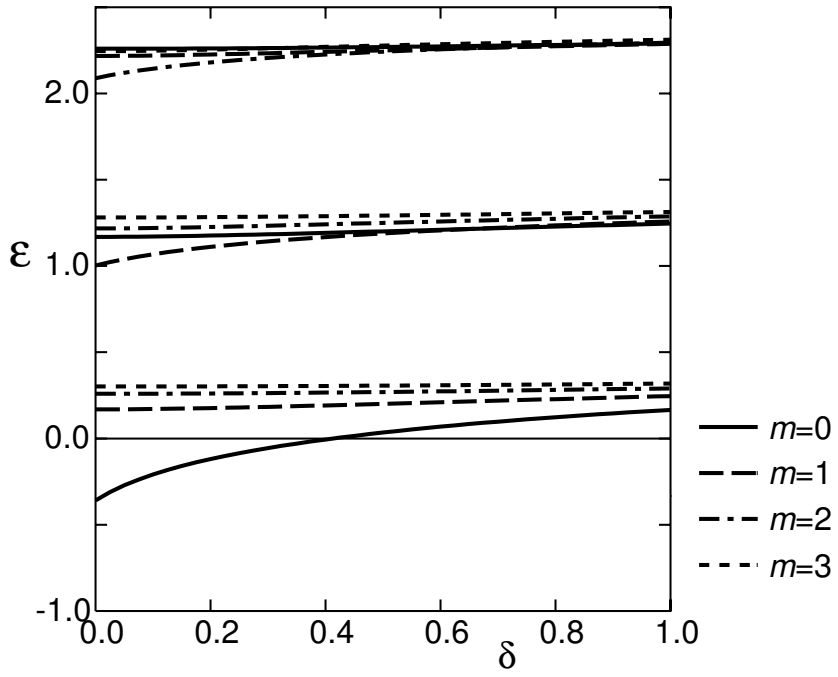
For $V(r) \propto 1/r$, the wavefunction with $L_z = 0$ has a cusp at the origin

Dependence on potential strength and potential range

$V(r) = \hbar\omega_c\alpha/\sqrt{\xi^2+\delta^2}$, $\xi = r/l_{\rm B}$, $\delta = d/l_{\rm B}$



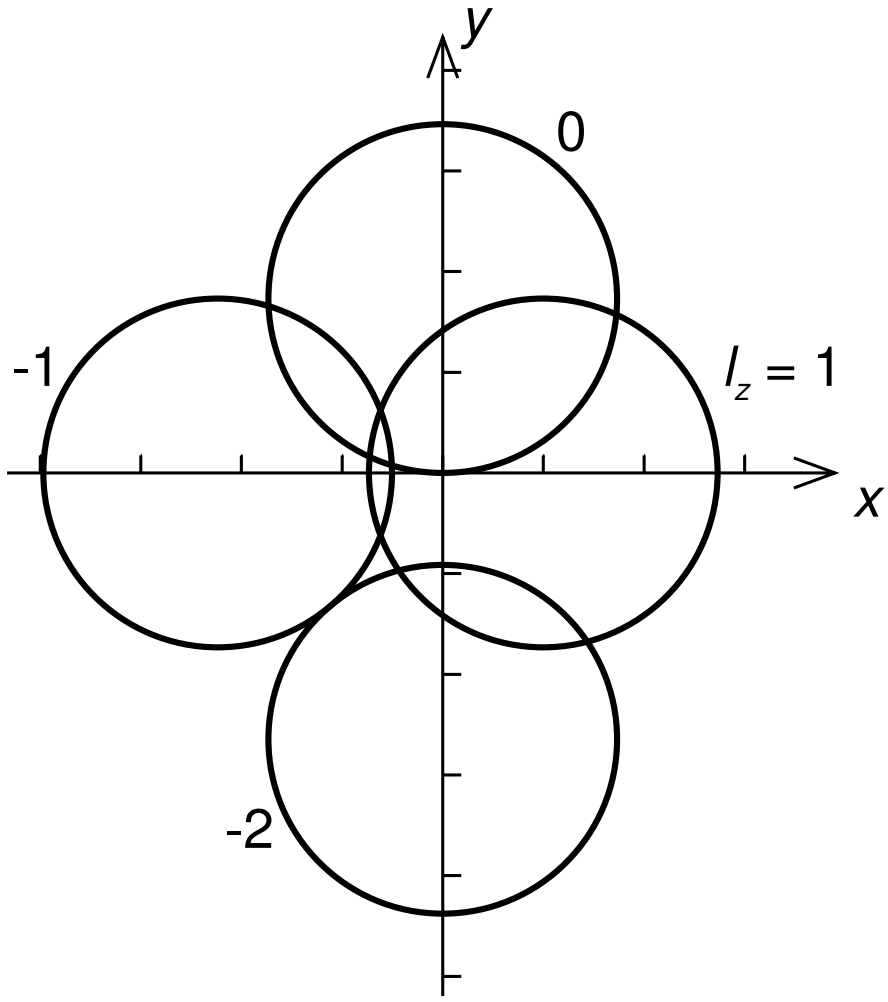
α **dependence at** $\delta = 0$



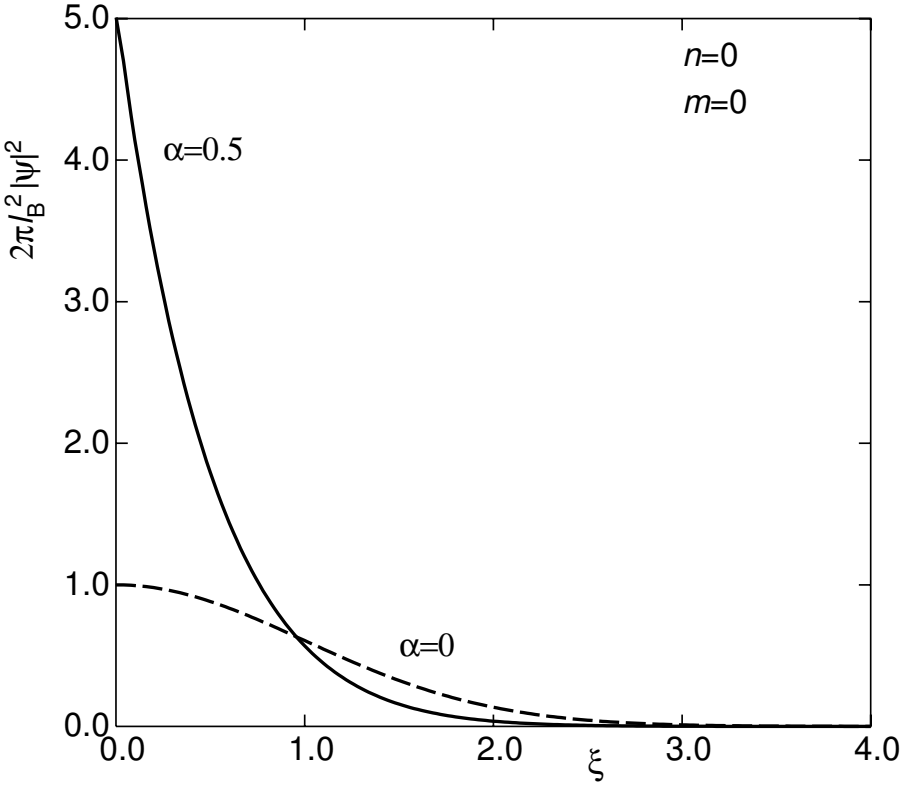
δ **dependence at** $\alpha = 0.5$

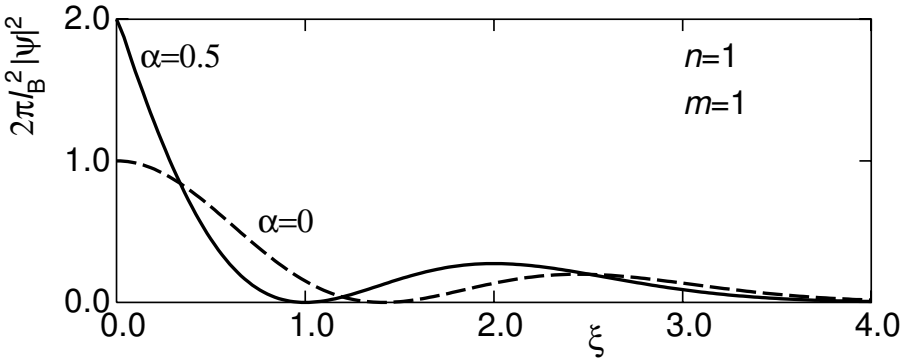
Explanation of the energy sequence by a classical picture

Classical orbits for states with $n = 1$, and $m = 0, 1, 2, 3$.



Cusp at the origin





$$|\psi_{n,n}(r,\theta)|^2 \simeq |\psi_{n,n}(0,\theta)|^2(1-4\alpha\frac{r}{l_{\rm B}}) \quad \textbf{for} \quad V(r)=\frac{\hbar\omega_c\alpha l_{\rm B}}{r}$$

§§2-2. 2-d system with linear dispersion

Graphene has k-linear spectrum around two equivalent points K and K'. (massless Dirac fermion)

$\boldsymbol{\kappa}$: momentum from K or K'

In the absence of impurity potential

$$H_0 = \frac{\gamma}{\hbar}\begin{pmatrix} 0 & \kappa_x + \mathrm{i}\kappa_y \\ \kappa_x - \mathrm{i}\kappa_y & 0 \end{pmatrix}$$

In the presence of magnetic field, we replace $\boldsymbol{\kappa}$ with $\boldsymbol{\pi}$, which can be rewritten with ladder operator a, $a^\dagger$:

$$H_0 = \frac{\sqrt{2}\gamma}{l_\mathrm{B}}\begin{pmatrix} 0 & a^\dagger \\ a & 0 \end{pmatrix}$$

Energy and eigenstates are given by eigenstates of ordinary 2-d system.

For $n < 0$, $n = 0$, and $n > 0$

$$E_{n,m} = \frac{\sqrt{-2n}\gamma}{l_{\rm B}}\,, \quad \psi_{n,m} = \frac{1}{\sqrt{2}} \begin{pmatrix} -|-n-1,m\rangle \\ |-n,m\rangle \end{pmatrix}\,, \quad (n<0)$$

$$E_{n,m} = 0\,, \quad \psi_{0,m} = \begin{pmatrix} 0 \\ |0,m\rangle \end{pmatrix}\,, \quad (n=0)$$

$$E_{n,m} = \frac{\sqrt{2n}\gamma}{l_{\rm B}}\,, \quad \psi_{n,m} = \frac{1}{\sqrt{2}} \begin{pmatrix} |n-1,m\rangle \\ |n,m\rangle \end{pmatrix}\,, \quad (n>0)$$

In the presence of impurity potential, we diagonalize the Hamiltonian using these states as bases.

Bound states around an impurity

- **We neglect mixing between K and K' for $1/r$-potential**
- **Two states with $L_z = -\hbar$ and $L_z = 0$ has non-zero amplitude at the origin.**

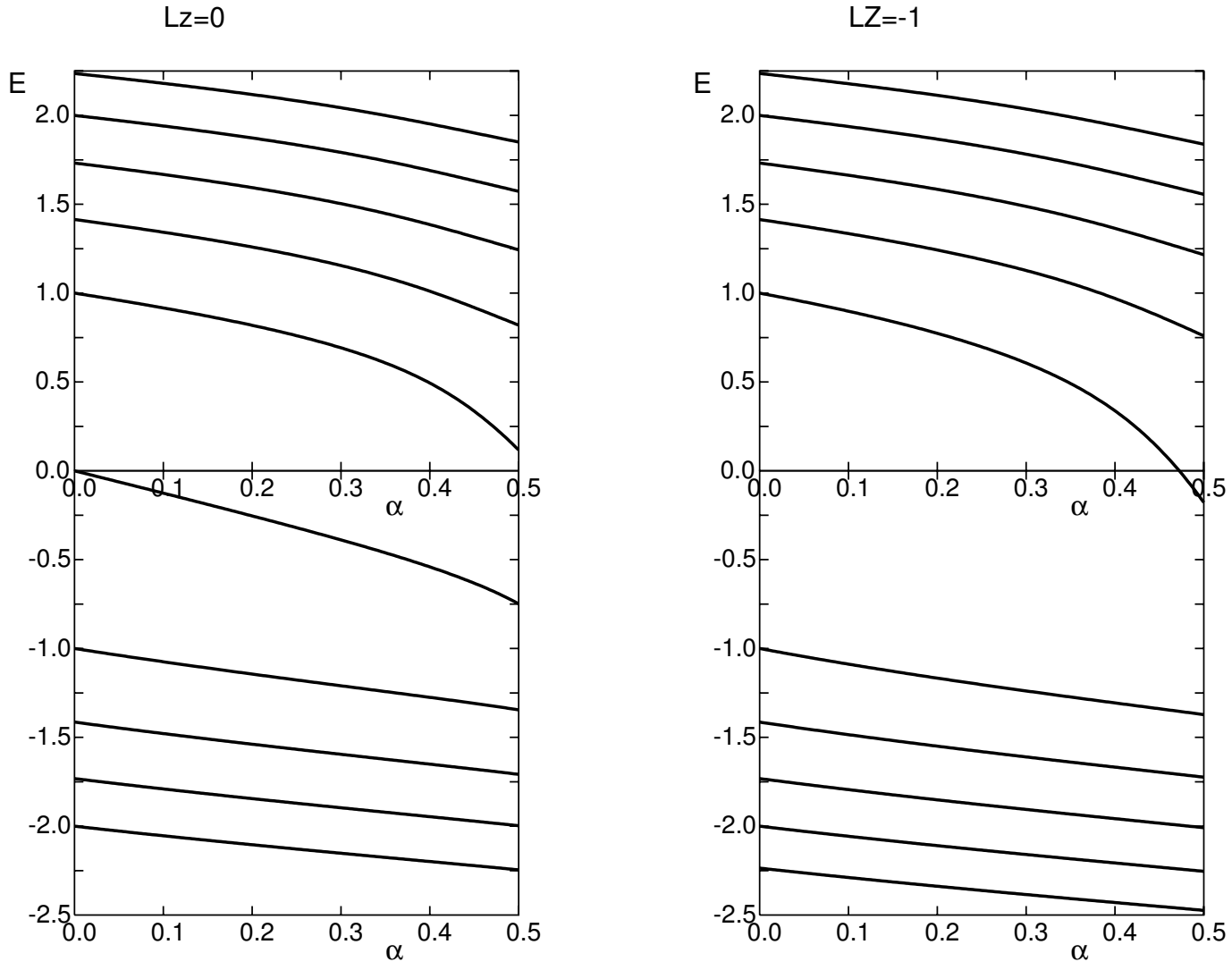
  remark:

  $L_z = (n-m)\hbar$ **for**

$$E_{n,m} = \frac{\sqrt{2n}\gamma}{l_{\mathrm{B}}}, \quad \psi_{n,m} = \frac{1}{\sqrt{2}} \begin{pmatrix} |n-1,m\rangle \\ |n,m\rangle \end{pmatrix}, \quad (n > 0)$$

- **for $n \neq 0$, $L_z = -\hbar$ is the lowest energy state for each Landau level**

Bound state energy as a function of potential strength



Behavior around the origin

for $L_z = 0$ and -1, the wave function diverges at the origin

$$\psi(r,\theta) \propto r^{\delta}, \quad \delta = \sqrt{\frac{1}{4} - \frac{\eta^2}{\gamma^2}} - \frac{1}{2} < 0$$

where

$$\eta = \frac{e^2}{4\pi\epsilon}, \quad \textbf{i.e.} \quad V(r) = \frac{\eta}{r}$$

for strong attraction, $\eta > \gamma/2$, the wave function diverges with oscillation.

cf. $\psi(r,\theta) \propto (1 - 2\alpha r/l_{\mathrm{B}})$ **for the parabolic case**

§3. Local Density of States (LDOS)

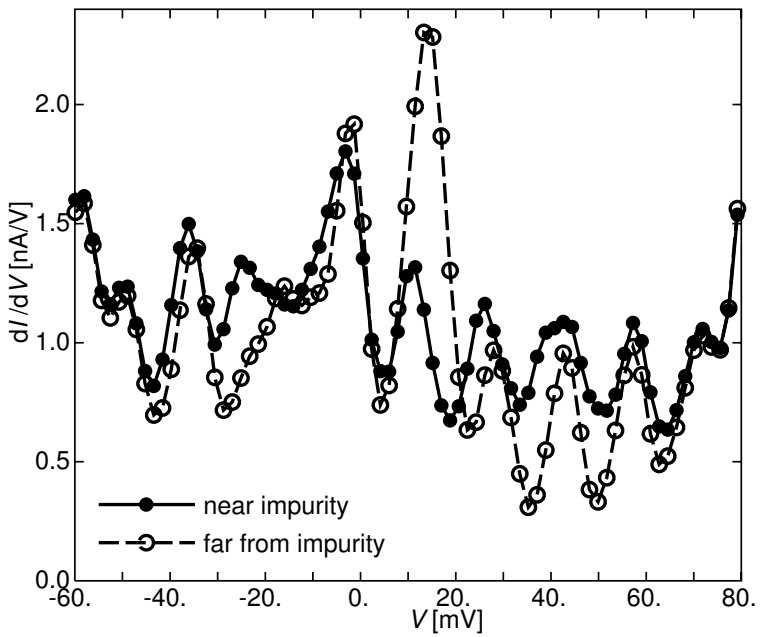
LDOS is observed by STS

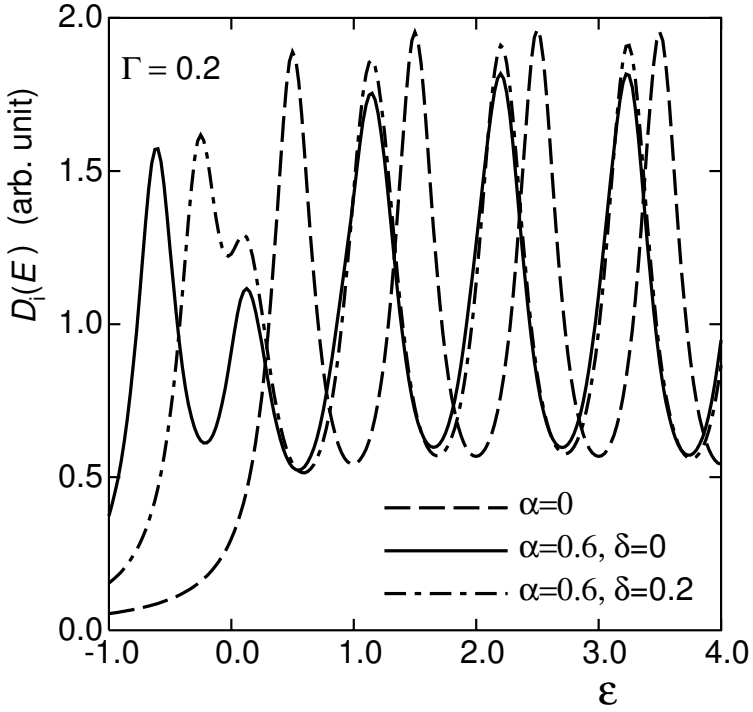
It is calculated by the following equation

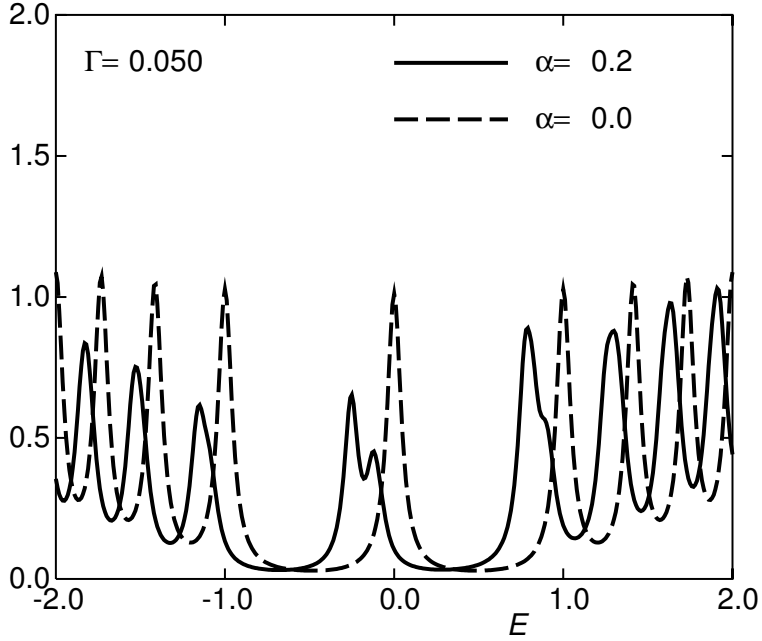
$$D(E, \boldsymbol{r}) = \frac{1}{\pi} \sum_n \sum_m \frac{\Gamma}{(E - E_{n,m})^2 + \Gamma^2} \left| \psi_{n,m}(\boldsymbol{r}) \right|^2 , \tag{1}$$

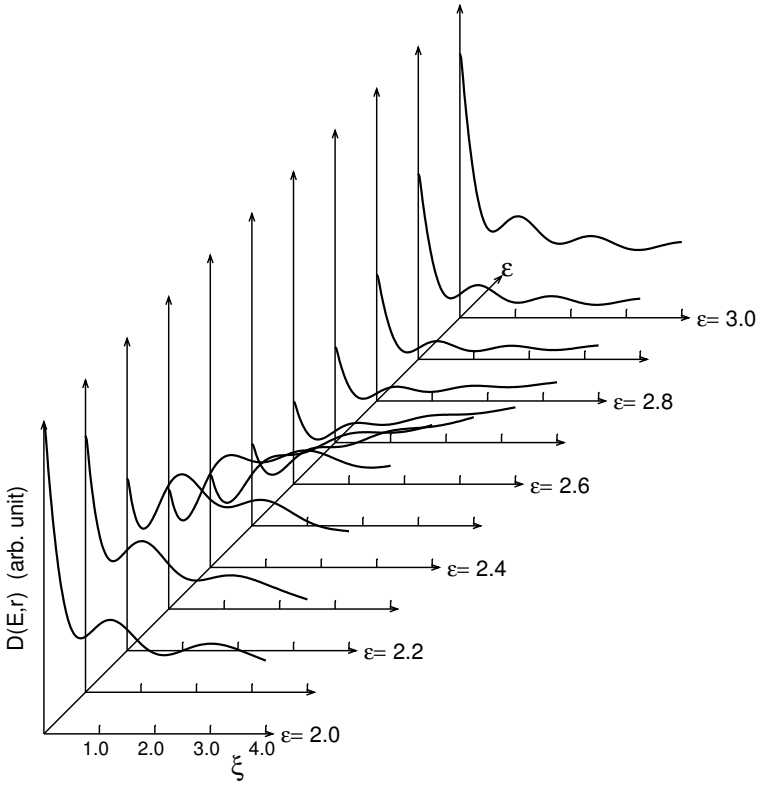
Γ is a parameter for the level broadening.

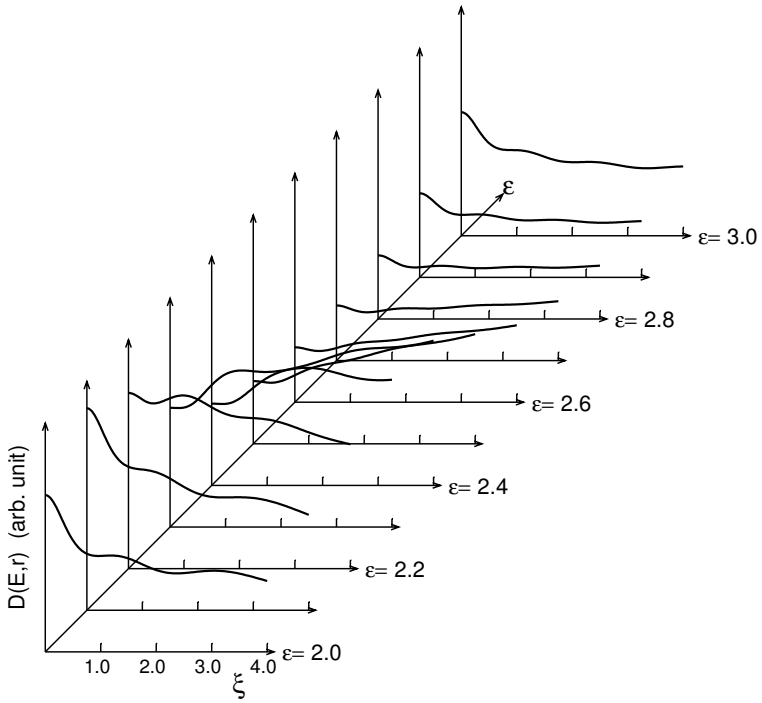
It is determined by comparison with experiment

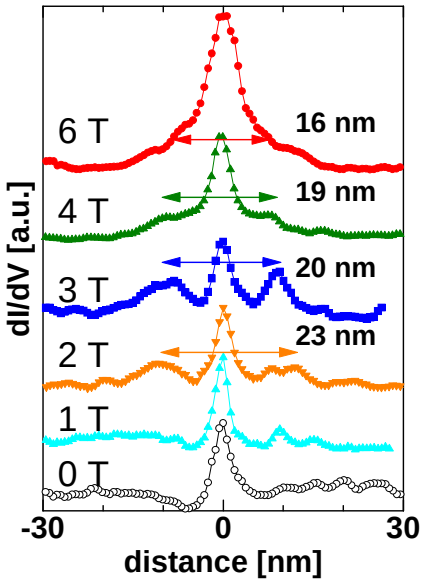

dI/dV [nA/V]
V [mV]
near impurity
far from impurity


Γ = 0.2
D_l(E) (arb. unit)
ε
α=0
α=0.6, δ=0
α=0.6, δ=0.2


Γ= 0.050
α= 0.2
α= 0.0
E



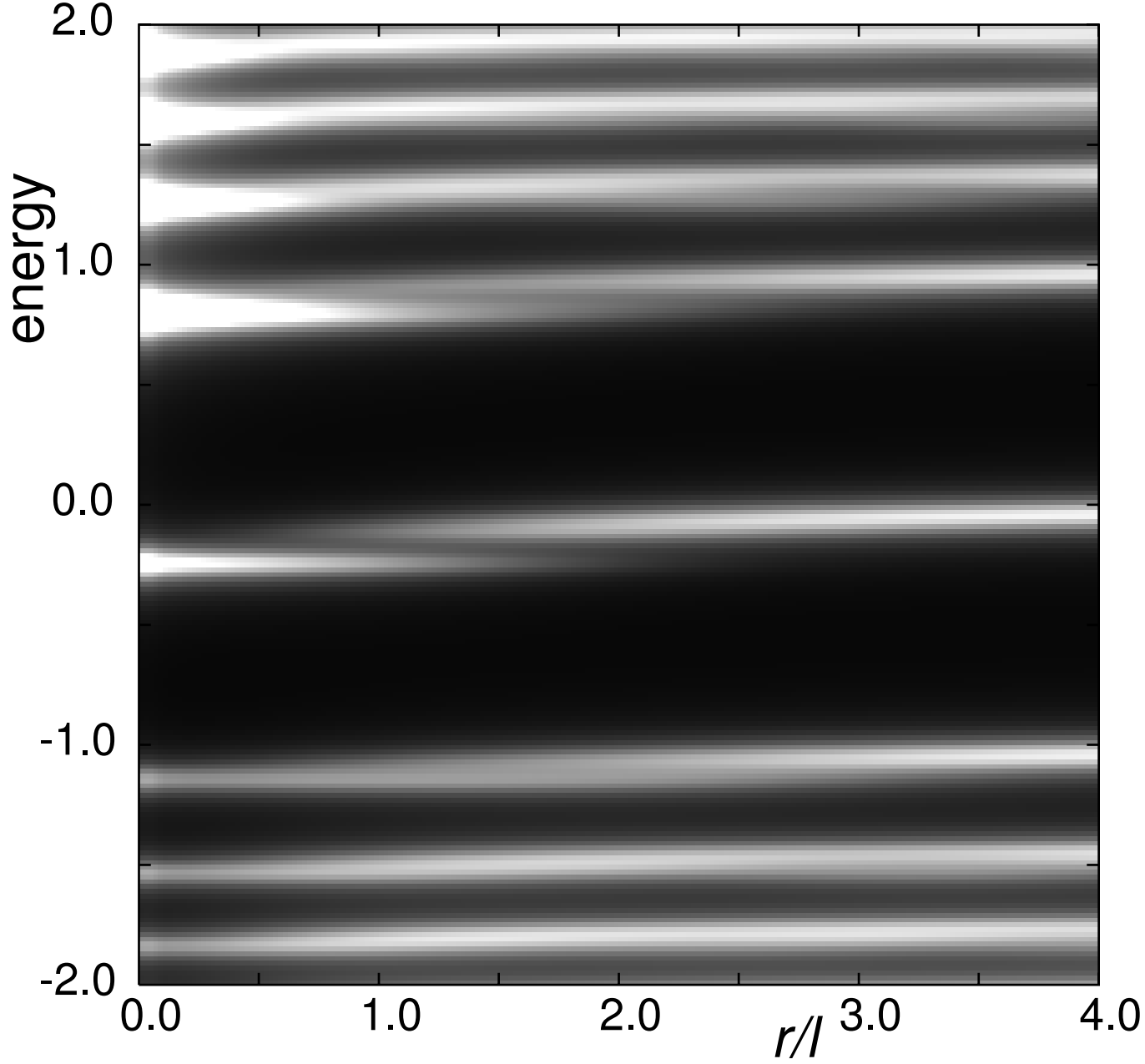


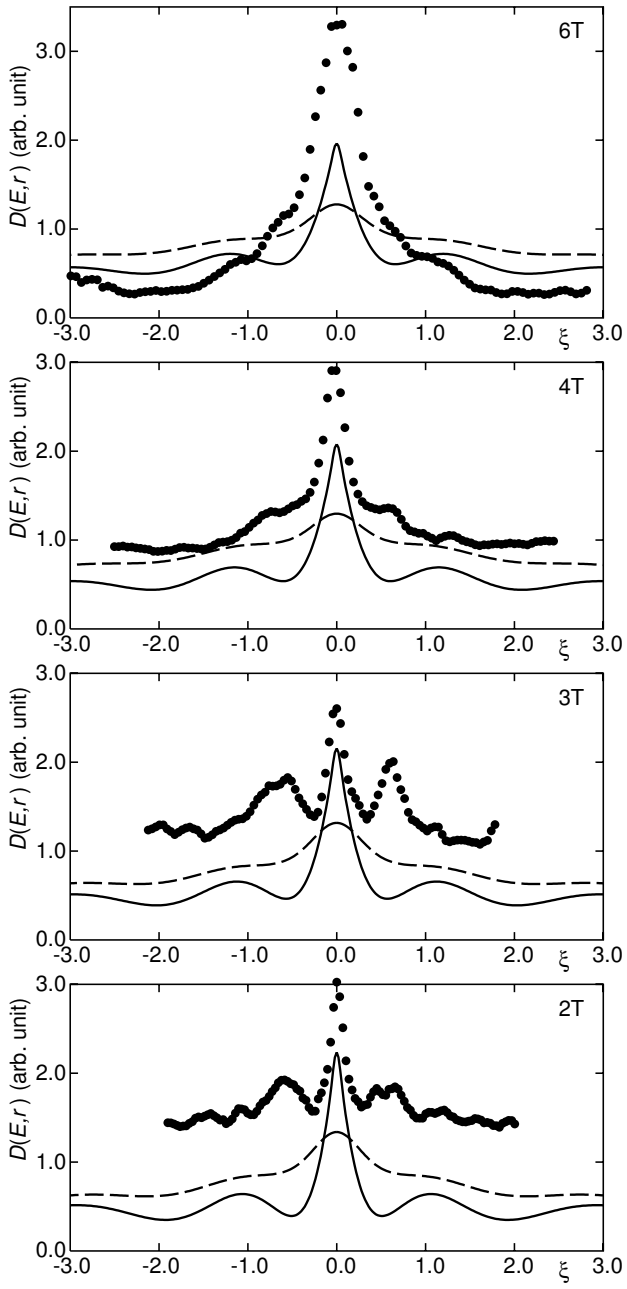


Left: $V(r) \propto 1/r$**, right:** $V(r) \propto 1/\sqrt{r^2 + d^2}$

Sharp peak, clear side peak are seen only for $1/r$ **potential**

$V(r) \propto 1/r$ **reproduces the experiment well**


2.0
1.0
0.0
-1.0
-2.0
energy
0.0
1.0
2.0
3.0
4.0
r/l


6T
4T
3T
2T
D(E,r) (arb. unit)
ξ
0.0
1.0
2.0
3.0
-3.0
-2.0
-1.0
0.0
1.0
2.0
3.0

§4. Summary

- **At the surface of HOPG graphite, 2-d electron systems are realized**
- **Bound states are formed around impurities**
- **Impurity potential is deduced to be $\propto 1/r$**
- **Calculated LDOS for the two systems (parabolic and linear) are similar for the electron band ($E > 0$)**
- **There is no peak of the LDOS in the hole band.**
- **Experiment on graphene is underway, and we are expecting to see the result in near future**