

Ferromagnetism and superconductivity in artificial crystals

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Overview

1. Artificial crystals designed in dot arrays

- Quantum dot system (Artificial atom, molecule, crystal)
- Design of Lieb and kagome lattices having flat-band
- Advantages of using dot arrays for flat-band system

2. Flat-band ferromagnetism in quantum dot arrays

- Stability of ferromagnetism in dot arrays
- Kagome lattice designed in quantum wire network

3. Sample structures

4. Superconductivity on a plaquette lattice

5. Summary

Artificial Material using Semiconductor Dots

Single dot

Atomic properties in an “artificial atom”

- Shell structure, Hund’s rule, and Kondo effect

Coupled dots

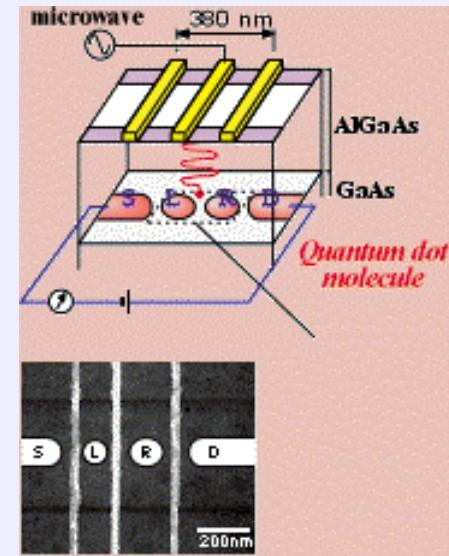
Molecular properties in an “artificial molecule”

- Bonding and anti-bonding level splitting

Dot arrays

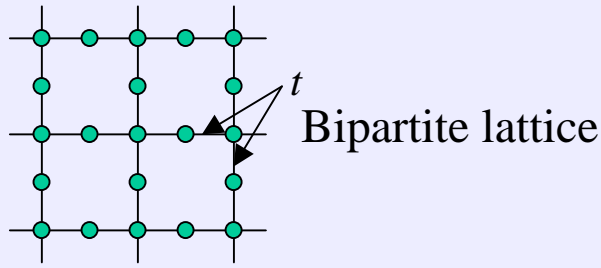
“Artificial crystals” by treating a dot as a building block

- Various lattice design
- Flat-band ferromagnetism
- Superconductivity

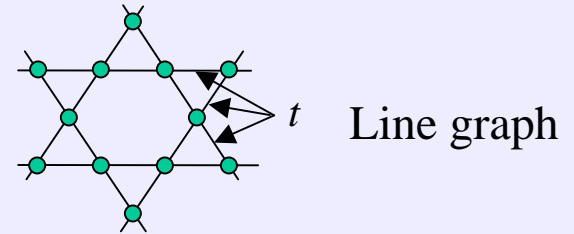


Lattice Structures having Flat-band

Lieb lattice

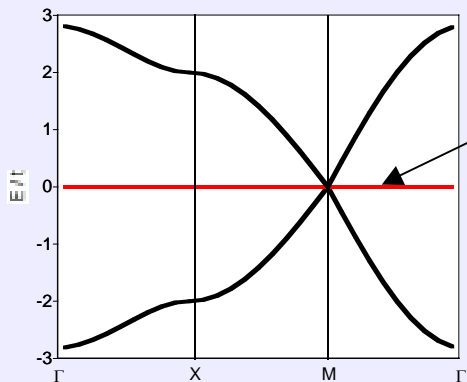


Kagome lattice



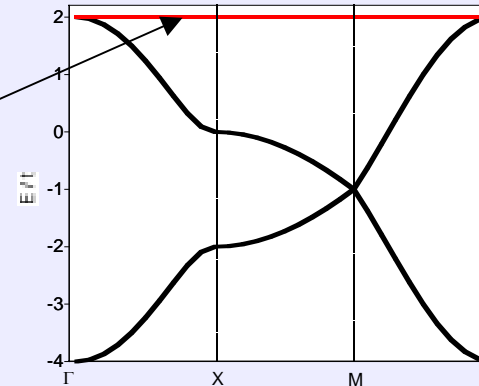
Single-particle band diagram

Tight-binding approximation



2D Lieb lattice

Flat-band



2D kagome lattice

Ferromagnetism appears when the flat band is half-filled.

Origin of Word “Kagome”

kago-me

kago (籠) = basket

me (目) = mesh (or pattern)



Basket



Flowers in basket

Search for Flat-band Ferromagnetism

Carbon network

Shima and Aoki, PRL **71**, 4389 ('93)

Fujita, Umeda, and Yoshida, PRB **51**, 13778 ('95)

Graphite sheet with edge (Nano graphite)

Fujita, Wakabayashi, Nakada, and Kusakabe, JPSJ **65**, 1920 ('96)

Kusakabe, Wakabayashi, Igami, Nakada, and Fujita, Mol. Cryst. Liq. Cryst. **305**, 445 ('97)

Ga or As atomic wire

Arita, Kuroki, Aoki, Yajima, Tsukada, Watanabe, Ichimaru, Onogi, and Hashizume, PRB **57**, R6854 ('98)

Yajima, Tsukada, Watanabe, Ichimura, Suwa, Onogi, and Hashizume, PRB **60**, 1456 ('99)

Okada and Oshiyama, JJAP **39**, 435 ('00)

Proposal for Flat-band Ferromagnetism in Dot Arrays

Tamura, Shiraishi, and Takayanagi, Jpn. J. Appl. Phys. **39** (2000) L241.

No clear evidence of flat-band ferromagnetism

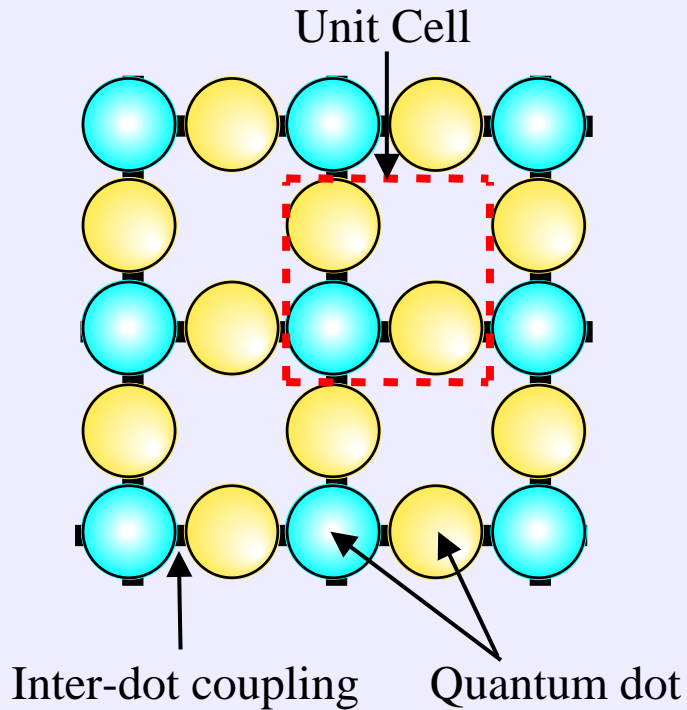
- Synthesis or fabrication is difficult.
- Filling cannot be freely changed.
- Jahn-Teller effect usually lifts flat-band degeneracy.

Possibility of flat-band ferromagnetism in dot arrays

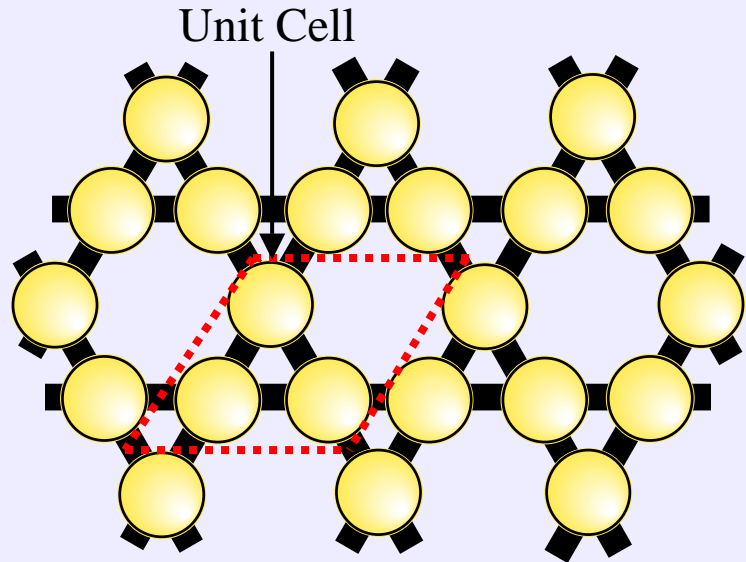
- Fabrication technology is well established.
- Various lattice designs are possible.
- Filling can be freely changed.
- No Jahn-Teller effect.

2D Lieb and Kagome Dot Arrays

Lieb lattice



Kagome lattice



Electrons transfer between nearest-neighboring dots

Hubbard Model for Dot Arrays

Hubbard Hamiltonian

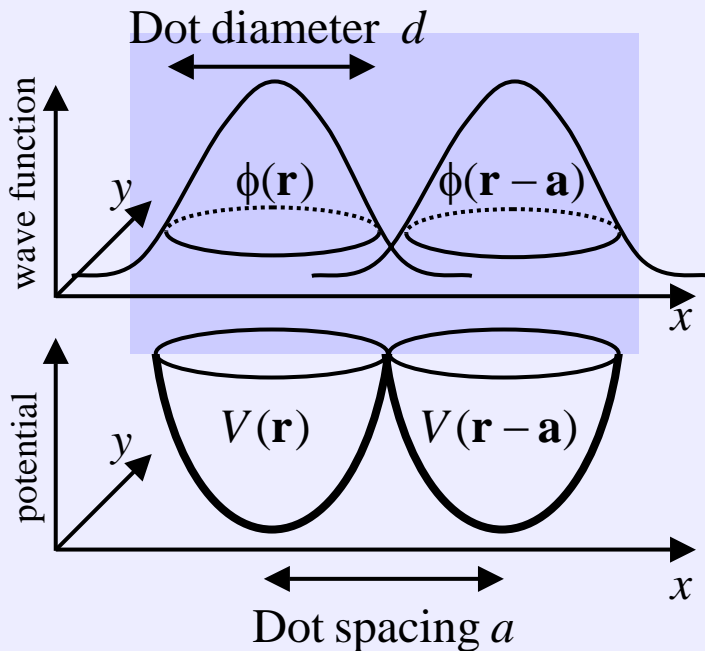
$$H = -t \sum_{(i,j),\sigma} c_{i\sigma}^+ c_{j\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow}$$

(i,j) is a pair of the nearest-neighbor sites

U is the on-site Coulomb repulsion

$$n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$$

Dot model in parabolic potentials



Parabolic potential

$$V(\mathbf{r}) = \frac{1}{2} m^* \omega^2 (r^2 - a^2)$$

Wave function

$$\phi(\mathbf{r}) = \frac{2}{\sqrt{\pi} d} e^{-\frac{2r^2}{d^2}}, \quad d \equiv 2 \sqrt{\frac{\hbar}{m^* \omega}}$$

Transfer integral

$$t = \int d\mathbf{r} \phi(\mathbf{r}) (H_0 + V(\mathbf{r})) \phi(\mathbf{r} - \mathbf{a}) = \hbar \omega \left(1 - \frac{7a^2}{2d^2} \right) e^{-\frac{a^2}{d^2}}$$

On-site Coulomb energy

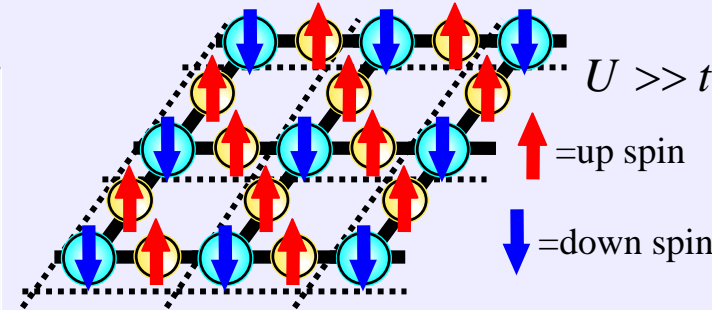
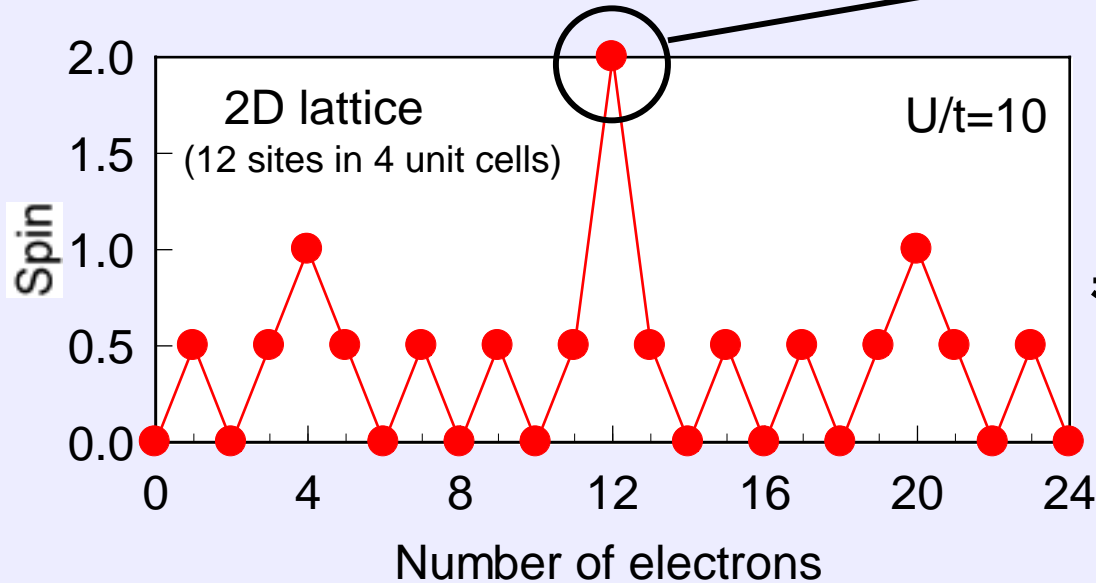
$$U = \iint d\mathbf{r}_1 d\mathbf{r}_2 \frac{|\phi(\mathbf{r}_1)|^2 |\phi(\mathbf{r}_2)|^2}{\kappa |\mathbf{r}_1 - \mathbf{r}_2|} = \frac{e^2}{\kappa} \frac{\sqrt{2\pi}}{d}$$

High-spin States in Lieb Lattice

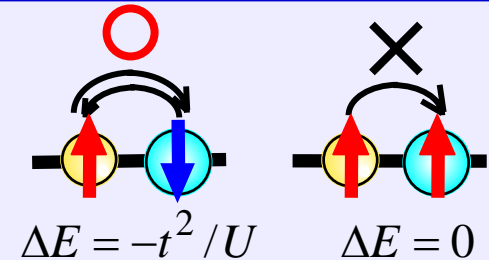
Exact diagonalization of Hubbard Hamiltonian

Total spin of the GS vs. N

Anti-ferromagnetic ordering



Kinetic exchange (2nd order)



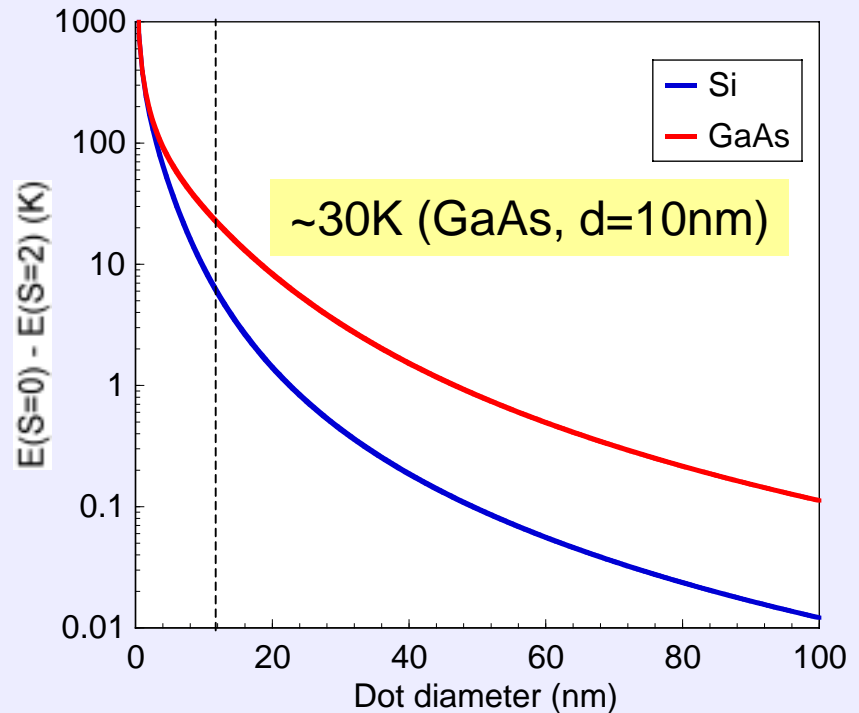
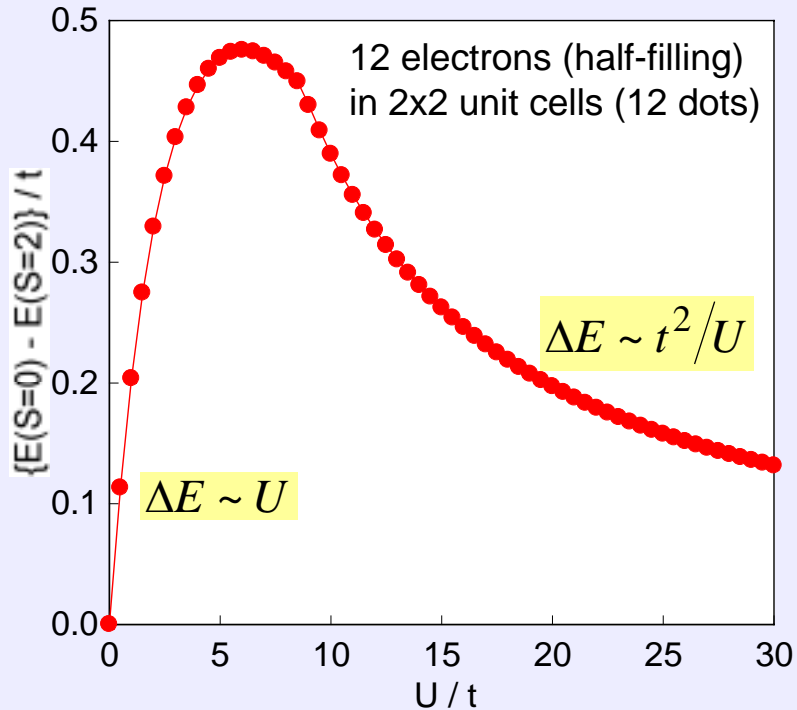
Lieb's theorem [E.H. Lieb: PRL **62** (1989) 1201]

When bands are half-filled in a bipartite lattice (one electron per site), the ground state has a spin $S = |N_A - N_B|/2$ (N_α is the number of α sites).

Stability of High Spin States

Tamura, Shiraishi, and Takayanagi, Phys. Rev. B. (2001)

Energy difference $\Delta E = E(S=0) - E(S=2)$ at half-filling



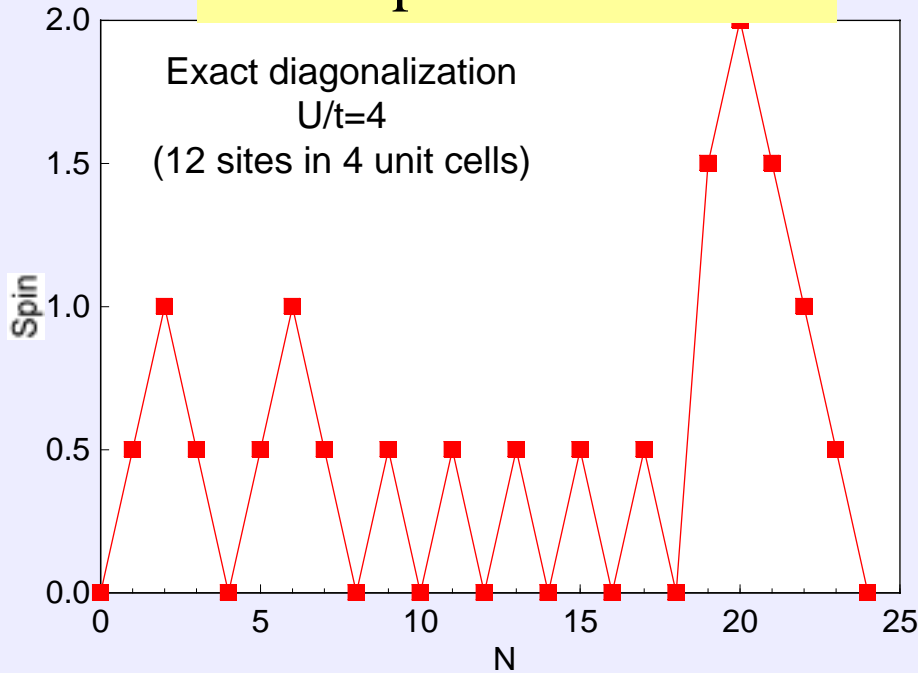
(Interdot spacing a) / (diameter d) = 1.5

GaAs: $m^* = 0.07$, $\kappa = 12$

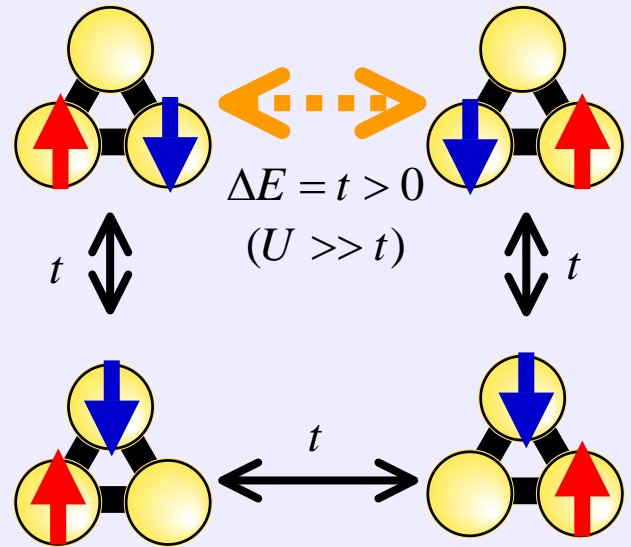
Si: $m^* = 0.2$, $\kappa = 13$

High-spin States in Kagome Lattice

Total spin the GS vs. N



Ring exchange (3rd order)

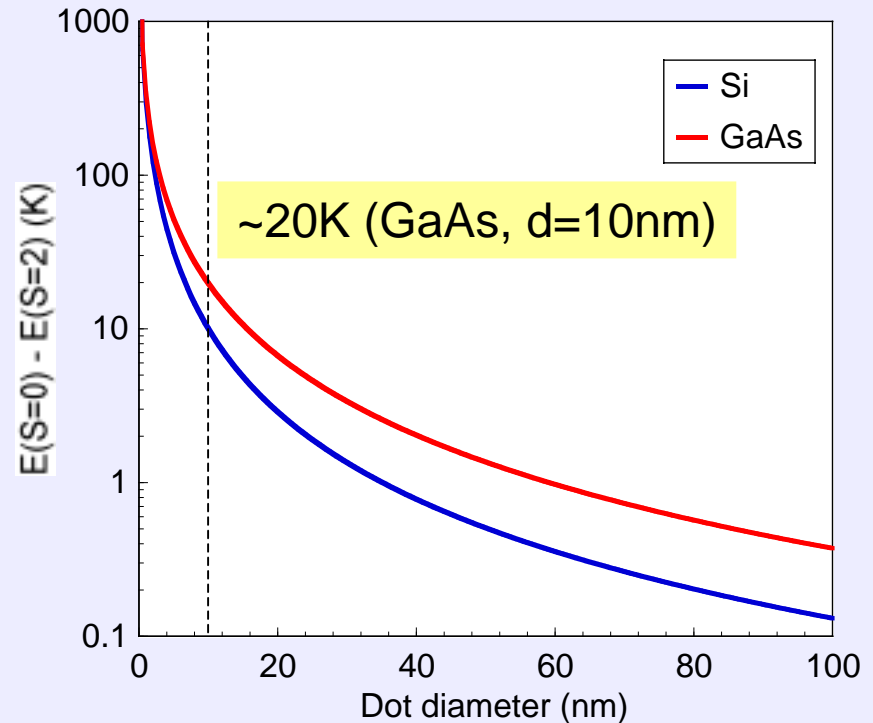
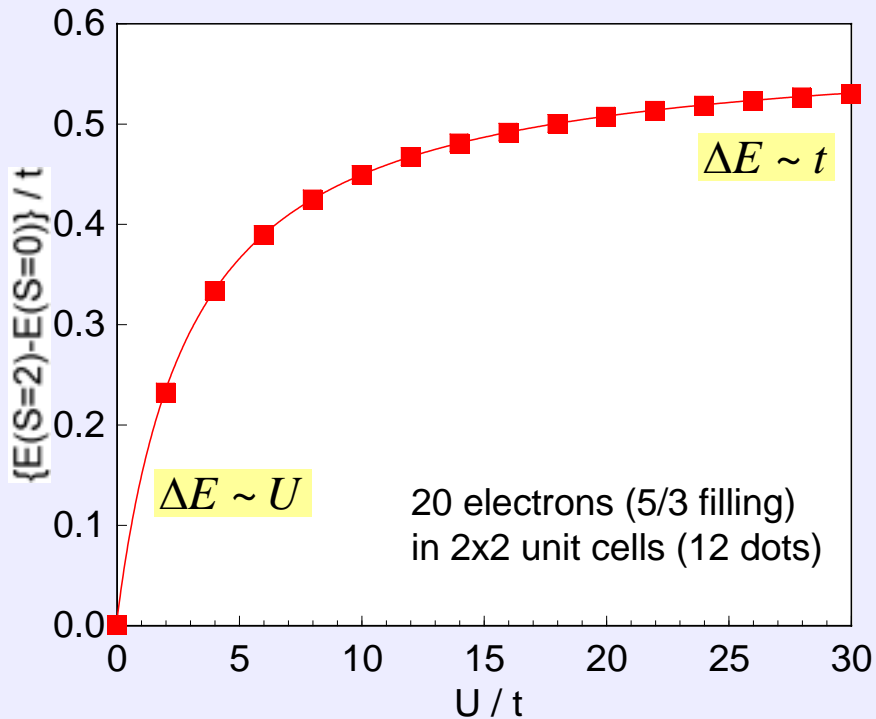


Mielke's theorem [A. Mielke: J. Phys. A25 (1992) 4335]

Kagome lattice shows a ferromagnetic behavior for the electron filling of $5/3 < n < 11/6$.

Stability of High Spin States

Energy difference $\Delta E = E(S=0) - E(S=2)$ at $n = 5/3$ filling



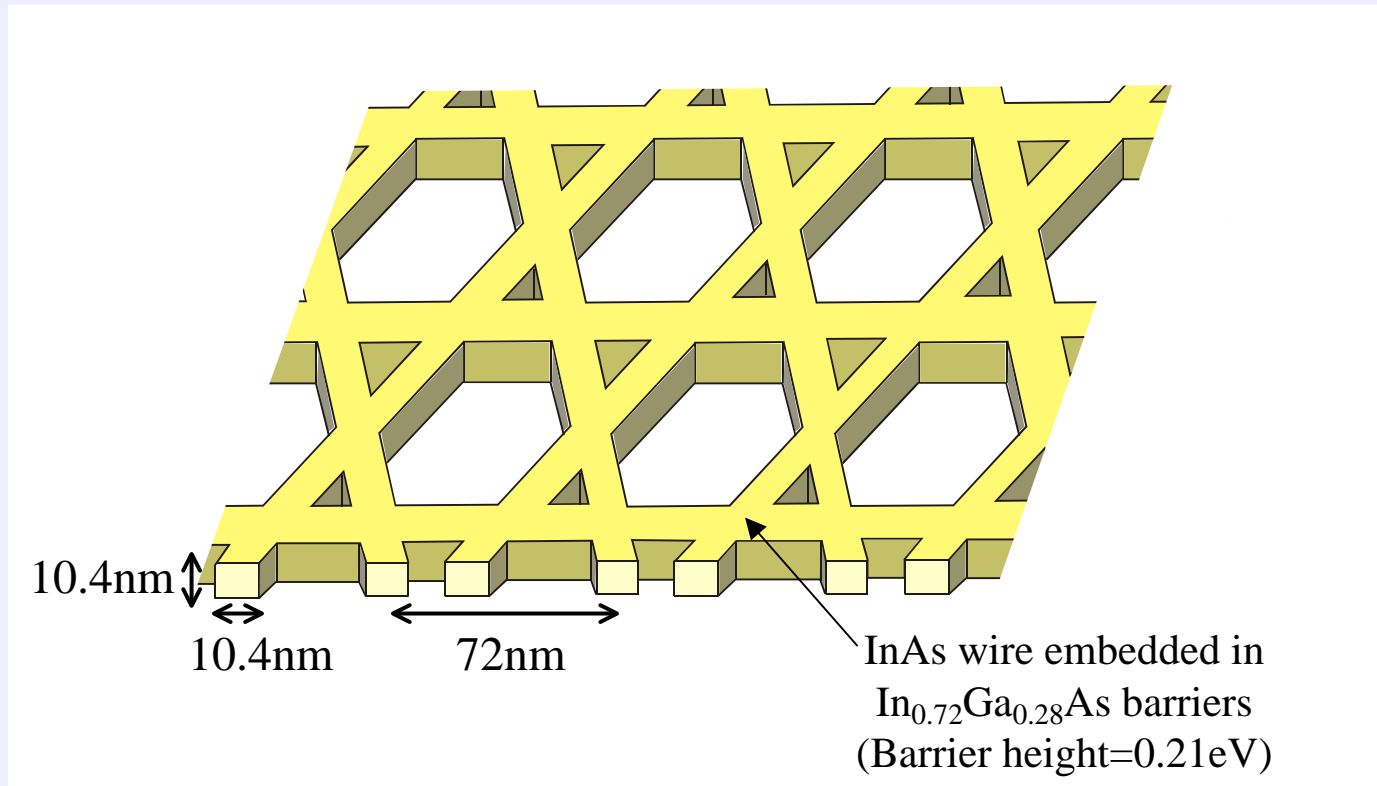
(Interdot spacing a) / (diameter d) = 1.5

GaAs: $m^* = 0.07$, $\kappa = 12$

Si: $m^* = 0.2$, $\kappa = 13$

Design of Kagome Solid

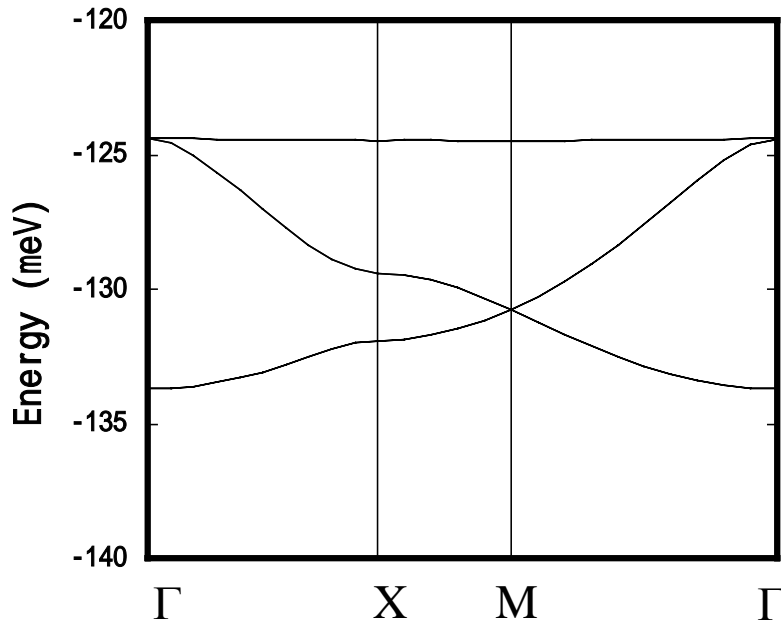
Kagome Network



Band Structure of Wire Network

Band calculation by local density functional approximation

Band structure



Parameter evaluation

$$\text{Band width} = 6t = 9.3 \text{ meV}$$

$$t = 1.55 \text{ meV}$$

$$\text{Hartree energy} = E_{\text{Intra-cell}} + E_{\text{Inter-cell}}$$

$$E_{\text{Intra-cell}} = N_{\text{cell}} \times n^2 \times U$$

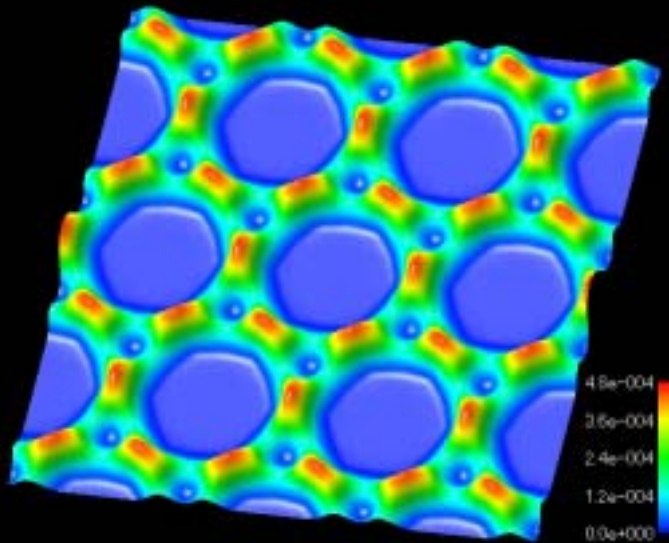
$$(N_{\text{cell}} = 3, n = 5/3)$$

$$E_{\text{Inter-cell}} = (-N_{\text{cell}}ne) \times \sum_{i \neq 0}^{\text{kagome}} \frac{q_i}{r_i}$$

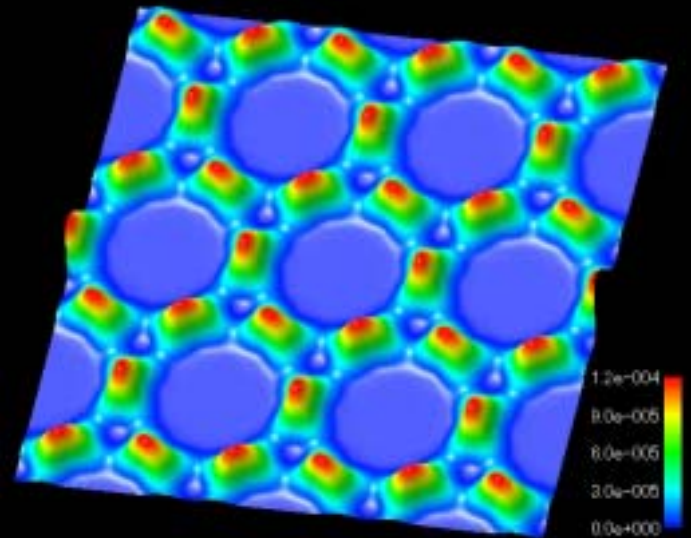
$$U = 6 \text{ meV}$$

Local spin density functional approximation

Charge distribution



Spin distribution



Number of electrons per dot

$4/3$

$5/3$

$6/3$

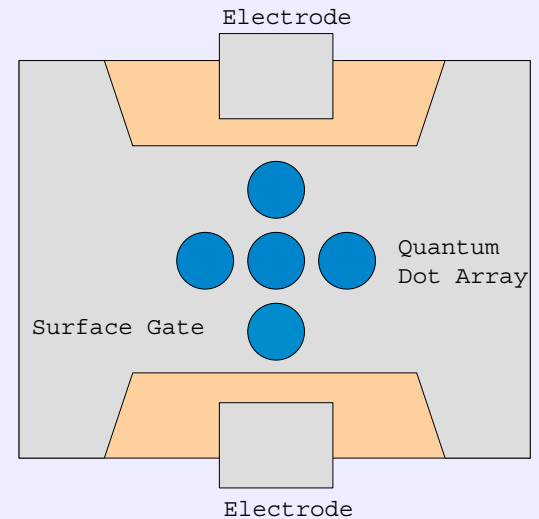
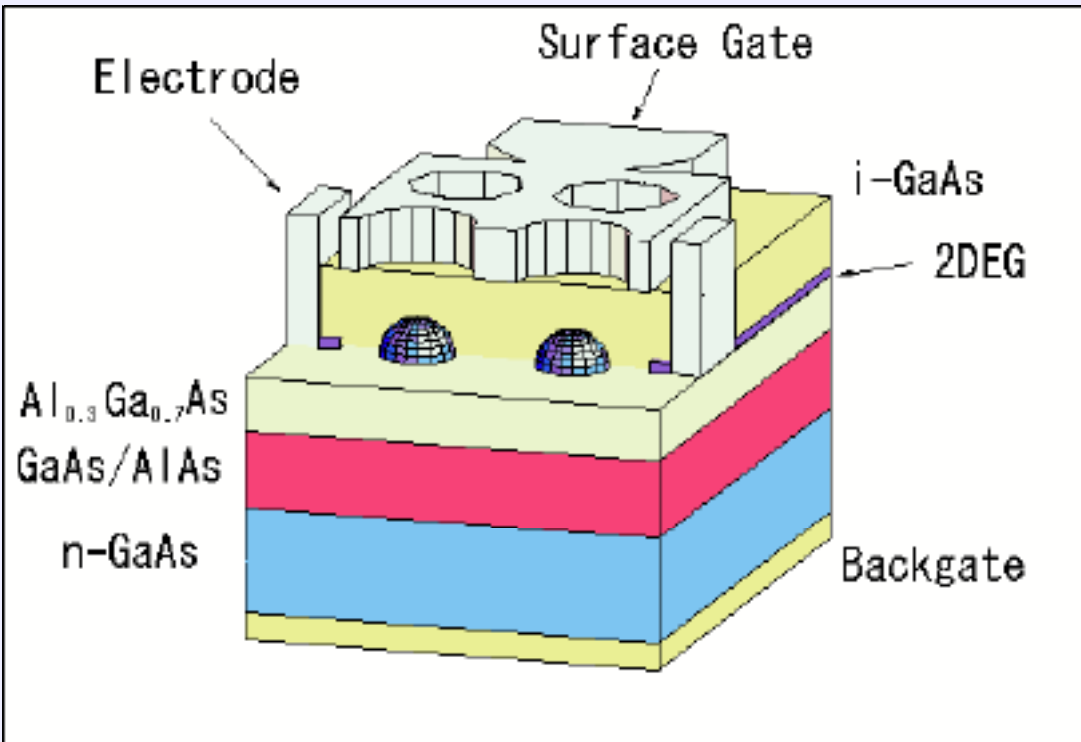
Flat band empty



Full filled

Half filled

Sample Structure

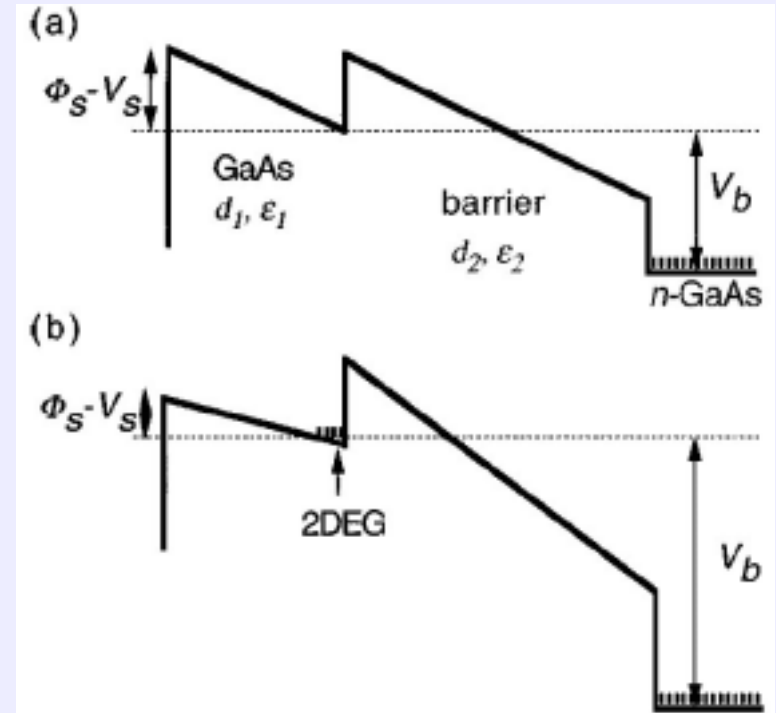
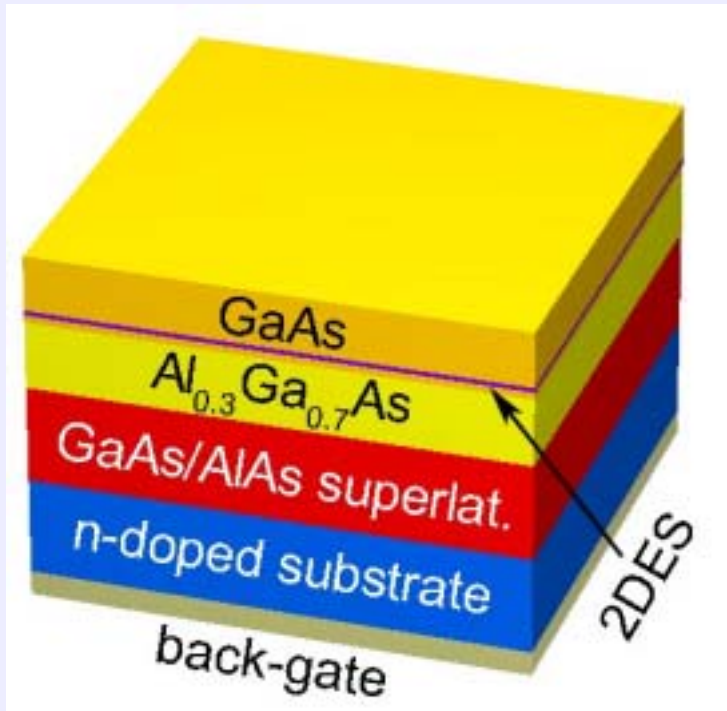


The two-dimensional electron gas (2DEG) in the heterostructure has initially **no electron**. The electron density increases as the back-gate voltage increases, and finally each dot has one electron.

	Thickness
Ti/Au	(Surface Gate)
i-GaAs	300 nm
Al _{0.3} Ga _{0.7} As	20 nm
GaAs/AlAs	2.5nm/2.5nm x100
n-GaAs	(Substrate)
AuGeNi/Au	(Back Gate)

Undoped back-gated HEMT structure

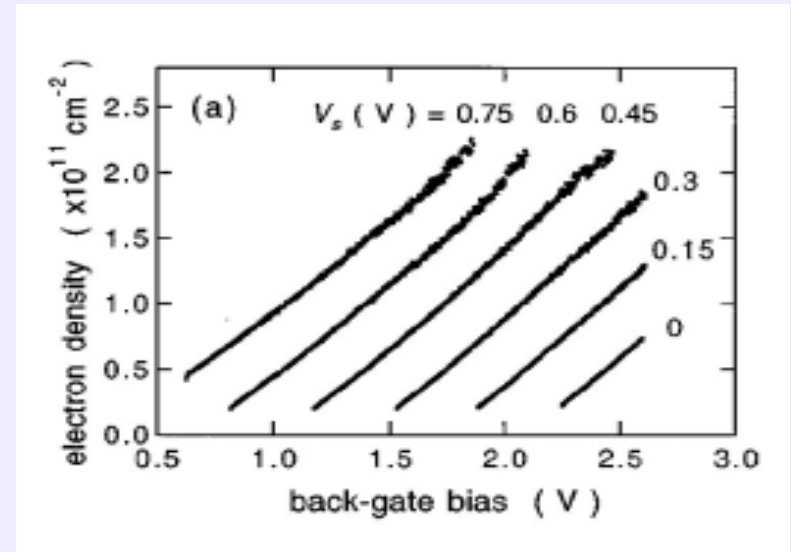
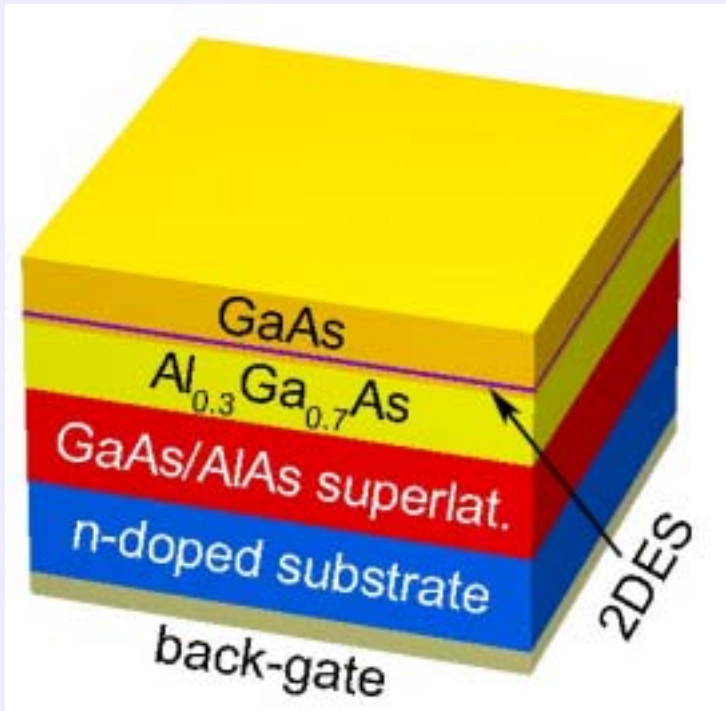
Band structure (schematic):



(Y. Hirayama, K. Muraki, and T. Saku, Appl. Phys. Lett. **72**, 1745 (1998))

Undoped back-gated HEMT structure

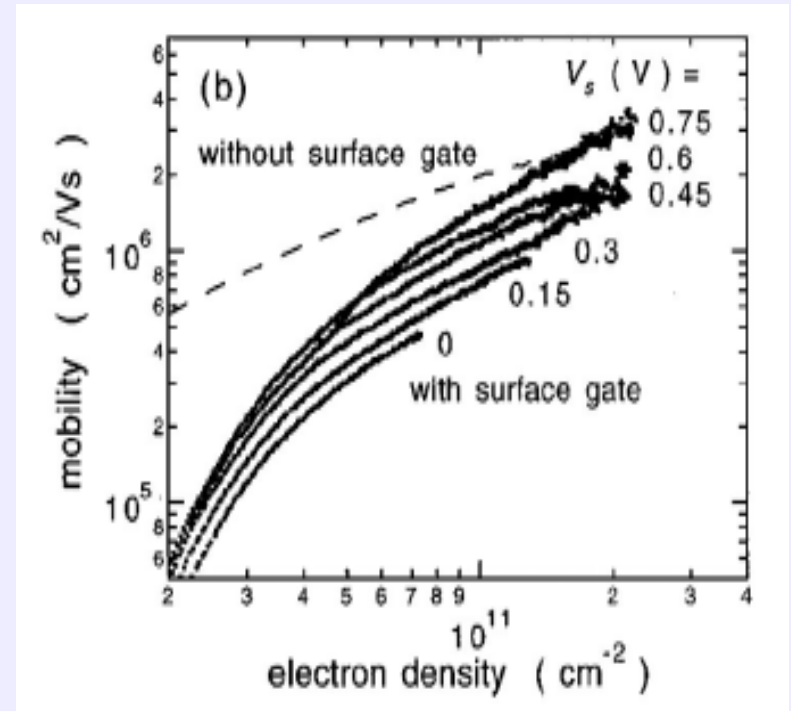
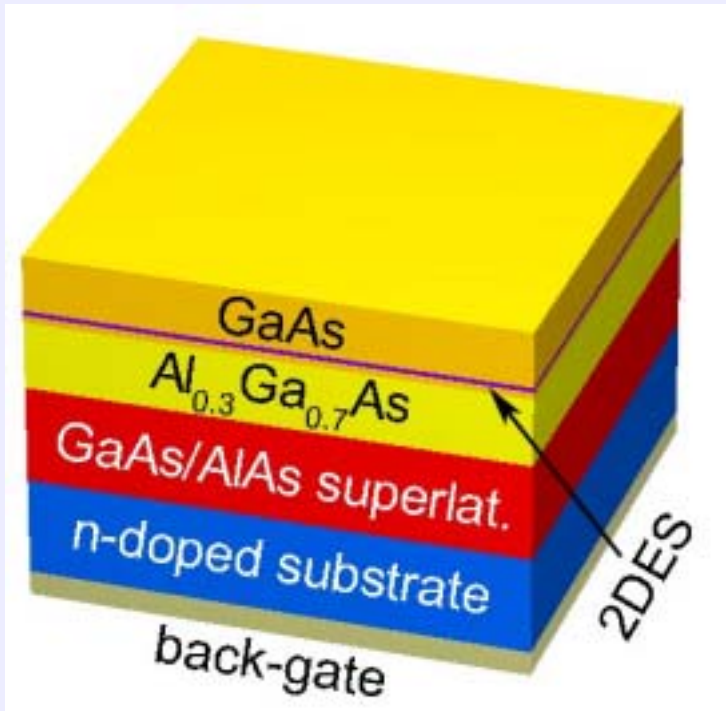
Electron density:



$$n = \frac{\epsilon_1}{d_1} (V_{fg} - \phi_{fg}) + \frac{\epsilon_1}{d_1} V_{bg}$$

Undoped back-gated HEMT structure

Electron mobility:

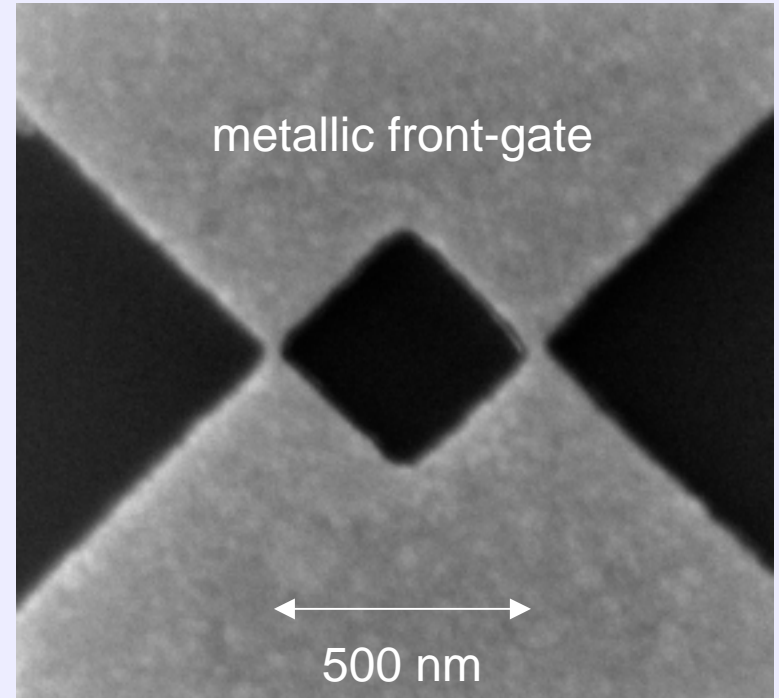
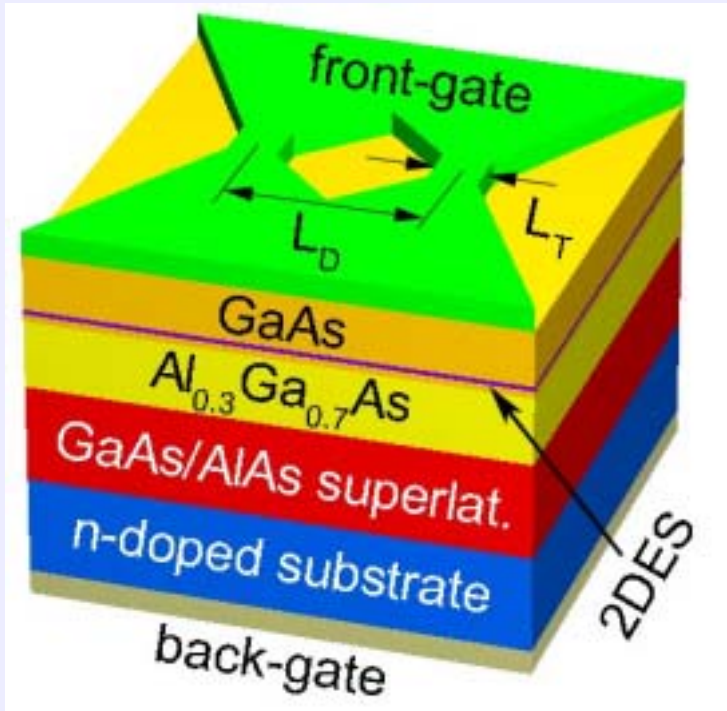


$$\mu = 3,000,000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}, n = 2 \times 10^{11} \text{ cm}^{-2} \rightarrow l_{el} = 22 \text{ } \mu\text{m}$$

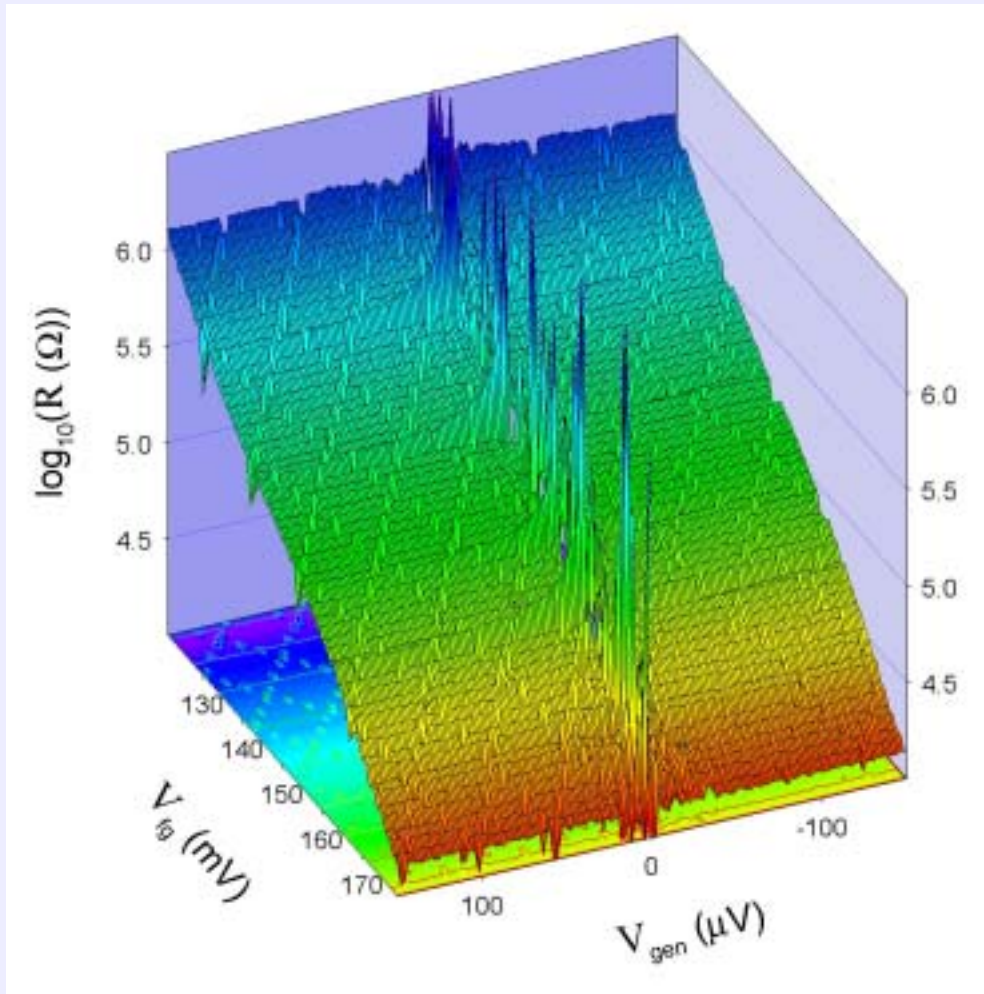
$$\mu = 200,000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}, n = 3 \times 10^{10} \text{ cm}^{-2} \rightarrow l_{el} = 570 \text{ nm}$$

Quantum dot with a single front-gate

Scanning electron micrograph



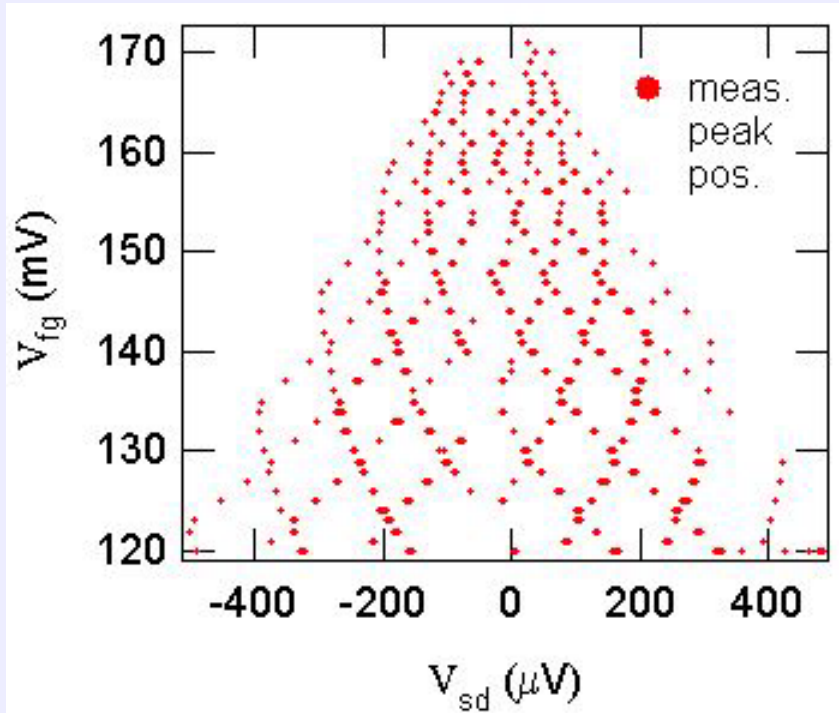
Single quantum dot – front-gate dependence



- Nice Coulomb diamond structure !
- Peaks at low bias related to DC measurement proc.
- Sample resistance changes by two orders of magnitude $\rightarrow V_{sd}$ changes

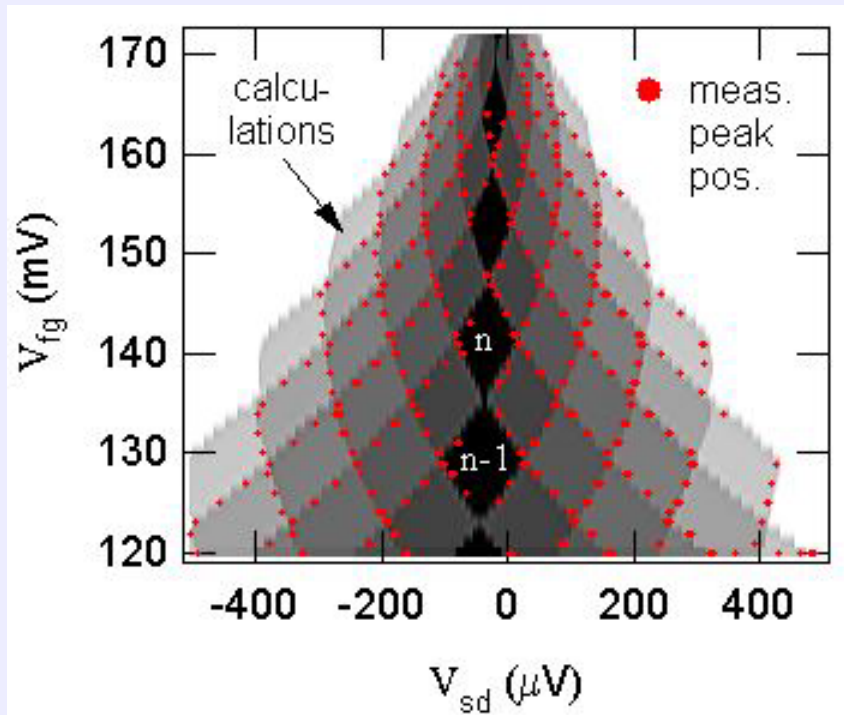
Single quantum dot – peak positions

Peak positions:

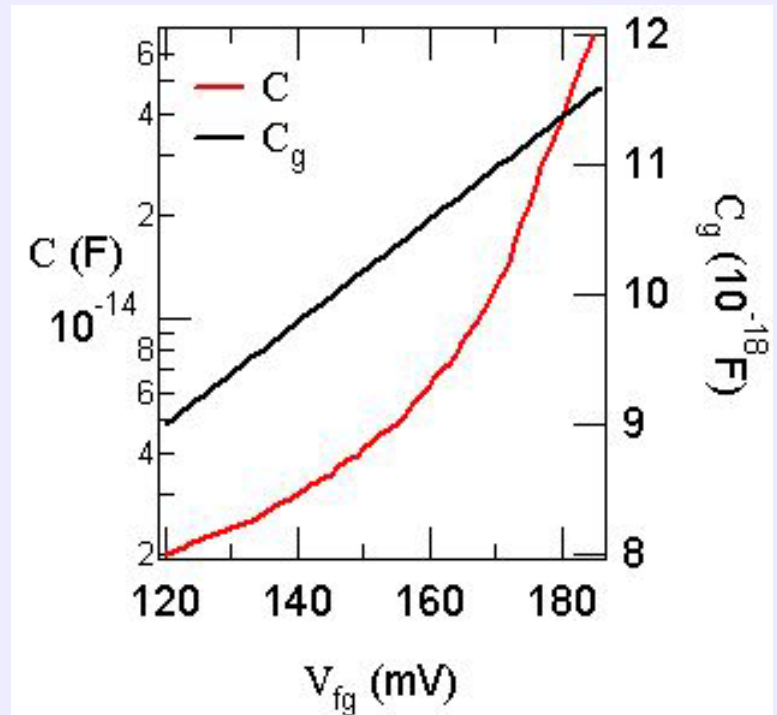


Single quantum dot – simulations

Peak positions:



Total and gate-capacitance:

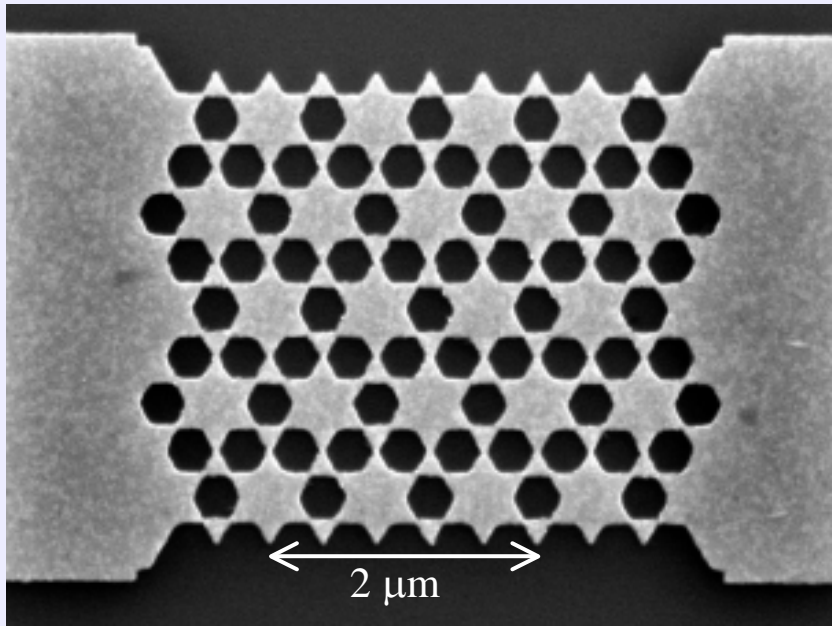


Front-gate has threefold impact:

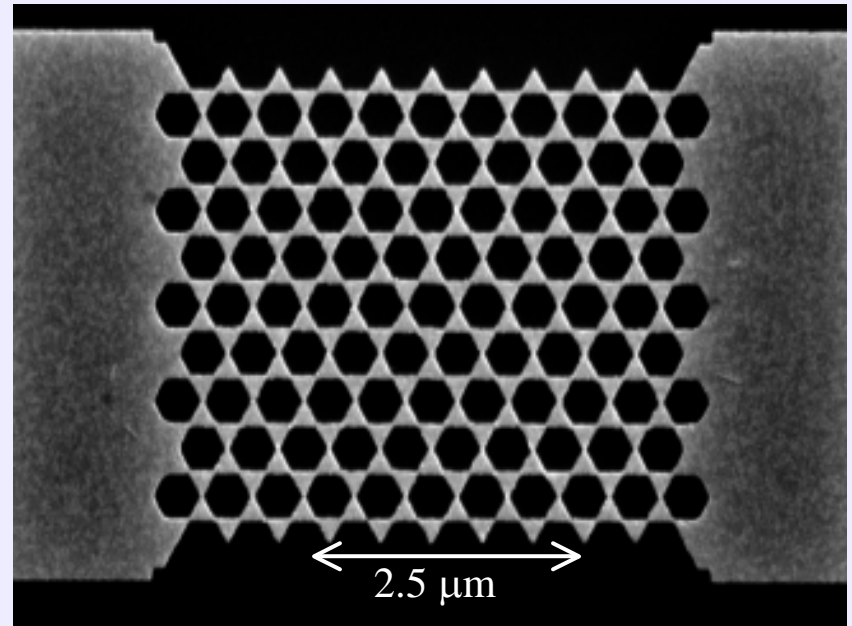
(a) shift dot spectrum, (b) change tunnel barriers, (c) change dot size

Quantum dot arrays

Kagome lattice:



Rhombic lattice:



Superconductivity with electronic mechanism

Kimura et.al., (2002)

Conventional BCS superconductors



High- T_c superconductors

d -wave superconducting pairing

Antiferromagnetic phase near the superconducting phase suggesting a strong antiferromagnetic fluctuation

Anomalous metal phase:

transport or magnetic properties, spin gap, etc...



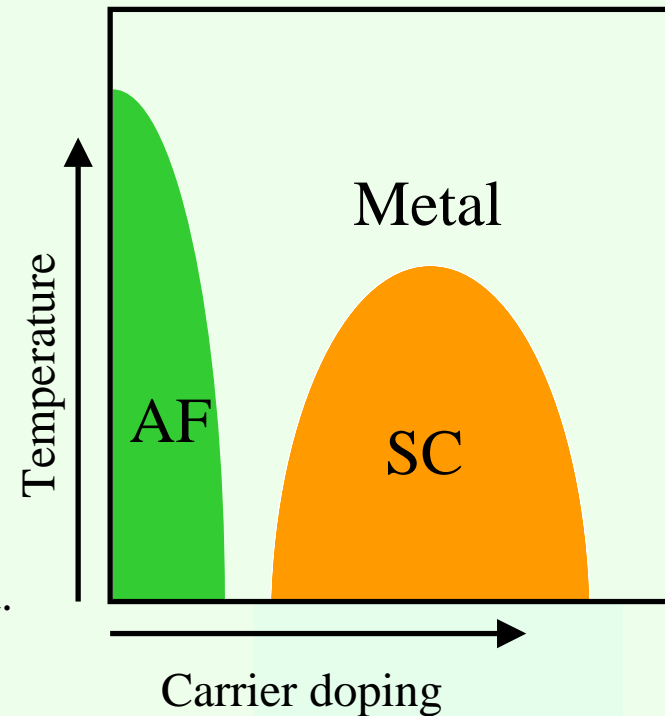
Possibility of electronic mechanism for superconductivity.

However, the phonon mechanism is not completely neglected.



In quantum-dot superlattices, we can study superconductivity with electronic mechanism and with negligible phonon.

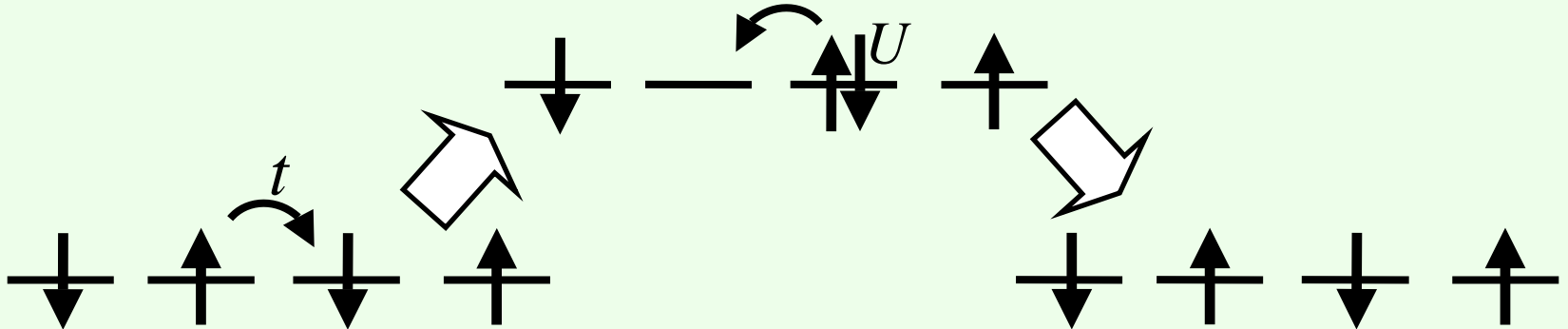
Phase diagram of High- T_c cuprate



Superconductivity of the Hubbard model

The **Hubbard model** is a possible relevant model for cuprates, including the interaction between electrons with opposite spins on lattice points.

A virtual process of the Hubbard model near/at the half-filling

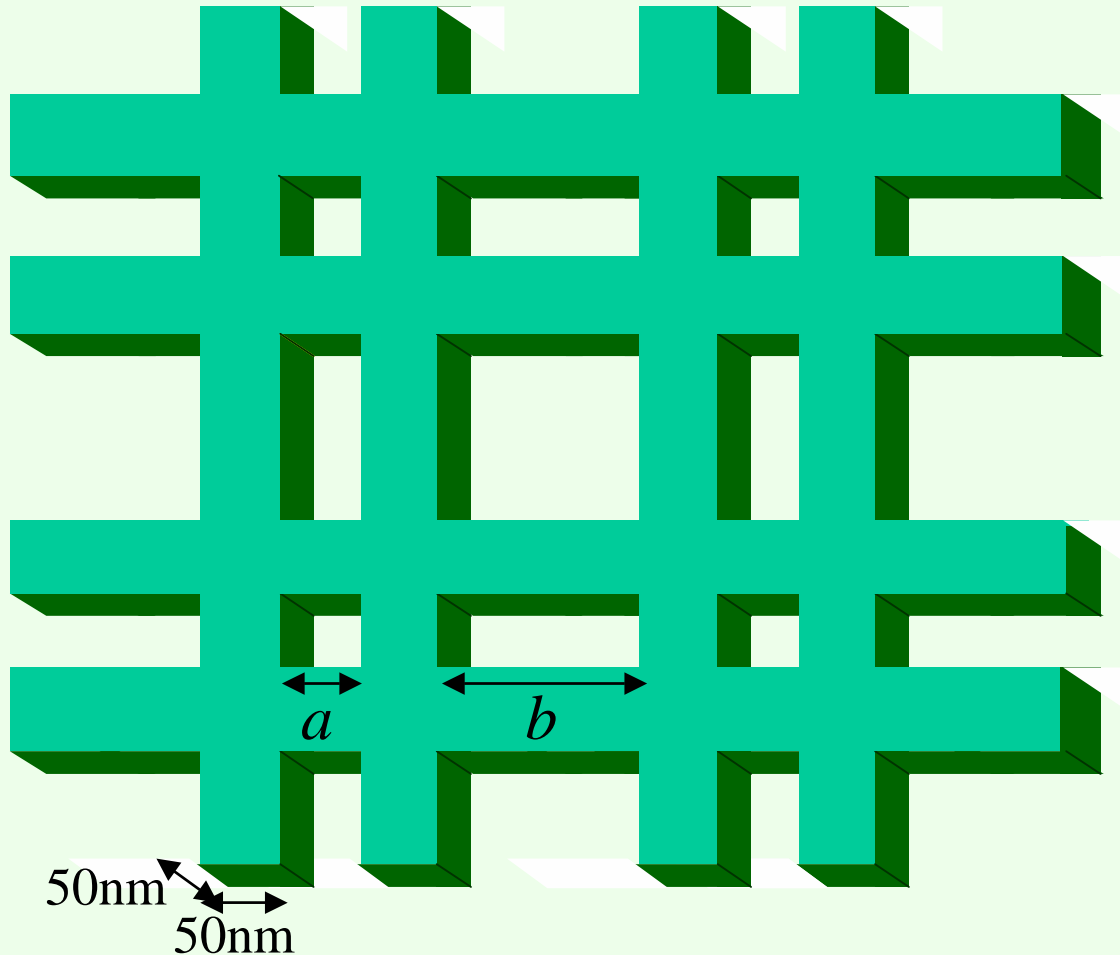


Effective antiferromagnetic coupling between adjacent spins $\approx 4t^2 / U$

We employ the fluctuation-exchange (**FLEX**) approximation (a self-consistent RPA). FLEX is an excellent tool to treat a strong **antiferromagnetic spin-fluctuation** and gives a **reliable** T_c (about 100K for cuprates).

Our lattice design with a quantum wire network

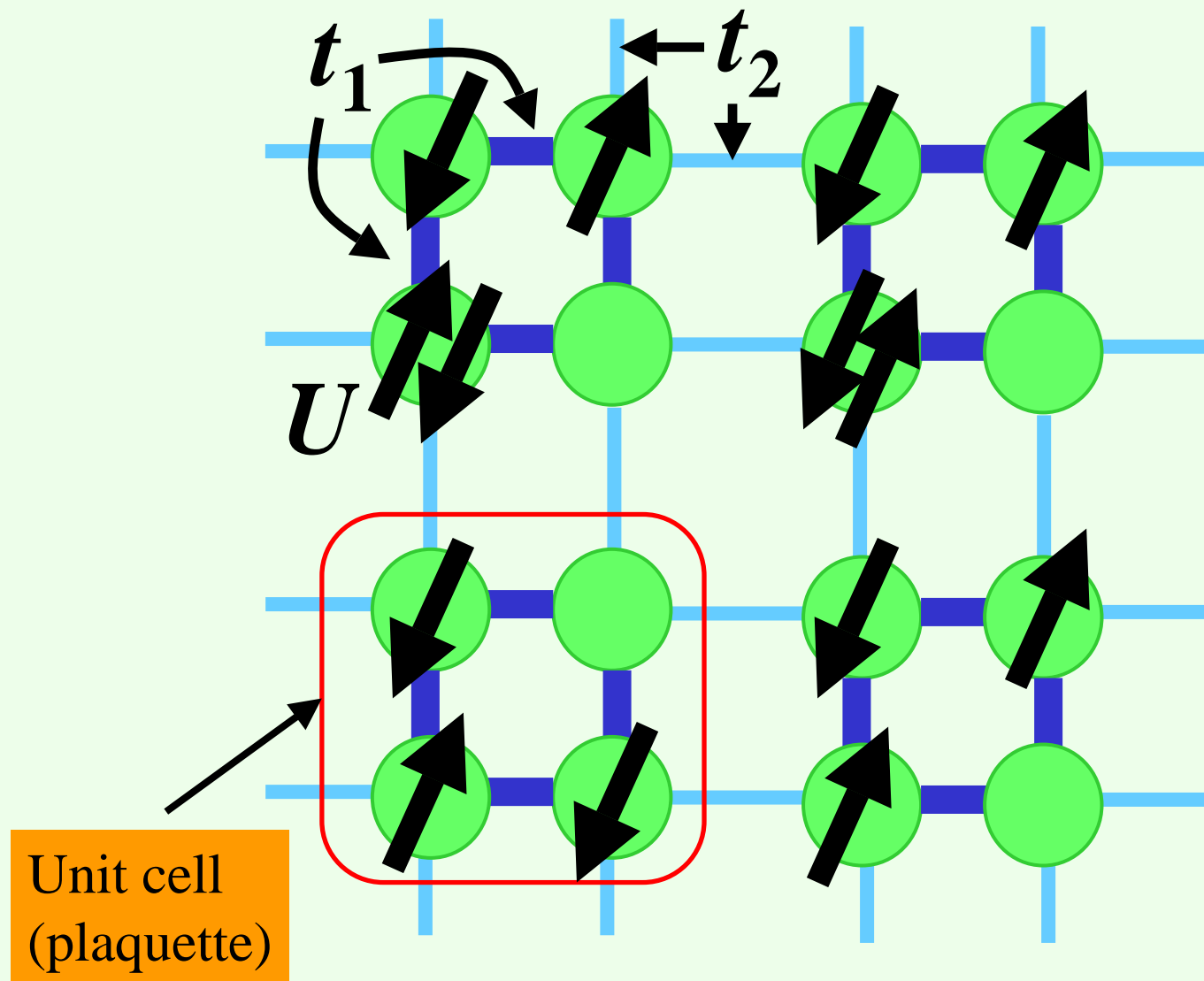
InAs wires embedded in $\text{In}_{0.776}\text{Ga}_{0.224}\text{As}$ with the barrier height=0.17eV



$a=b=61.1\text{nm}$ for a square lattice

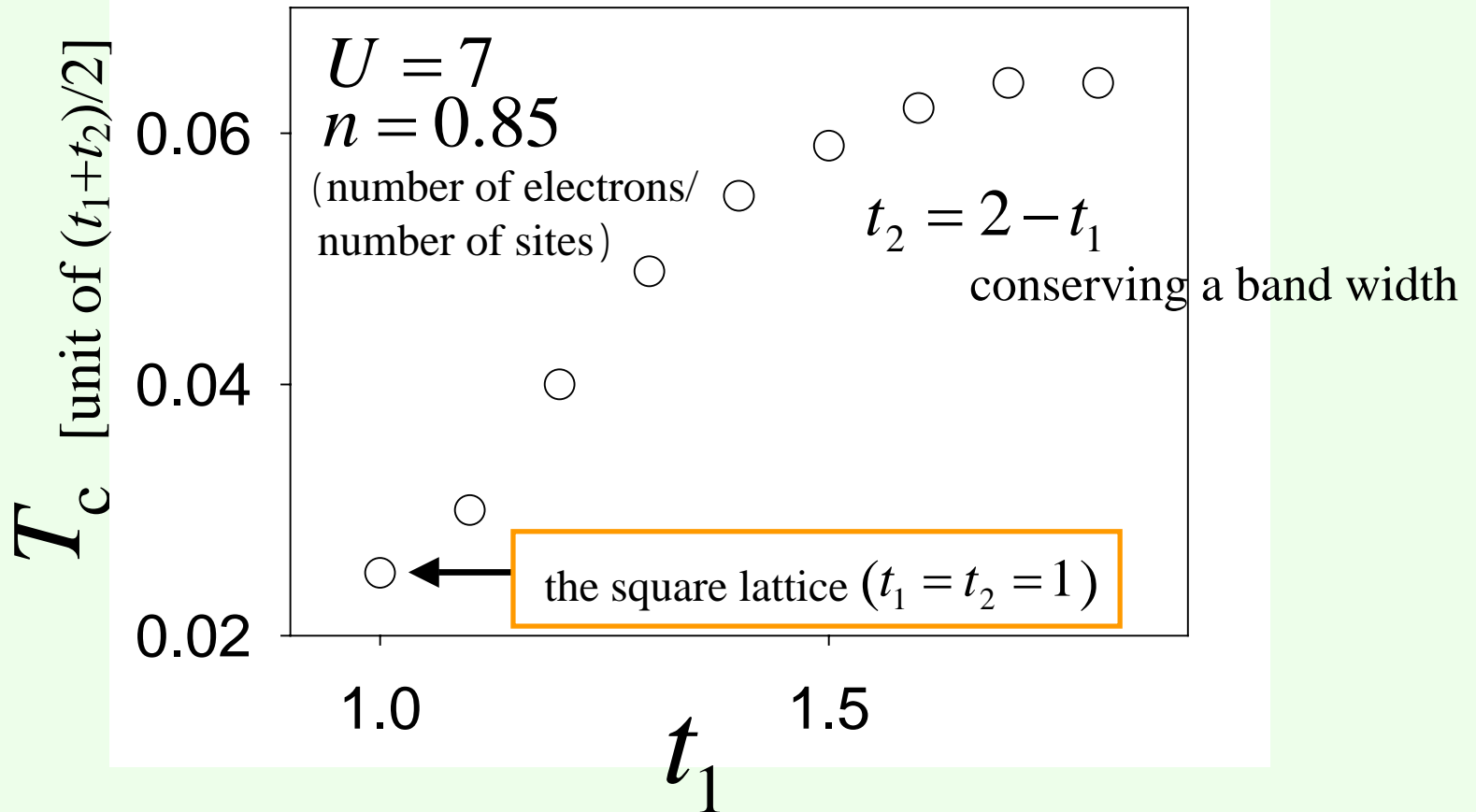
$a=38.8\text{nm}$ and $b=83.4\text{nm}$ for a plaquette lattice

The Hubbard model on a plaquette lattice



A square lattice is reproduced at $t_1 = t_2$.

Lattice structure dependence of T_c



For our design with an InAs wire network:

$T_c \approx 40$ mK for a square lattice.

$T_c \approx 90$ mK for a plaquette lattice.

How is T_c of the Hubbard model decided?

1. A self-consistent calculation with FLEX approximation

→ The Green's function $G(\vec{k})$ and the antiferromagnetic spin susceptibility $\chi(\vec{k})$

2. Solving the Eliashberg's equation

→ Determination of T_c and the superconducting gap function $\phi(\vec{k})$

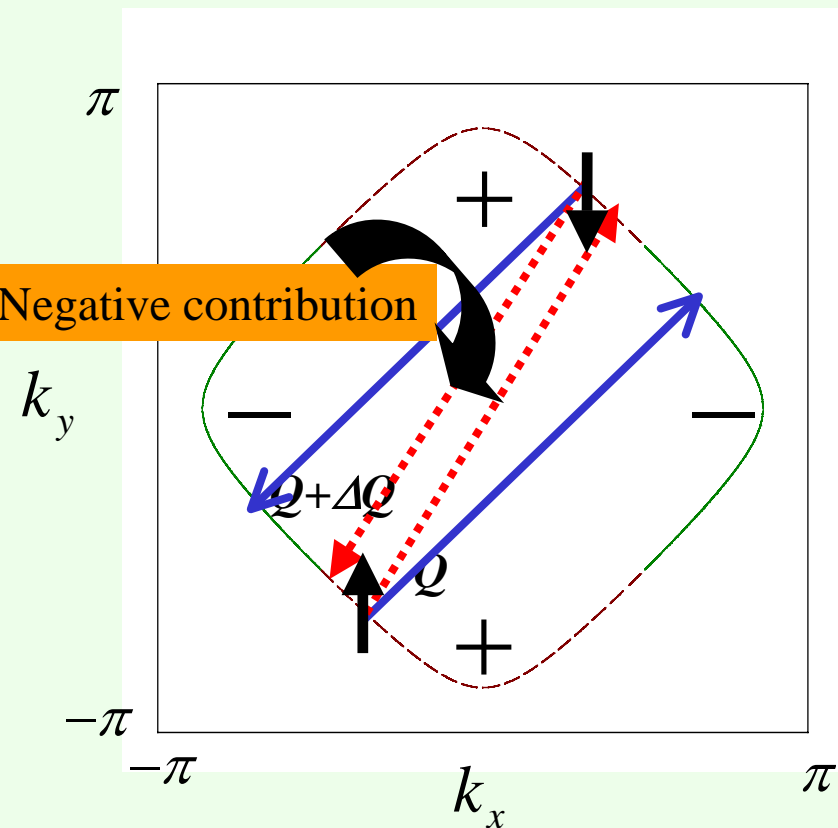
The Eliashberg's equation

$$\phi(\vec{k}) = - \sum_{\vec{k}'} \frac{V_{\text{eff}}(\vec{k} - \vec{k}')}{2\xi(\vec{k})} \tanh\left(\frac{\xi(\vec{k}')}{2k_B T}\right) \phi(\vec{k}')$$

$$V_{\text{eff}} \approx - \frac{\langle \chi(\vec{k} - \vec{k}') \phi(\vec{k}) \phi(\vec{k}') \rangle}{\langle \phi(\vec{k})^2 \rangle} \quad \langle \dots \rangle : \text{average over Fermi surfaces}$$

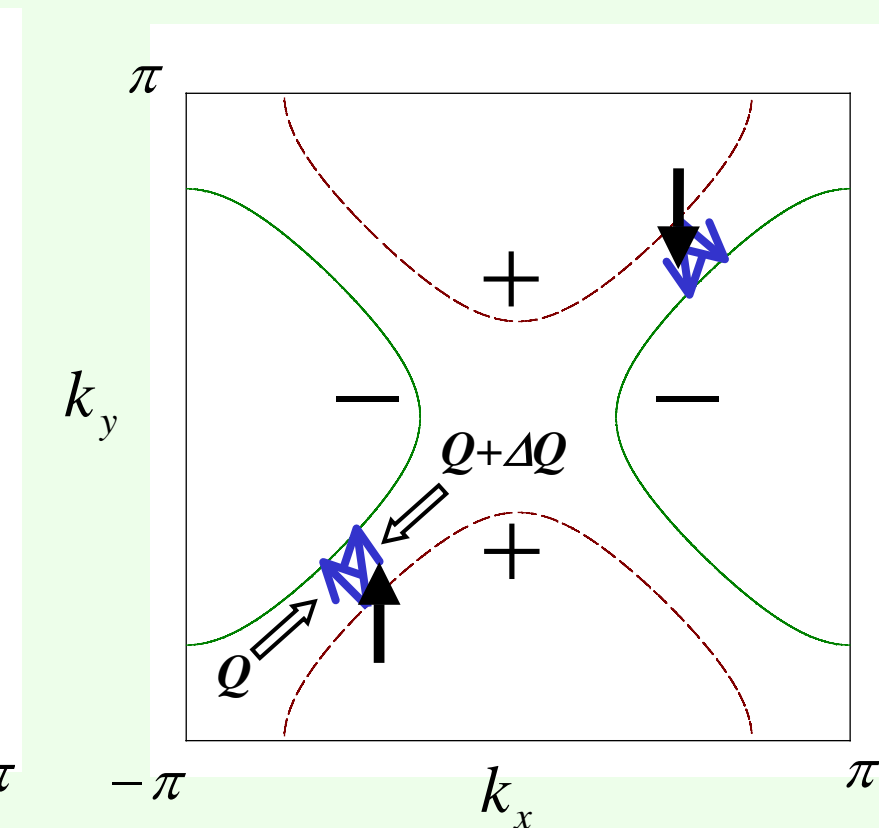
Generally speaking, we obtain a larger T_c for larger V_{eff} .

Why is T_c of the plaquette lattice enhanced?



Square lattice

A Pair scattering (Red dashed lines) connects points where the gap functions have the same sign, resulting in a negative contribution to superconductivity.



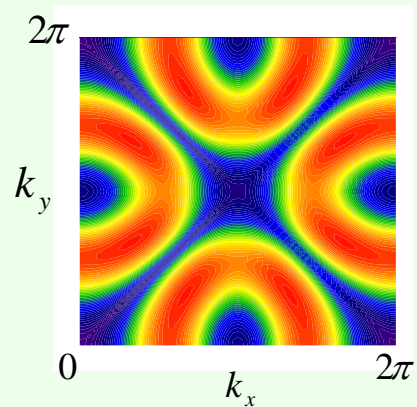
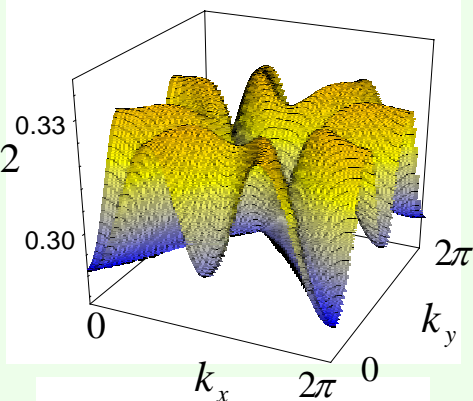
Plaquette lattice

Because of disconnected Fermi surfaces, pair-scatterings with negative contribution to superconductivity are absent.
 → a very high- T_c

Green function

(a)

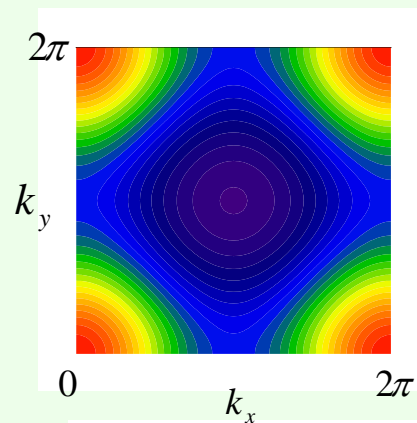
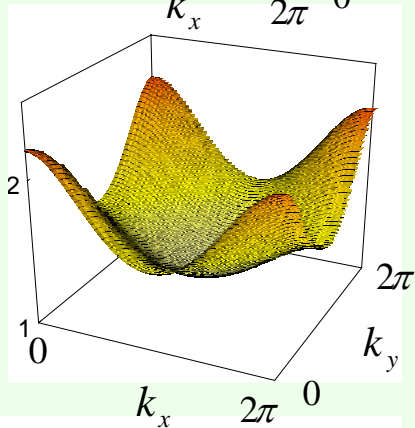
$$|G|^2$$



Spin susceptibility

(b)

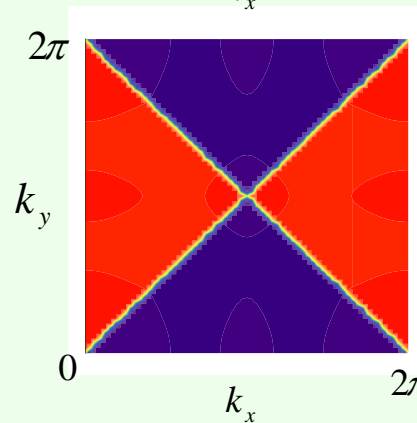
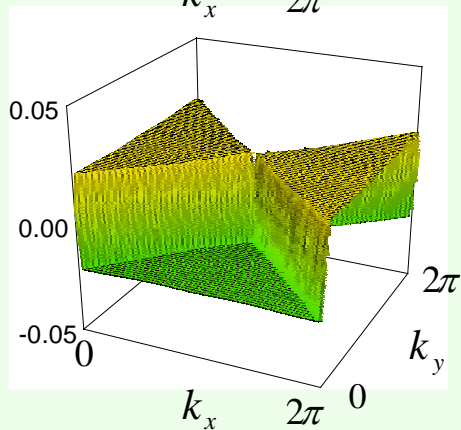
$$\chi$$



Gap function

(c)

$$\phi$$



Summary

- Material design using semiconductor dot arrays is proposed.
- Flat-band ferromagnetism in dot arrays is discussed.
- Advantages of using semiconducting materials for dot-array ferromagnets are pointed out.
- Superconductivity using dot arrays are proposed.