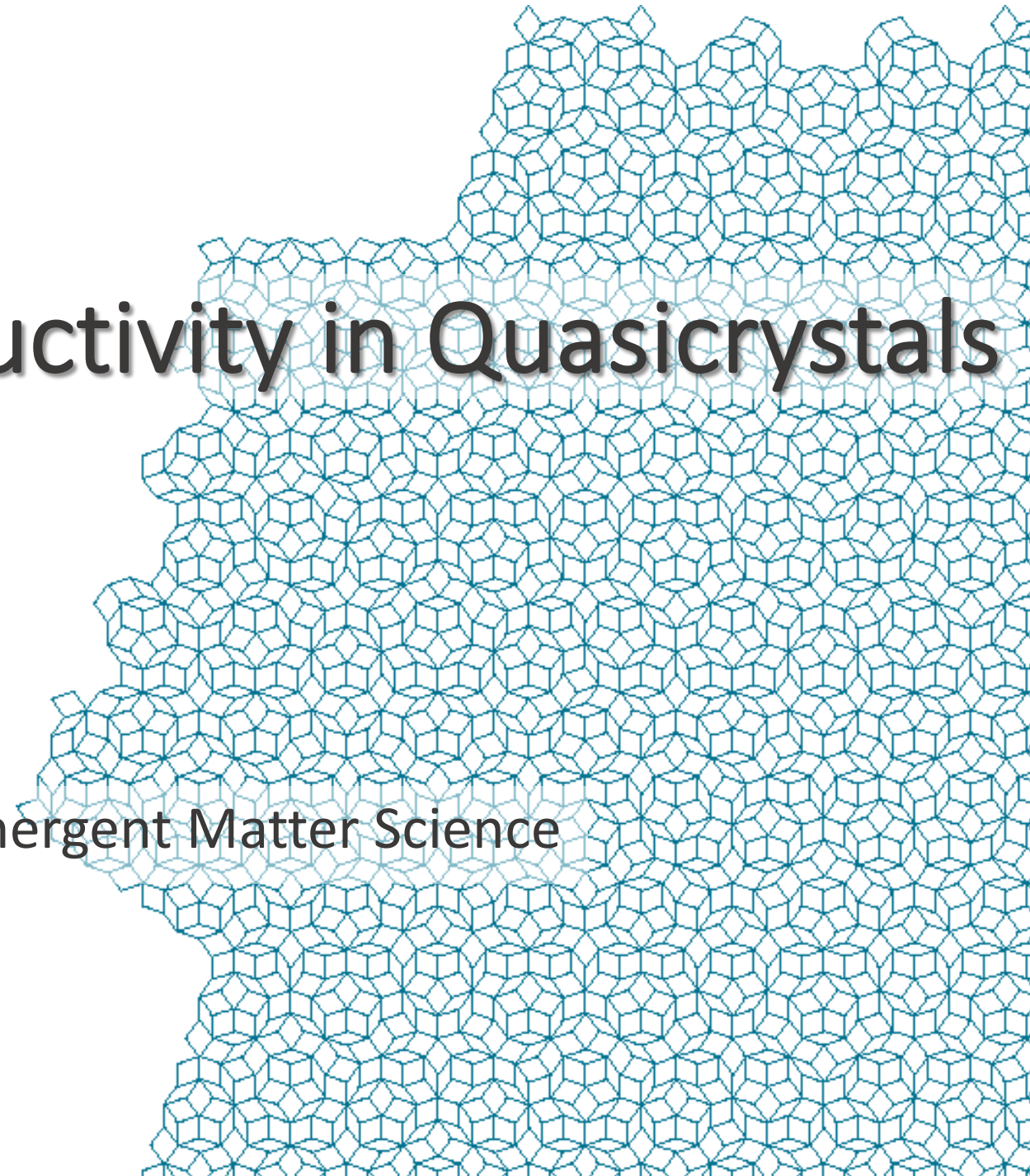


Superconductivity in Quasicrystals



RIKEN Center for Emergent Matter Science
Shiro Sakai

Feb. 1, 2021

Collaborators

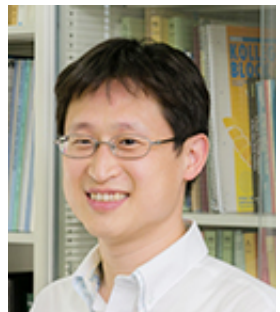
Nayuta Takemori (Okayama University, A03)



Akihisa Koga (Tokyo Institute of Technology, A04)



Ryotaro Arita (University of Tokyo, RIKEN)

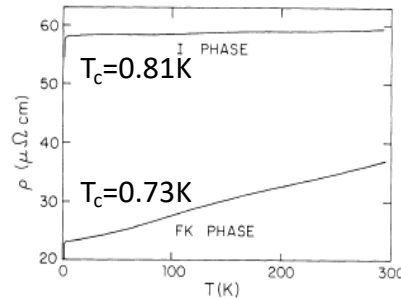


Superconducting quasicrystal?

Al-Zn-Mg

Wong *et al.*, PRB **35**, 2494 (1987)

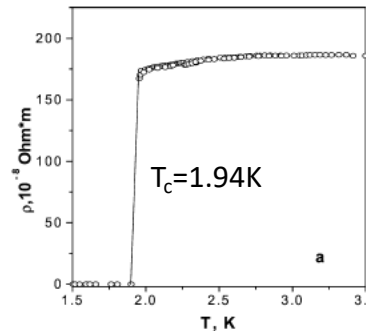
Graebner and Chen, PRB **58**, 1945 (1987)



- No magnetization data.
- Later identified as approximant.

Al-Cu-Mg, Al-Cu-Li

Wagner *et al.*, PRB **38**, 7436 (1988)



- No magnetization data.

Ti-Zr-Ni

Azhazha *et al.*, Phys. Lett. A **303**, 87 (2002)

- No magnetization data.
- Possible mixture of other phase.

For the discovery of a new superconductor, we would have

- Zero resistivity
- Meissner effect
- Identification of crystal structure
- Reproducibility

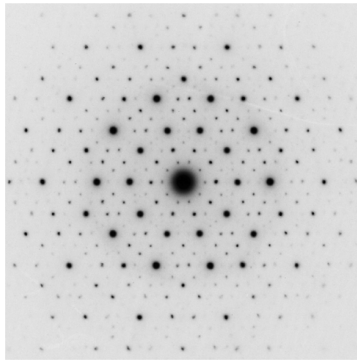
by K. Kitazawa

Discovery of superconductivity in quasicrystal

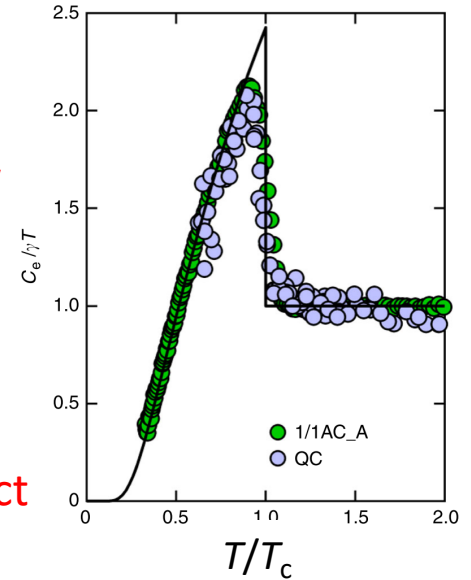
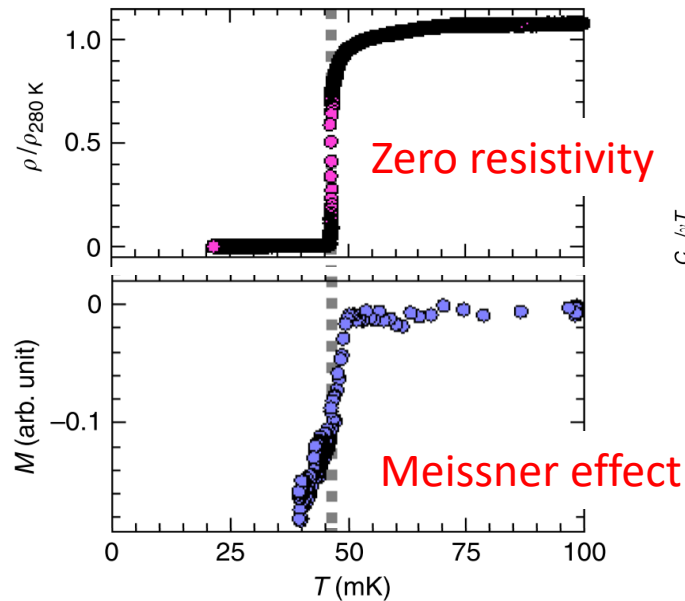
K. Kamiya^{1,5}, T. Takeuchi², N. Kabeya³, N. Wada¹, T. Ishimasa⁴, A. Ochiai³, K. Deguchi¹, K. Imura¹ & N.K. Sato¹

Al-Zn-Mg alloy

$T_c = 50\text{mK}$



Structure identification



Bulk property

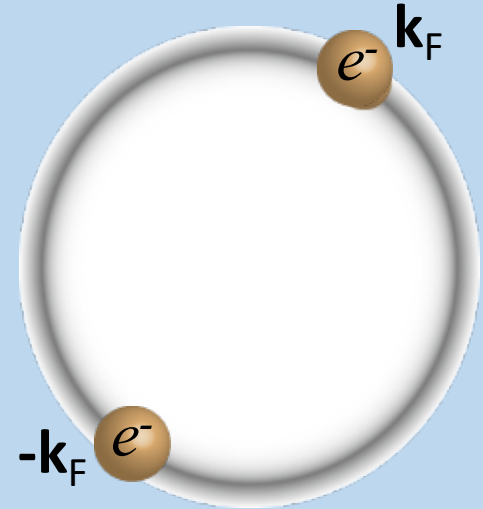
First example of electronic long-range order in QC

Top 10 Breakthroughs of 2018 in Physics World

What's the issue?

Standard understanding of superconductivity

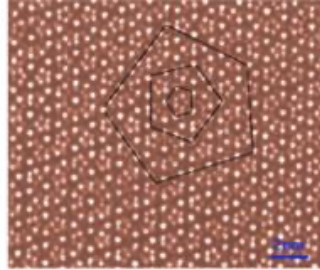
- Presence of Fermi surface
- Cooper pair
= (2 el. with $\mathbf{k}_F$ and $-\mathbf{k}_F$)
- Many properties calculated in momentum space.



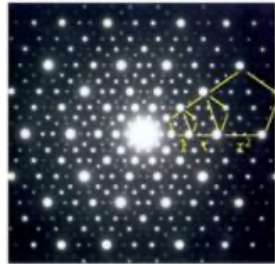
Quasicrystal: No momentum space, no Fermi surface

How can we understand a superconducting QC?

Note: Two different reciprocal spaces



$$\rho(\mathbf{r}) = \langle c_{\mathbf{r}}^{\dagger} c_{\mathbf{r}} \rangle \quad \text{Local density}$$



$$S(\mathbf{q}) = \int \rho(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r}$$

$\mathbf{q}$: F. T. of *absolute* coordinate $\mathbf{r}$

Figures from
<https://www.kek.jp/ja/newsroom/2011/12/08/1200/>

In periodic systems, Fermi surface is defined by a peak in

$$A(\mathbf{k}, \omega = E_F) = -\frac{1}{\pi} \text{Im} G(\mathbf{k}, \omega = E_F)$$

$\uparrow$
 F. T. of $G(\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, t) = -i \langle T c_{\mathbf{r}_1}(t) c_{\mathbf{r}_2}^{\dagger}(0) \rangle$

$\mathbf{k}$: F. T. of *relative* coordinate

This is not well defined in QC.

What's the issue?

Anderson's theorem

P. Anderson, J. Phys. Chem. Solids **11**, 26 (1959)

s-wave superconductivity is robust against weak (nonmagnetic) disorder

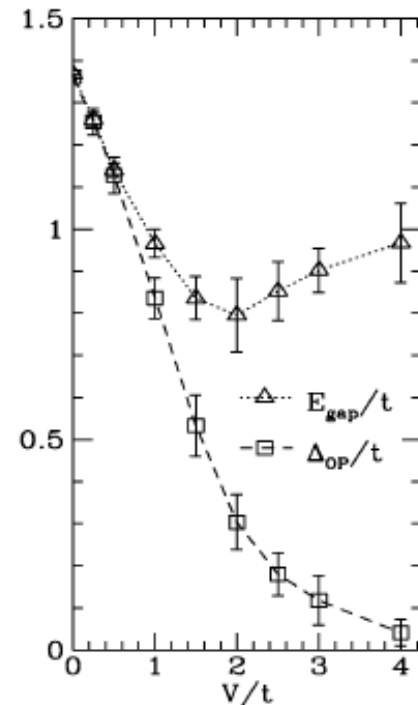
But, strong disorder can destroy SC!

Figure from A. Ghosal, M. Randeria, and N. Trivedi, PRL **81**, 3940 (1998).

Normal state: metal $\rightarrow$ Anderson insulator

What about quasicrystal?

Normal state: critical wave function



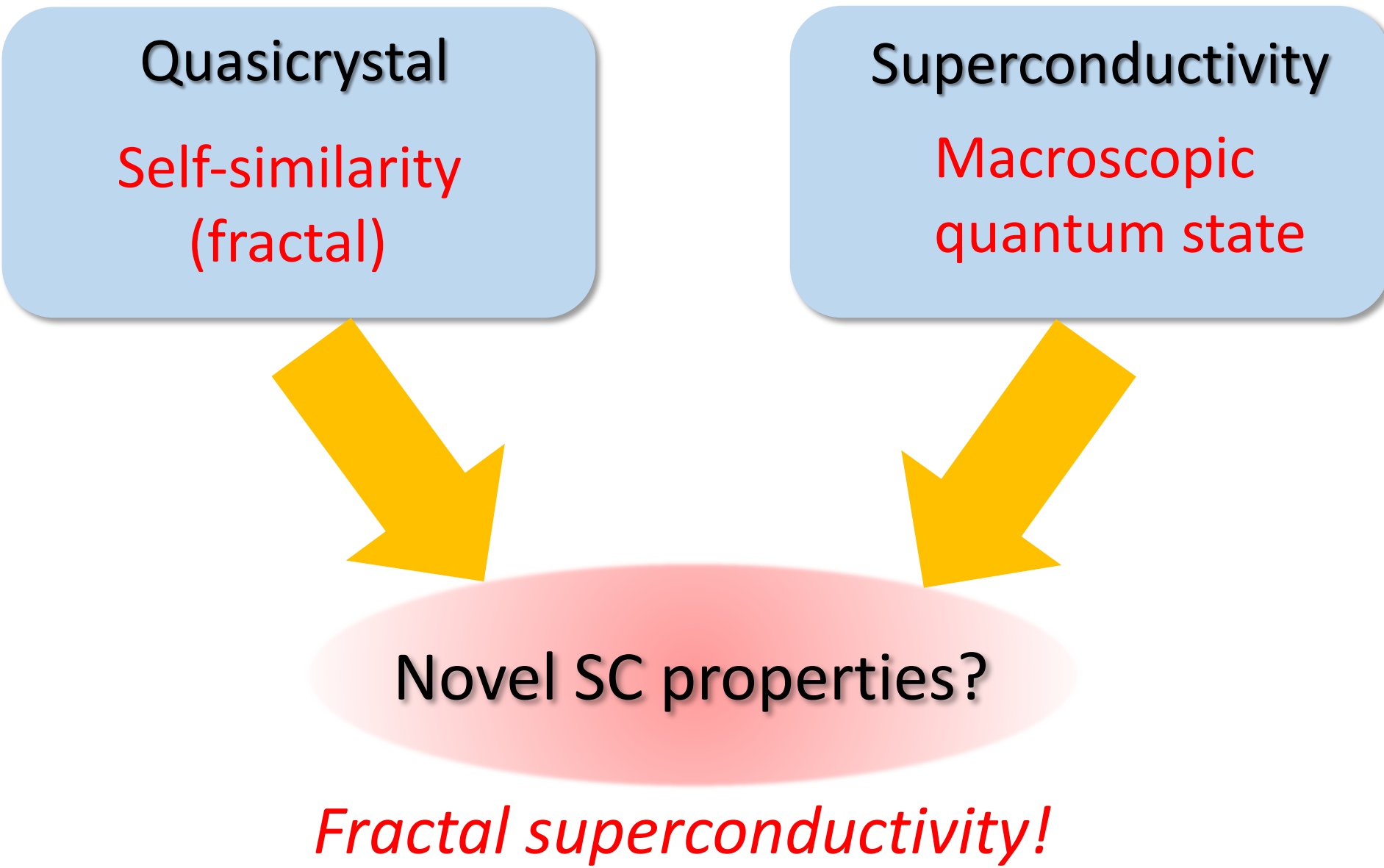
What's the issue?

Quasicrystal

Self-similarity
(fractal)

Superconductivity

Macroscopic
quantum state



```
graph TD; A[Quasicrystal<br/>Self-similarity<br/>(fractal)] --> D([Novel SC properties?]); B[Superconductivity<br/>Macroscopic<br/>quantum state] --> D; D --- C[Fractal superconductivity!]
```

Novel SC properties?

Fractal superconductivity!

How to address the issues?

- No momentum space
- Nonuniform (but not random)



DFT for approximants?

M. Saito, T. Sekikawa, and Y. Ono,
Phys. Status Solidi B 2000108 (2020):
Conductivity and specific heat



Simplified model for QC?

Essence:

- Quasiperiodicity
- Pairing attraction

Our approach

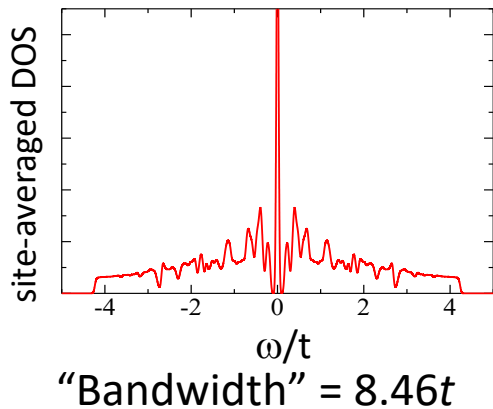
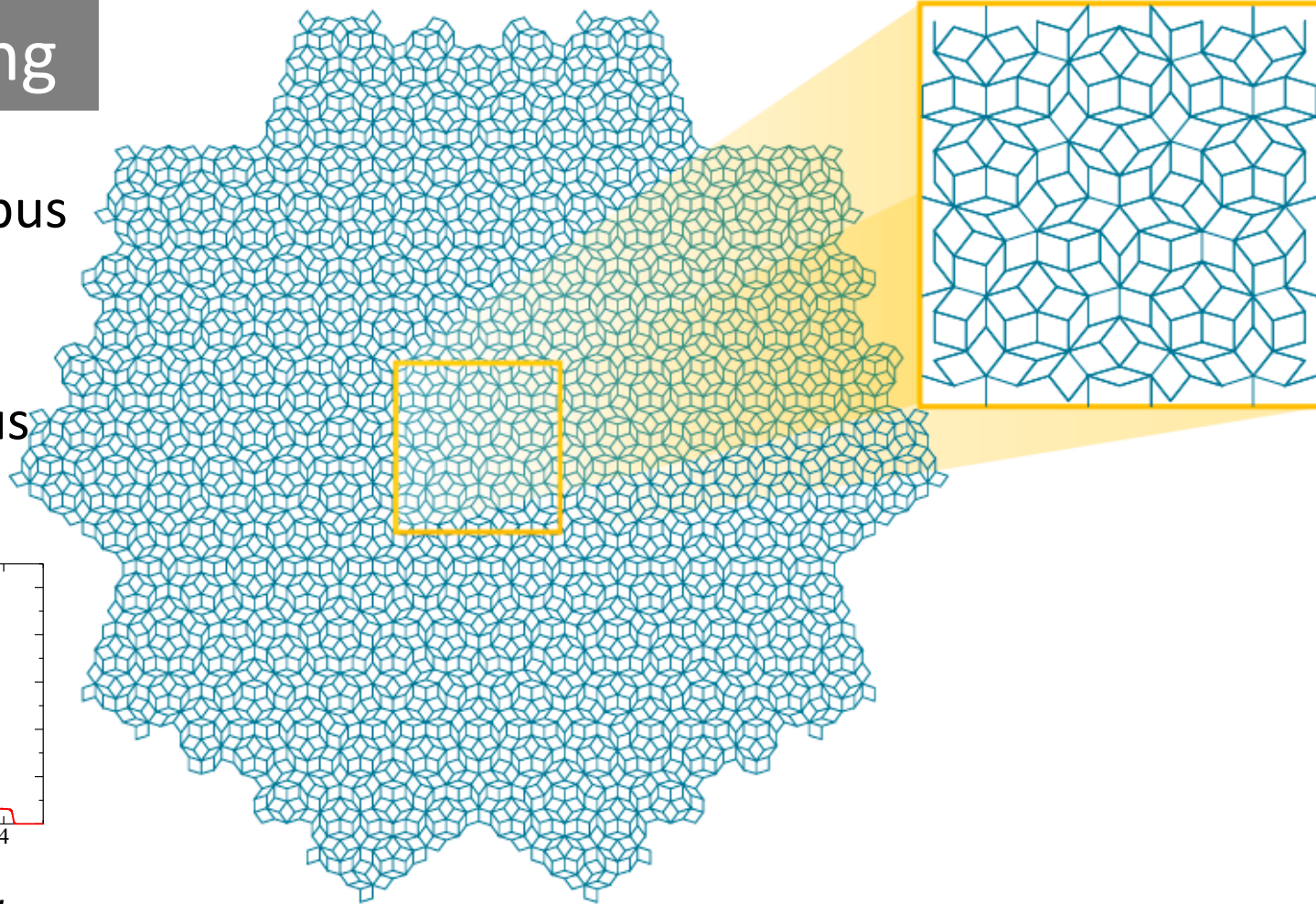
cf. 1D: M. Tezuka and A. M. Garcia-Garcia, PRA **82**, 043613 (2010).

Model of quasiperiodicity

Penrose tiling

Vertex of rhombus
→ lattice point

Edge of rhombus
→ hopping t



Five-fold rotational symmetry

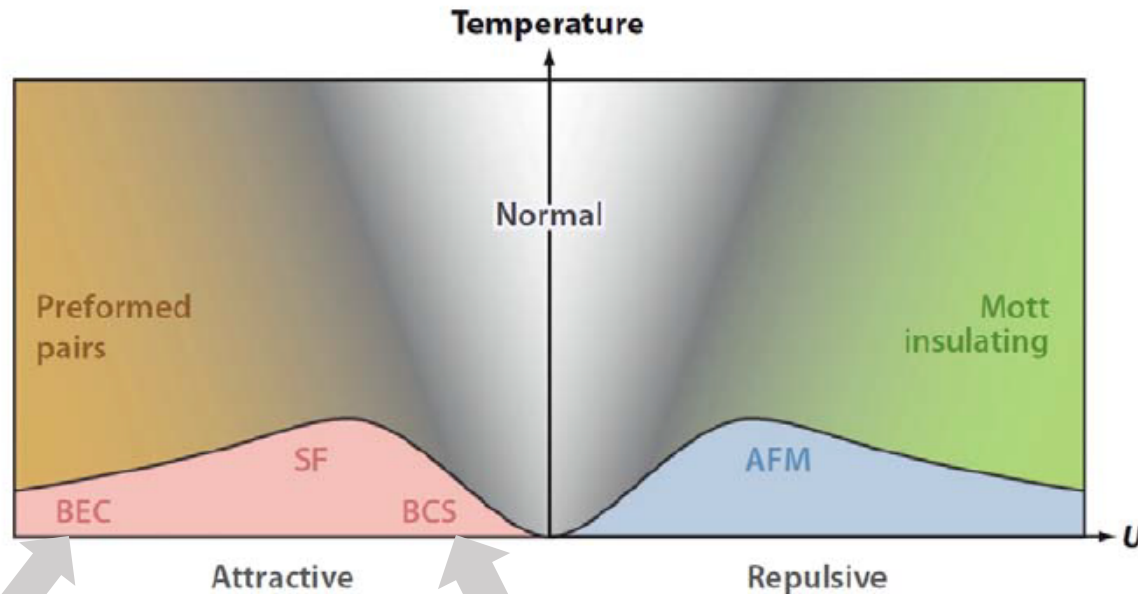
Model with pairing attraction

Attractive Hubbard model

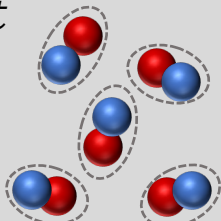
$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$U < 0$$

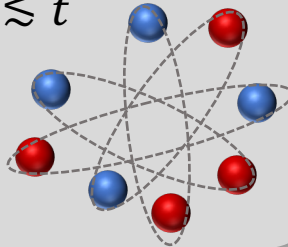
Cubic lattice
Half filling



Strong attraction
 $|U| \gg t$



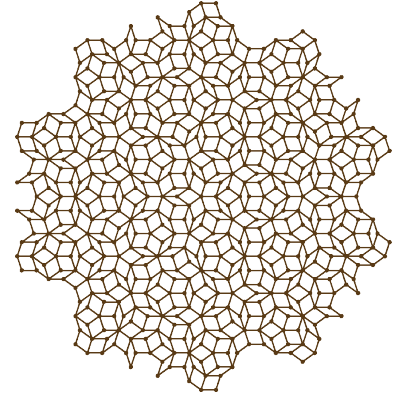
Weak attraction
 $|U| \lesssim t$



- SC at low T for any $U < 0$.
- BCS-BEC crossover with U .

Attractive Hubbard model on Penrose tiling

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad \text{on}$$



Inhomogeneity $\rightarrow$ Real-space approaches

Bogoliubov-de Gennes theory (BdG)

- Static mean field (one-body approx., weak U)
- Large size ~ 1 million sites : Y. Nagai, JPSJ **89**, 074703 (2020)

Real-space dynamical mean-field theory (RDMFT)

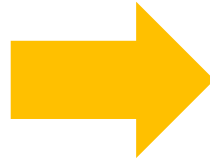
- Dynamical mean field (many-body physics, weak-to-strong U)
- $< 10,000$ sites

A. Georges *et al.*, RMP **68**, 13 (1996)

M. Potthoff and W. Nolting, PRB **59**, 2549 (1999)

Bogoliubov - de Gennes theory (BdG)

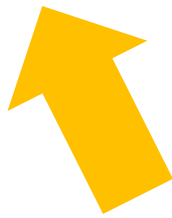
Eigenenergy
Eigenstates



$$n_{i\sigma} = \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$$

$$\Delta_i = U \langle c_{i\uparrow} c_{i\downarrow} \rangle$$

Site-dependent local quantities

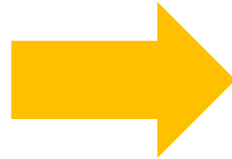


$$\hat{H}_{BdG} = \begin{pmatrix} Un_{1\downarrow} - \mu & -t & \cdots & \Delta_1 & 0 & \cdots \\ -t & Un_{2\downarrow} - \mu & \cdots & 0 & \Delta_2 & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\ \Delta_1 & 0 & \cdots & -Un_{1\uparrow} + \mu & t & \cdots \\ 0 & \Delta_2 & \cdots & t & -Un_{2\uparrow} + \mu & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \end{pmatrix}$$

: 2N x 2N matrix

Real-space dynamical mean-field theory (RDMFT)

Site-dependent
impurity problem



$$\hat{\Sigma}_i(i\omega_n) = \begin{pmatrix} \Sigma_i^{nor}(i\omega_n) & \Sigma_i^{ano}(i\omega_n) \\ \Sigma_i^{ano}(i\omega_n) & -\Sigma_i^{nor}(-i\omega_n) \end{pmatrix}$$

$$\hat{g}_0(i\omega_n)^{-1} = \hat{G}_{ii}(i\omega_n)^{-1} + \hat{\Sigma}_i(i\omega_n)$$

Exact diag.

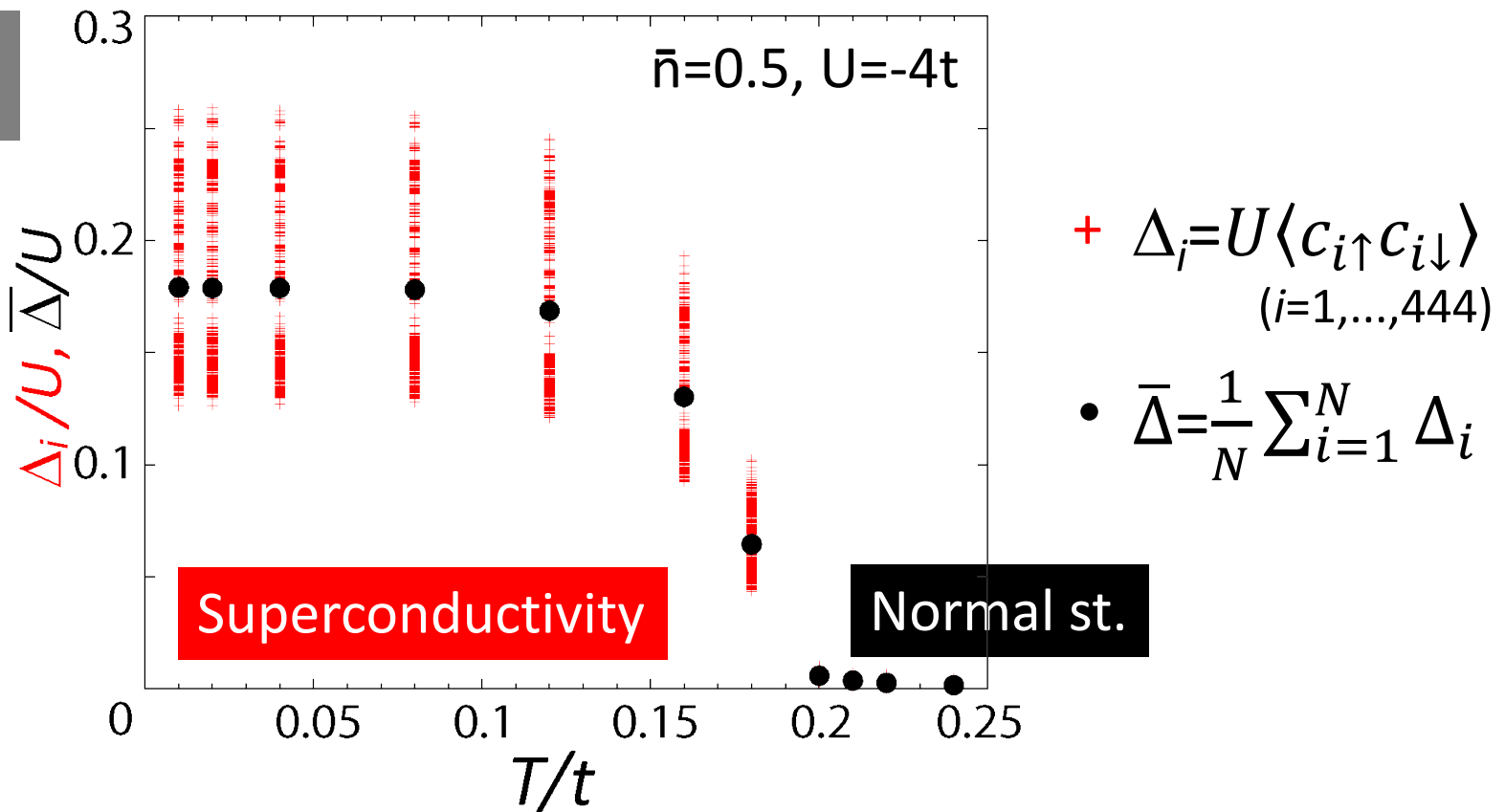
Site- & energy-dependent local self-energy

$$\hat{G}(i\omega_n)^{-1} = \begin{pmatrix} i\omega_n + \mu - \Sigma_1^{nor} & -t & \dots & -\Sigma_1^{ano} & 0 & \dots \\ -t & i\omega_n + \mu - \Sigma_2^{nor} & \dots & 0 & -\Sigma_2^{ano} & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\ -\Sigma_1^{ano} & 0 & \dots & i\omega_n - \mu + \Sigma_1^{nor} & t & \dots \\ 0 & -\Sigma_2^{ano} & \dots & t & i\omega_n - \mu + \Sigma_2^{nor} & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \end{pmatrix}$$

: 2N x 2N matrix

- *Geometry of the Penrose lattice comes in the one-body part.*
- *Nonlocal correlations are neglected.*

Local SC order parameter



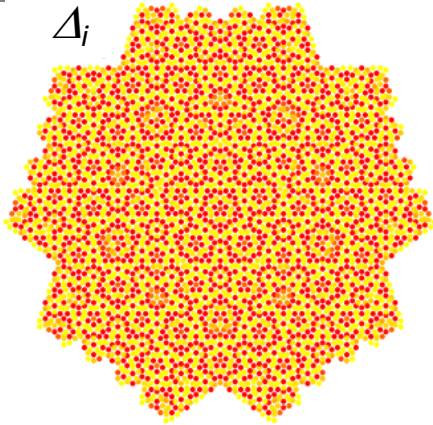
- Superconductivity occurs at low T .
- Transition occurs *simultaneously* at every sites.

Three different superconducting states

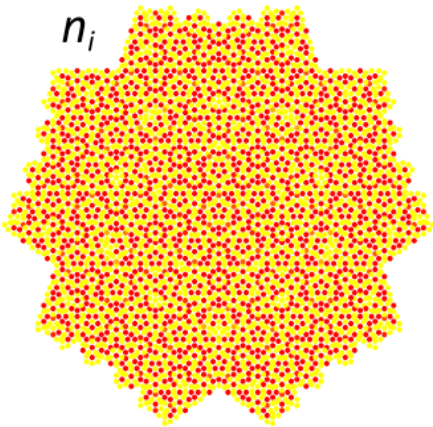
$T=0.01t$

$\bar{n}=0.5, U=-16t$

Δ_i

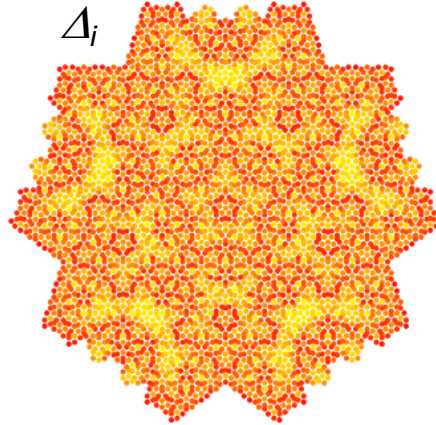


n_i

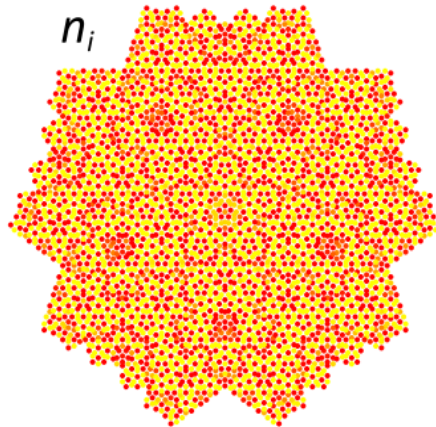


$\bar{n}=0.9, U=-8t$

Δ_i

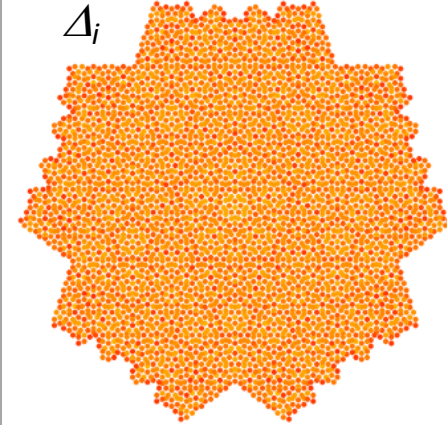


n_i

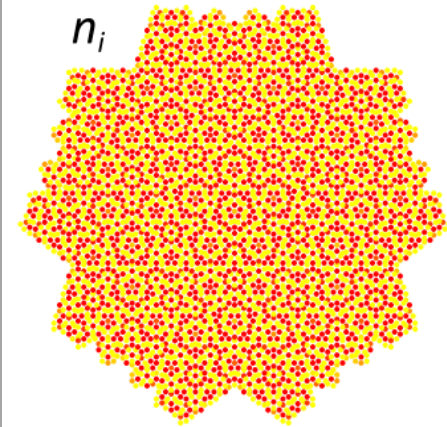


$\bar{n}=0.5, U=-2t$

Δ_i



n_i



large
small

Δ_i

Order similar to n_i

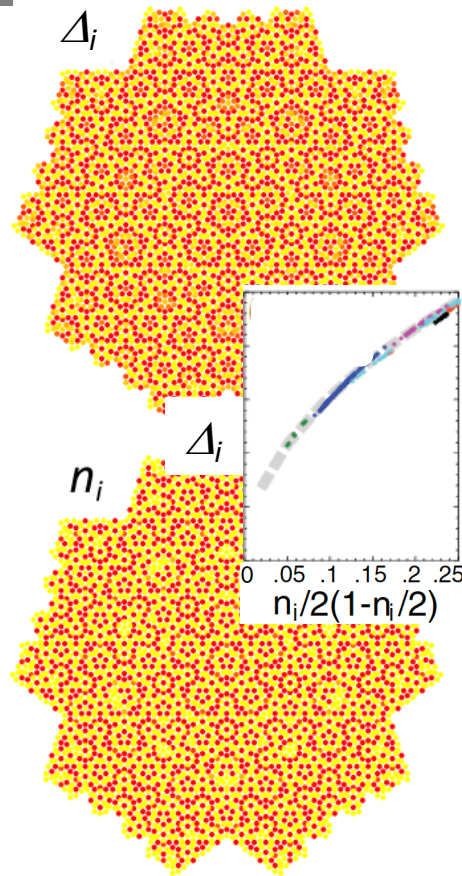
Order different from n_i

No clear pattern

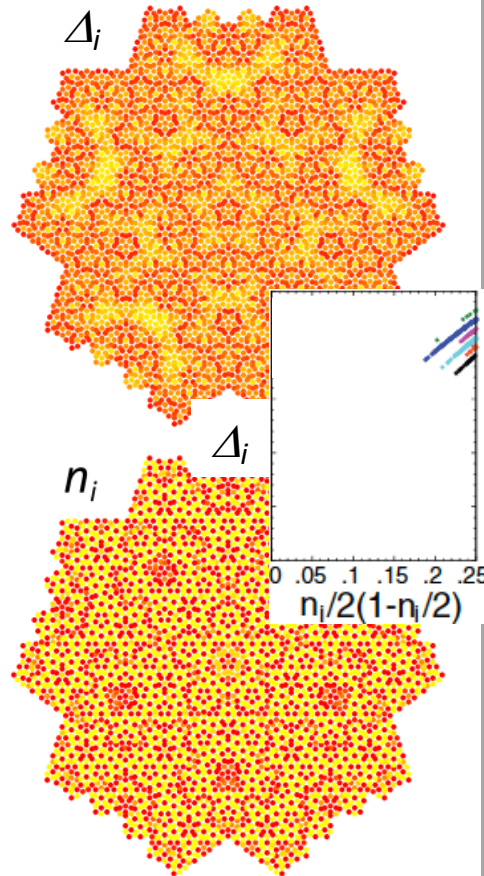
Three different superconducting states

$T=0.01t$

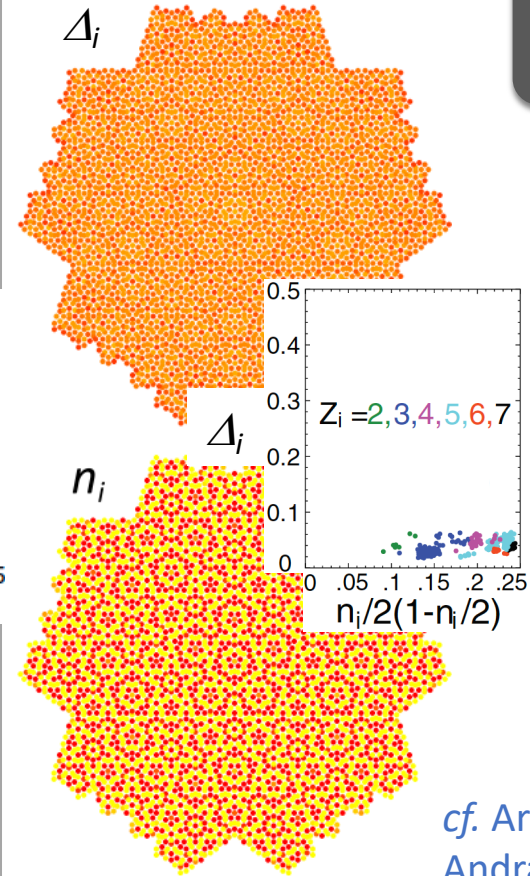
$\bar{n}=0.5, U=-16t$



$\bar{n}=0.9, U=-8t$



$\bar{n}=0.5, U=-2t$



large
small

Δ_i	Order similar to n_i	Order different from n_i	No clear pattern
------------	------------------------	----------------------------	------------------

→ Determined by n_i

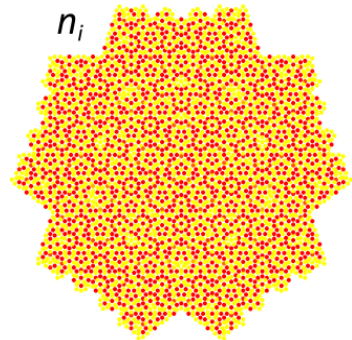
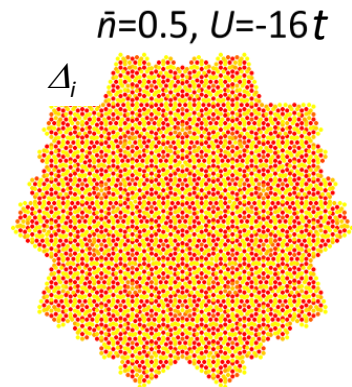
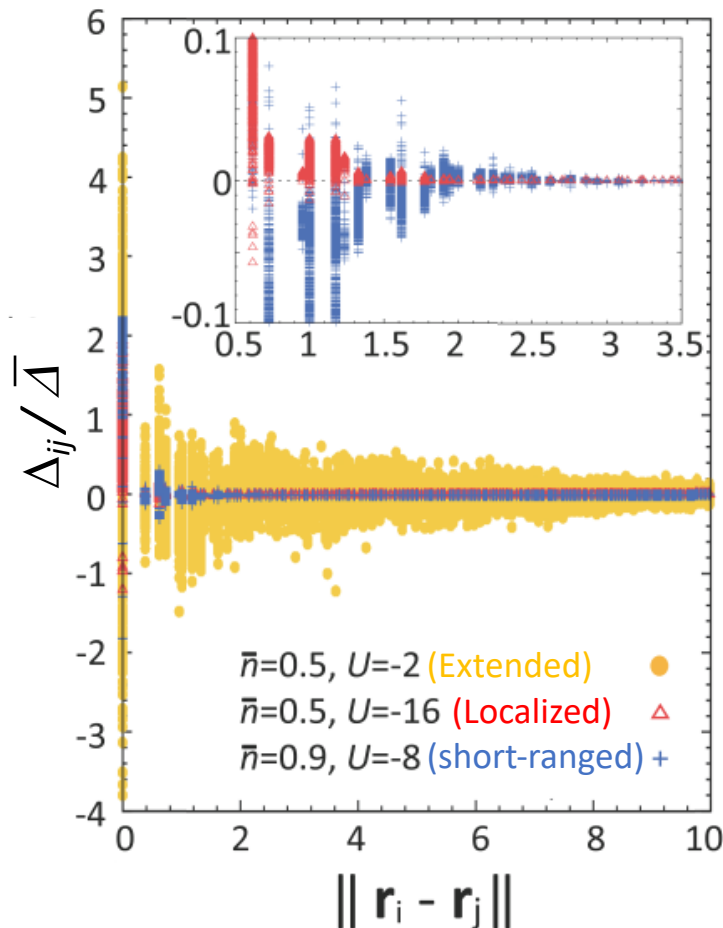
→ Determined by Z_i

→ Determined by LDOS(?)

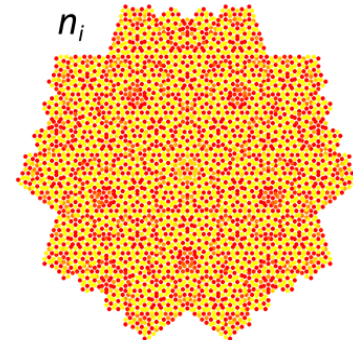
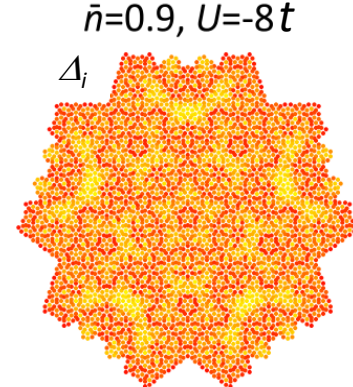
cf. Araujo and Andrade, PRB **100**, 014510 (2019)

Spatial extension of Cooper pairs

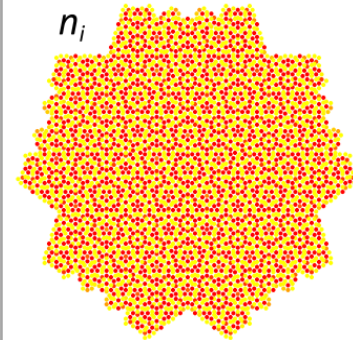
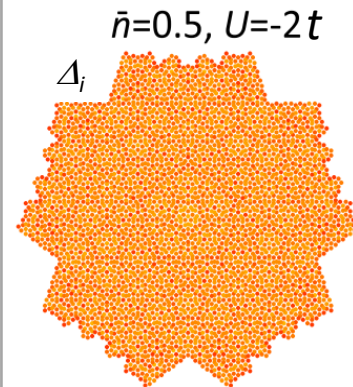
$\Delta_{ij} = \langle c_{i\uparrow} c_{j\downarrow} \rangle$: Off-site SC order parameter



Red (n_i)



Blue (z_i)



Yellow (LDOS)

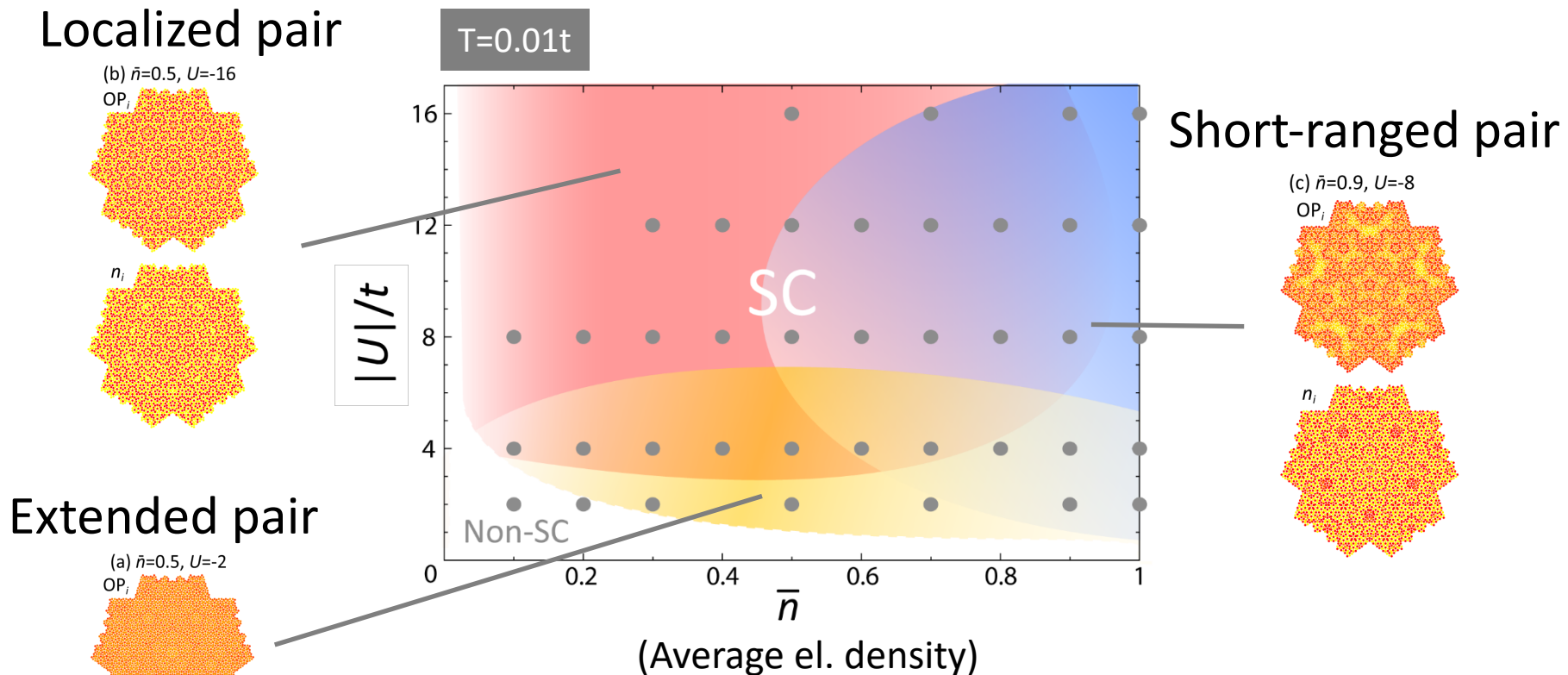
Cooper pairs are

Localized

Short-ranged

Extended

Crossover of three different SC states



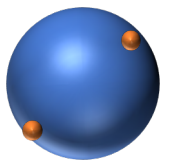
cf. Cooper instability in quasiperiodic system

Y. Zhang *et al.*, arXiv:2002.06485

$$|\Psi_A\rangle = \sum_{mn}^{\tilde{\epsilon}_{m,n}>0} a_{mn} \hat{c}_{m\uparrow}^\dagger \hat{c}_{n\downarrow}^\dagger |\text{FS}\rangle$$

$$\langle \Psi_A | \hat{H} | \Psi_A \rangle < 0 \text{ for any } U < 0$$

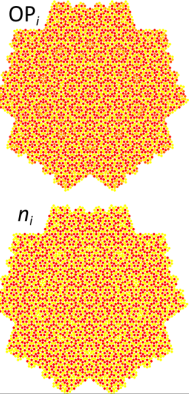
$$\Delta \propto \exp \left[\frac{1}{\alpha U} \right]$$



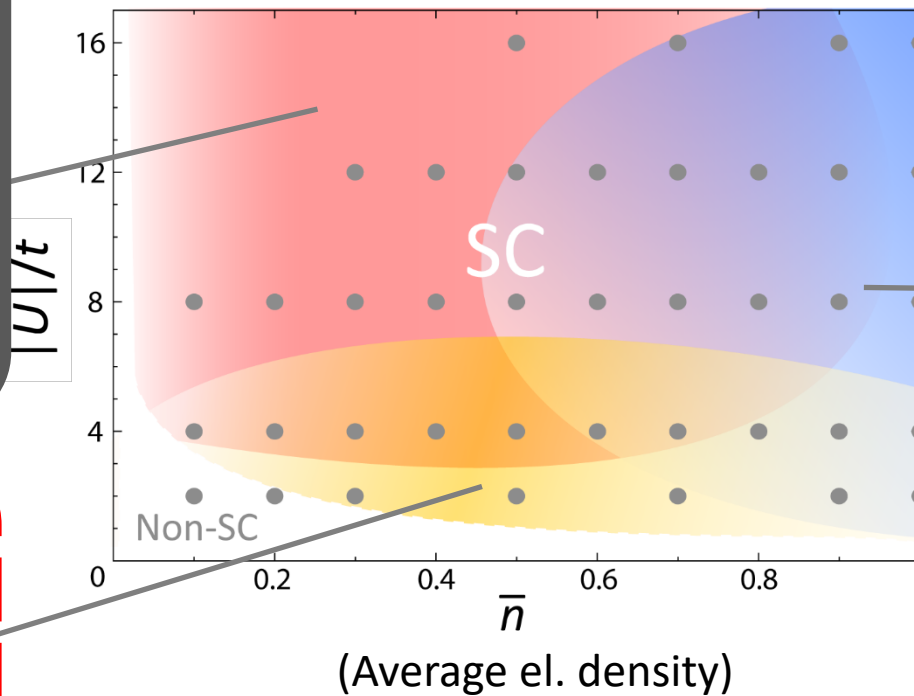
Crossover of three different SC states

Localized pair

(b) $\bar{n}=0.5, U=-16$

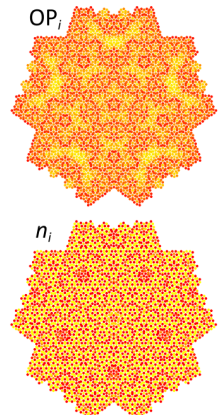


BEC: Lattice structure may be irrelevant



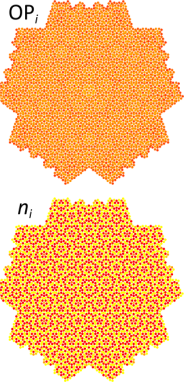
Short-ranged pair

(c) $\bar{n}=0.9, U=-8$



Extended pair

(a) $\bar{n}=0.5, U=-2$



Extended without Fermi surface!
What's happening?

Unusual pairing in momentum space (1)

Cooper pair on periodic lattice: $c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow}$

FT of relative coordinate $i-j$

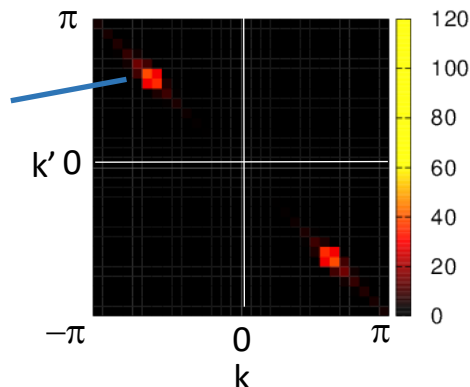
➔ $c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\downarrow}$ for aperiodic lattice

FT of i and j , respectively

Square lattice

$|\langle c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\downarrow} \rangle|$ for $k_x=k_y=k$ and $k'_x=k'_y=k'$

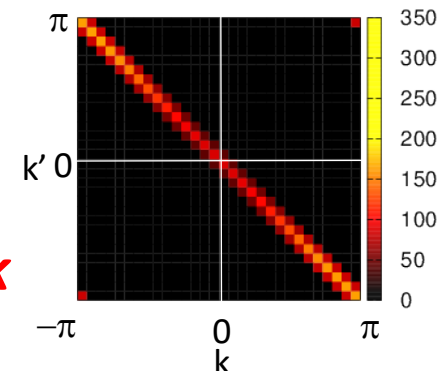
BCS ($U=-t$, $n=0.5$)



Fermi momentum

Finite only along $k'=-k$

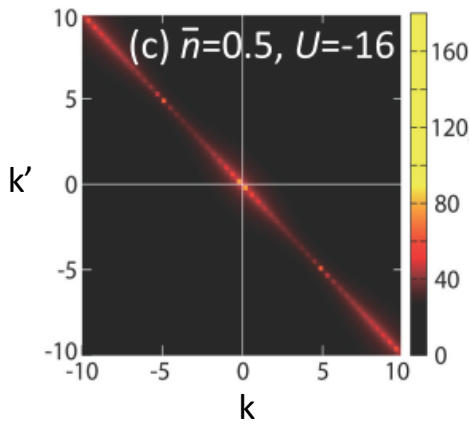
BEC ($U=-16t$, $n=0.5$)



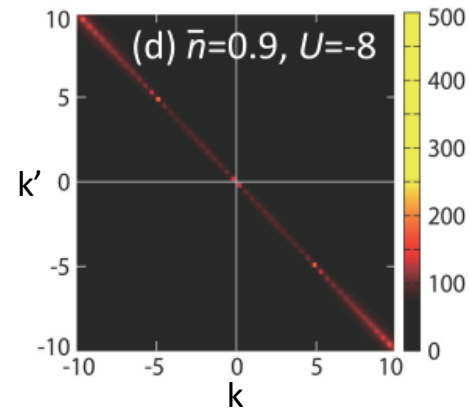
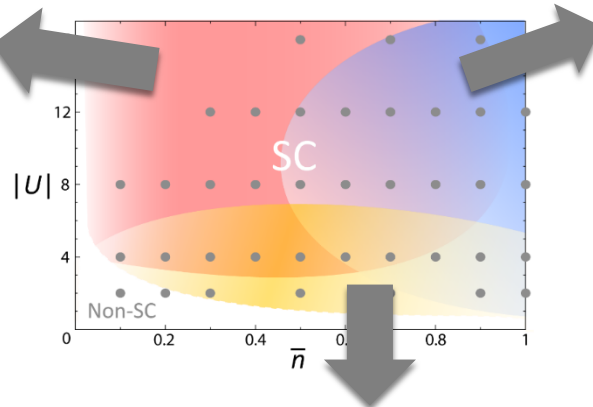
Unusual pairing in momentum space (2)

$$|\langle c_{\mathbf{k}\uparrow} c_{\mathbf{k}'\downarrow} \rangle| \text{ for } k_x = k_y = k \text{ and } k'_x = k'_y = k'$$

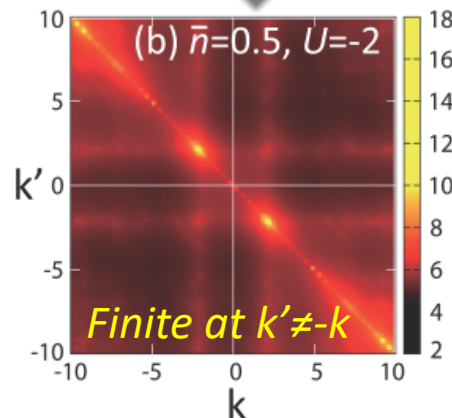
Penrose lattice



Localized pair
→BEC-like



Short-ranged pair
→BEC-like



Extended pair

*Different from both
BCS and BEC characteristics*

What about the property?

Universal properties in BCS theory

$$\frac{2E_g^0}{T_c} \cong 3.52$$

$$E_g(T): \text{Energy gap}$$
$$E_g^0 = E_g(0)$$

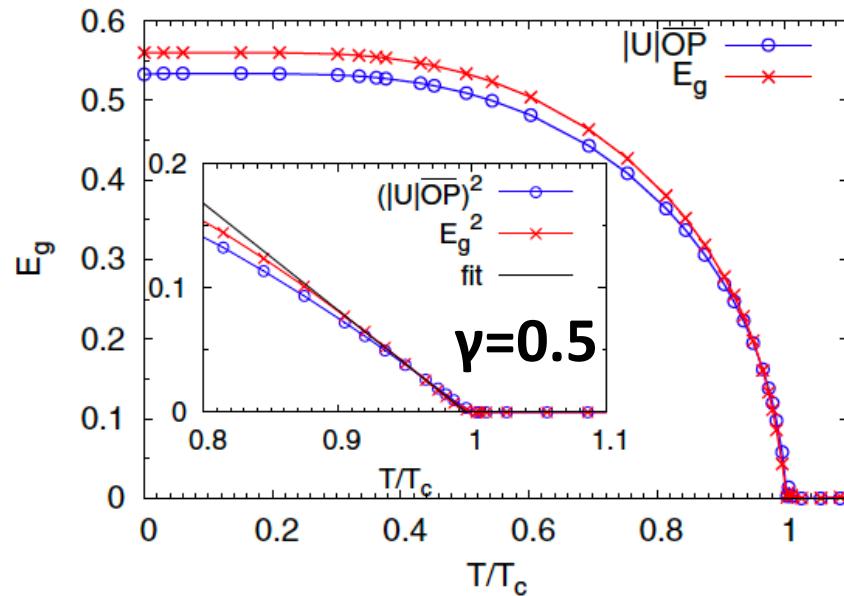
$$\frac{E_g(T)}{E_g^0} \cong A_1 \left(1 - \frac{T}{T_c}\right)^\gamma, A_1 \cong 1.74, \gamma = \frac{1}{2}$$

$$\frac{\Delta C_e}{C_{en}} \cong 1.43 : \text{Jump of specific heat}$$

Does these relations hold in quasiperiodic SC?

The gap & T_c

BdG
 $U=-3t$



cf. Amorphous SC

amorphous metal	T_c [K]	$2\Delta_0$ [meV]	$\frac{2\Delta_0}{kT_c}$	λ
Bi	6,1	2,42	4,60	2,2 - 2,46
Ga	8,4	3,32	4,60	1,94 - 2,25
<u>$Sn_{0.9}Cu_{0.1}$</u>	6,76	2,6	4,46	1,84
<u>$Pb_{0.9}Cu_{0.1}$</u>	6,5	2,66	4,75	2,0
<u>$Pb_{0.75}Bi_{0.25}$</u>	6,9	2,96	4,98	2,76
<u>$In_{0.8}Sb_{0.2}$</u>	5,6	2,13	4,40	1,69
<u>$Tl_{0.9}Te_{0.1}$</u>	<u>4,2</u>	1,67	4,6	1,70

Strong coupling SC

Bergmann, Phys. Rep. **27**, 159 (1976)

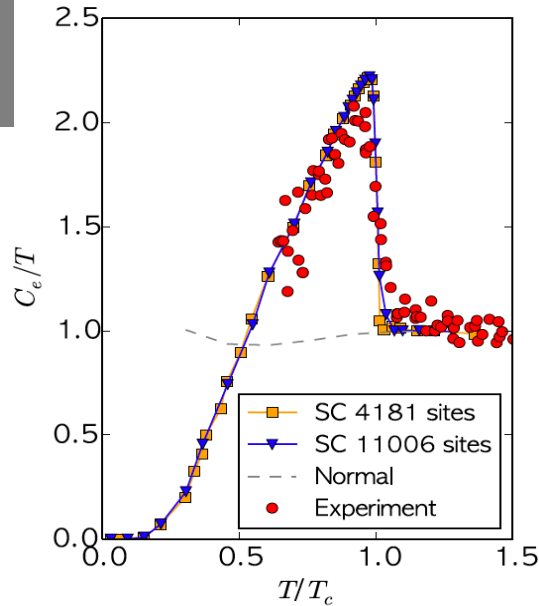
	Penrose				Square		BCS
	1591	4181	11 006	Ext	2500	10 000	
$\frac{2E_g^0}{T_c}$	3.35	3.38	3.38	3.38	3.46	3.45	3.52
A_1	1.61	1.63	1.69	1.70	1.70	1.70	1.74

$2E_g^0/T_c$: Small but substantial shift to a **lower** value $\leftrightarrow$ Amorphous SC

A_1 : No significant change

Jump of specific heat

BdG
U=-3t



$$S = 2 \sum_{\alpha} \left\{ \ln(1 + e^{-\beta E_{\alpha}}) + \frac{\beta E_{\alpha}}{e^{\beta E_{\alpha}} + 1} \right\}$$

$$C_e = T \frac{dS}{dT}$$

Experiment: Kamiya *et al.*, Nature Commun. **9**, 154 (2018)

	Penrose				Square		BCS
	1591	4181	11 006	Ext	2500	10 000	
$\frac{\Delta C}{C_{en}}$	1.13	1.21	1.21	1.21	1.40	1.39	1.43

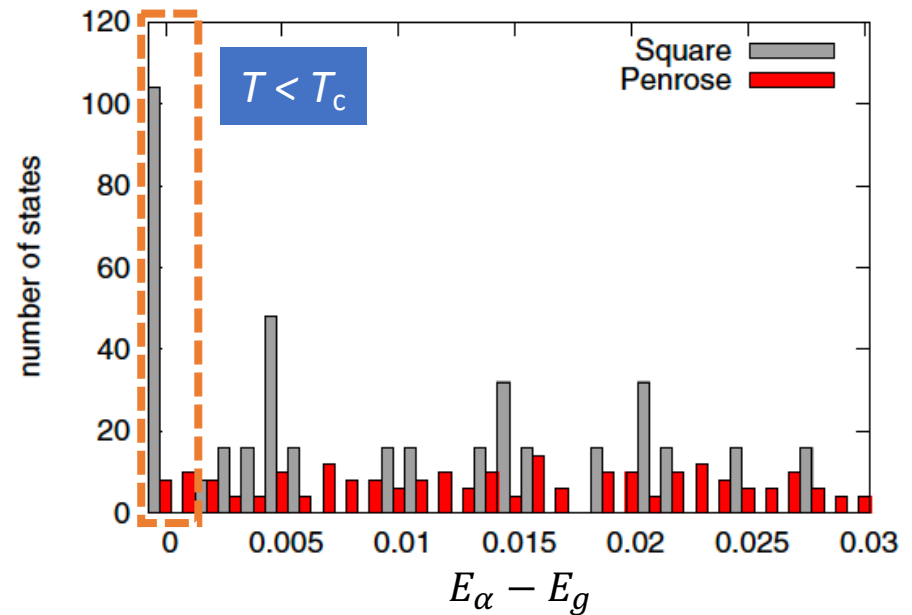
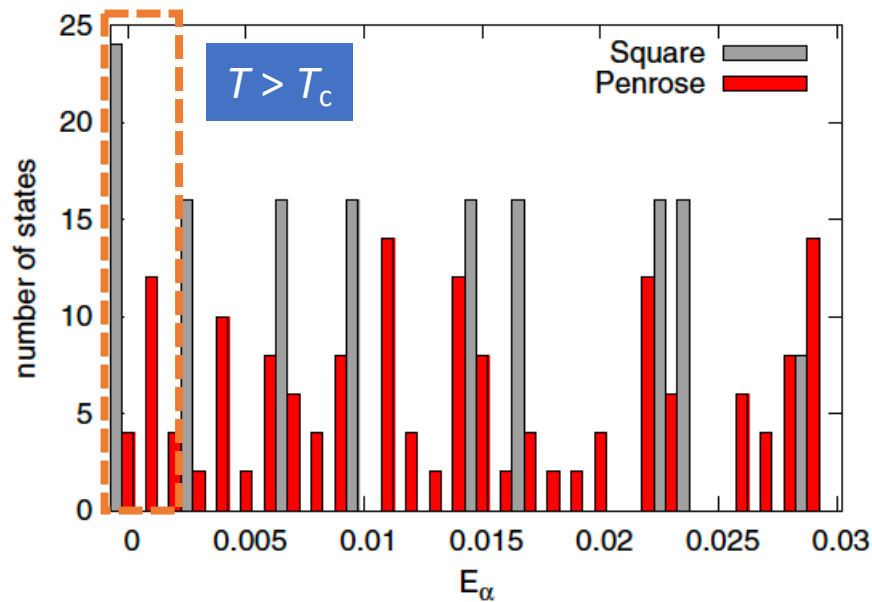
~15 % smaller Jump

Absence of coherence peak

BdG
U=-3t

$$C_e = 2\beta \sum_{\alpha} \left(-\frac{\partial f(E_{\alpha})}{\partial E_{\alpha}} \right) \left(E_{\alpha}^2 + \frac{\beta}{2} \frac{\partial E_{\alpha}^2}{\partial \beta} \right)$$

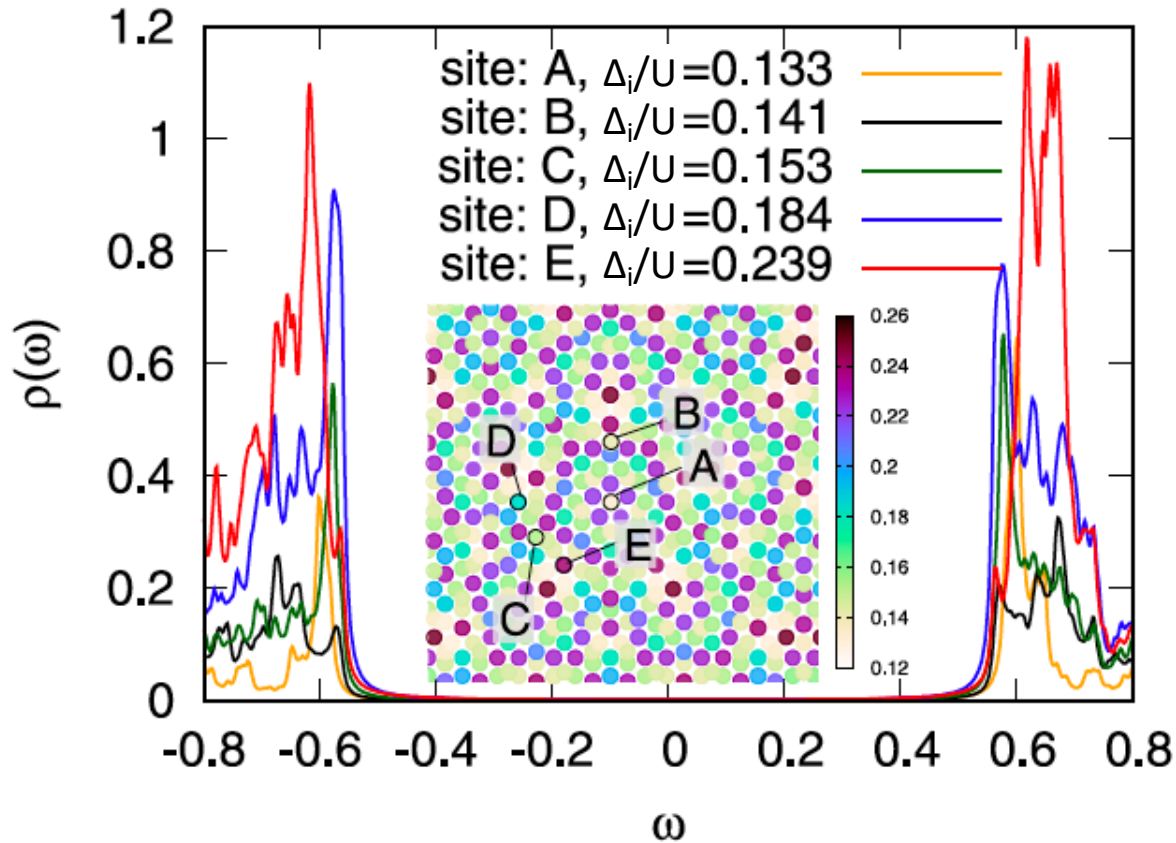
Only around E_F



Absence of Fermi surface $\Rightarrow$ Absence of coherence peak
 $\Rightarrow$ Smaller jump

Local density of states

BdG
 $U=-3t$



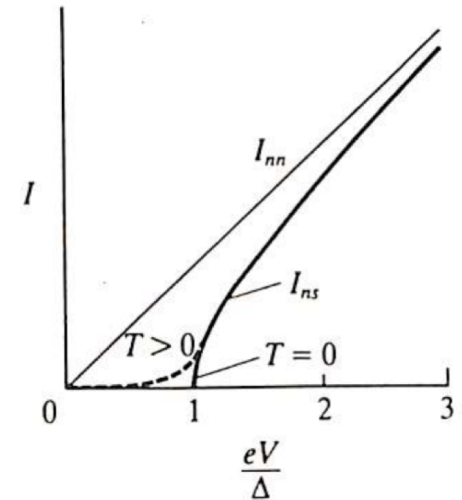
- The spectral gap is much more uniform than $\langle c_{i\uparrow}c_{i\downarrow} \rangle$.
- The weight of spectral peaks significantly depends on sites.

I-V characteristics (1)

Normal metal
(periodic)

Super-
conductor

$$I(V) \propto \int_{-\infty}^{\infty} \rho(E)[f(E) - f(E + eV)]dE$$



$T = 0$

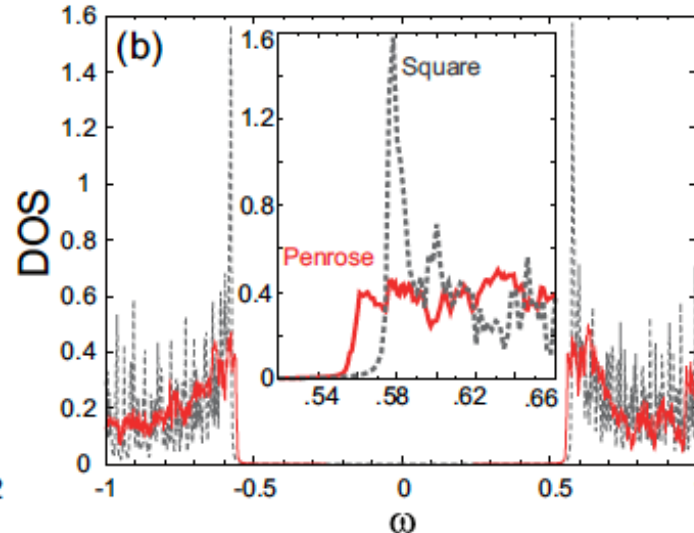
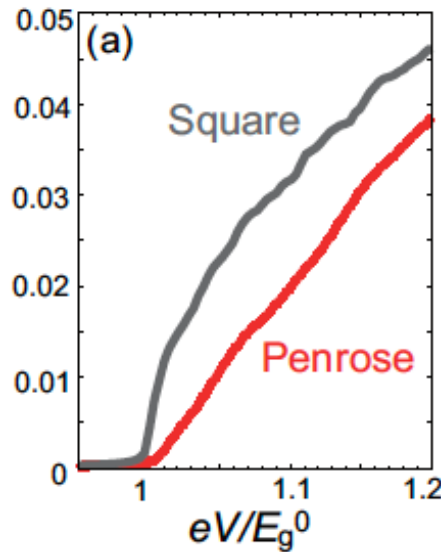


Fig. from M. Tinkham,
INTRODUCTION TO
SUPERCONDUCTIVITY

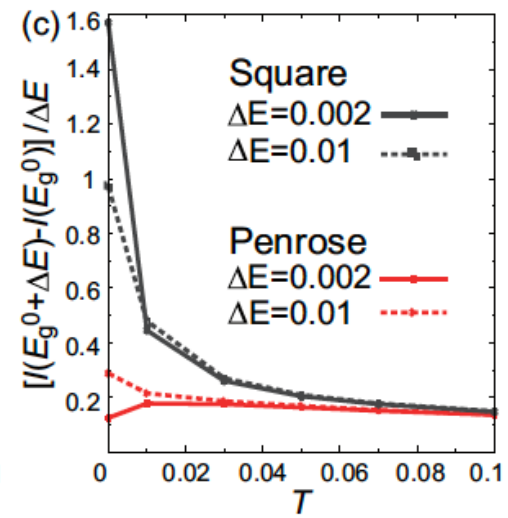
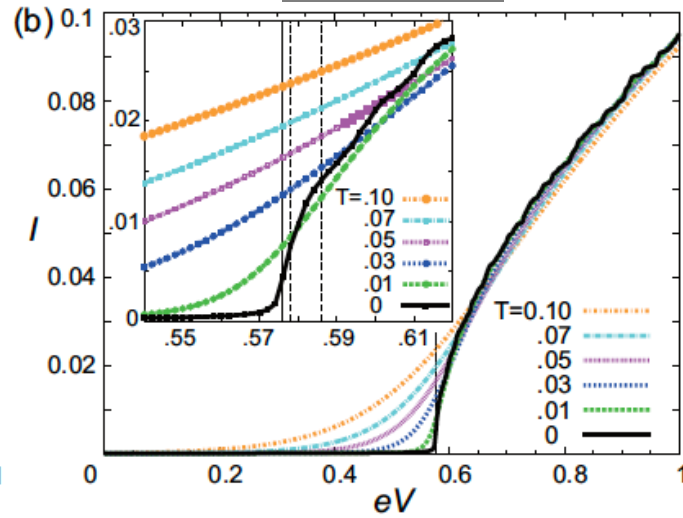
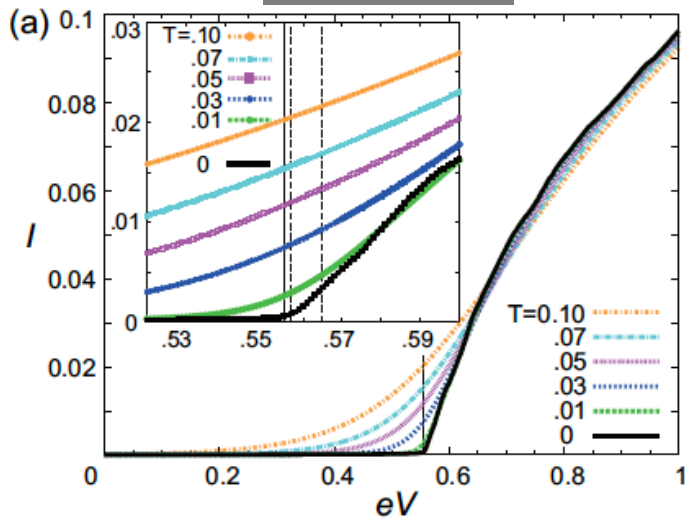
Finite gradient at the threshold voltage ➡ Absence of coherence peak

I - V characteristics (2)

Any signature at finite T ?

Penrose

Square



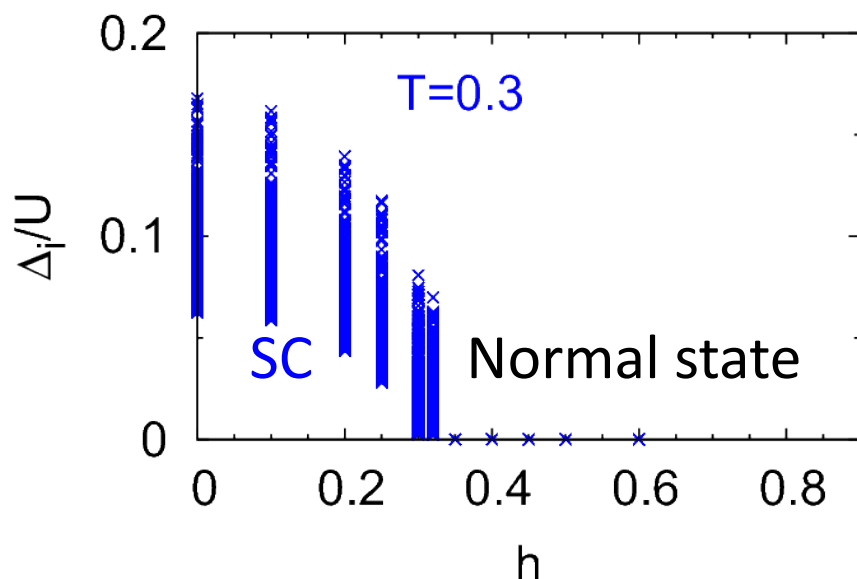
Weakly T -dependent slope signals quasiperiodic SC.

Effect of magnetic field

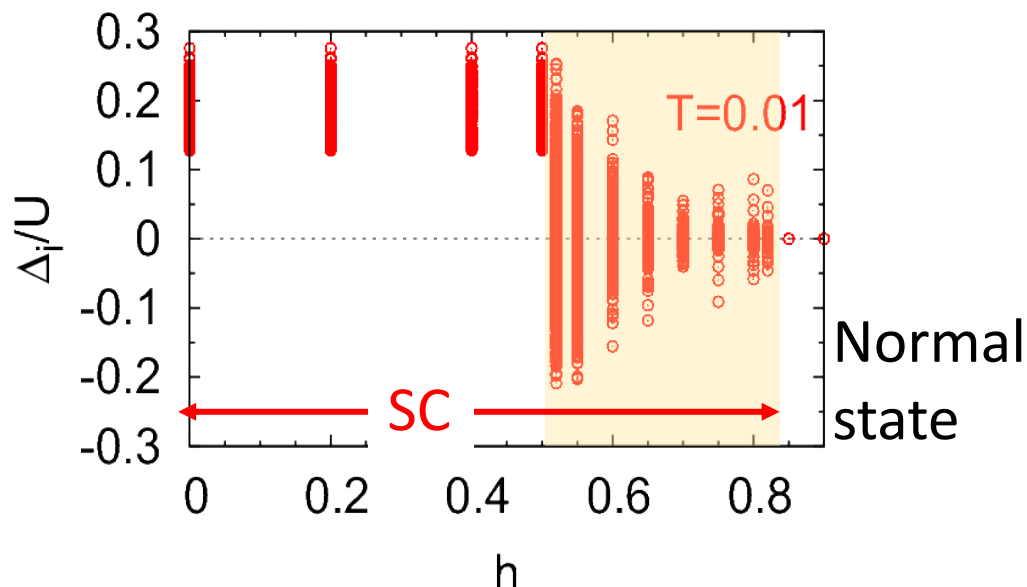
BdG
11006 sites
 $\bar{n}=0.5$
 $t=1, U=-3$

Only Zeeman effect, no orbital motion : Magnetic field parallel to plane

$$T_c(h=0)=0.34$$

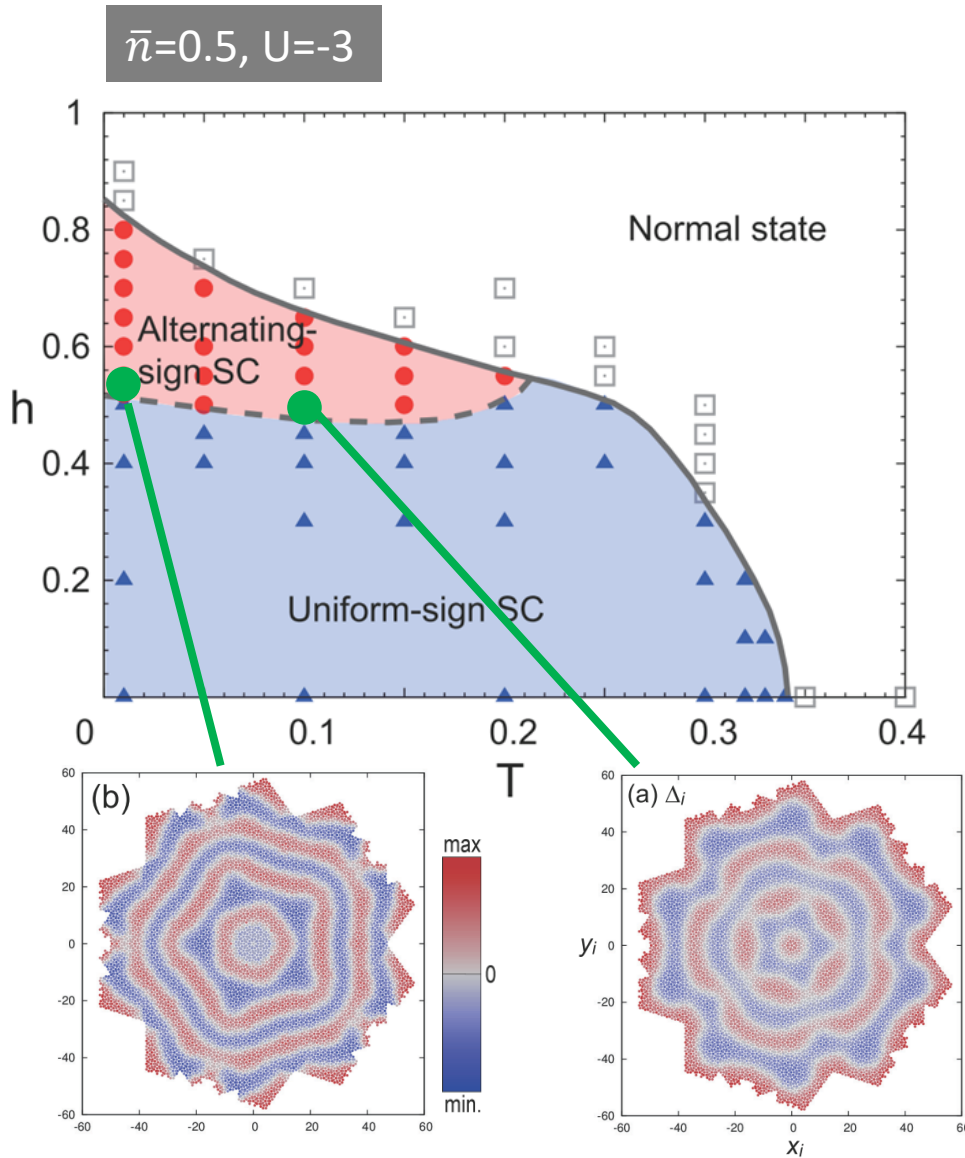


- 1st order transition.
- $\Delta_i \geq 0$.



- Strange behavior before H_c .
- Both positive and negative Δ_i .

FFLO-like state in quasiperiodic systems



FFLO in periodic systems

Fulde and Ferrell, PR **135**, A550 (1964).

Larkin and Ovchinnikov, ZETF **47**, 1136 (1964).

$$\langle c_{\mathbf{k}+\mathbf{q}\uparrow} c_{-\mathbf{k}\downarrow} \rangle$$

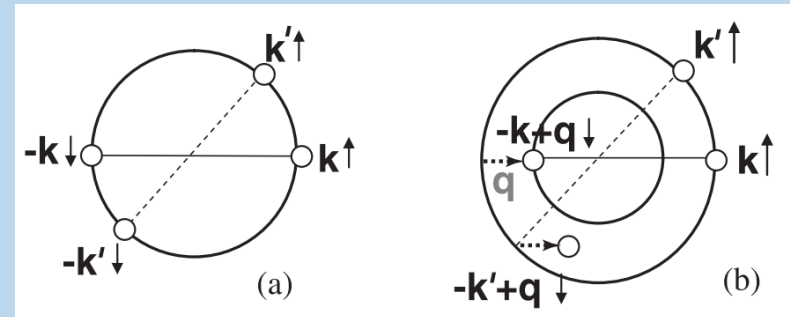


Fig. from Matsuda and Shimahara, JPSJ **76**, 051005 (2007).

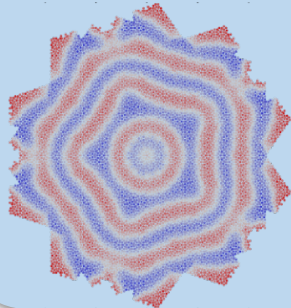
Even without Fermi surface, the sign change occurs!

Impurities
(random potential)

Quasiperiodic
potential



FFLO-like states



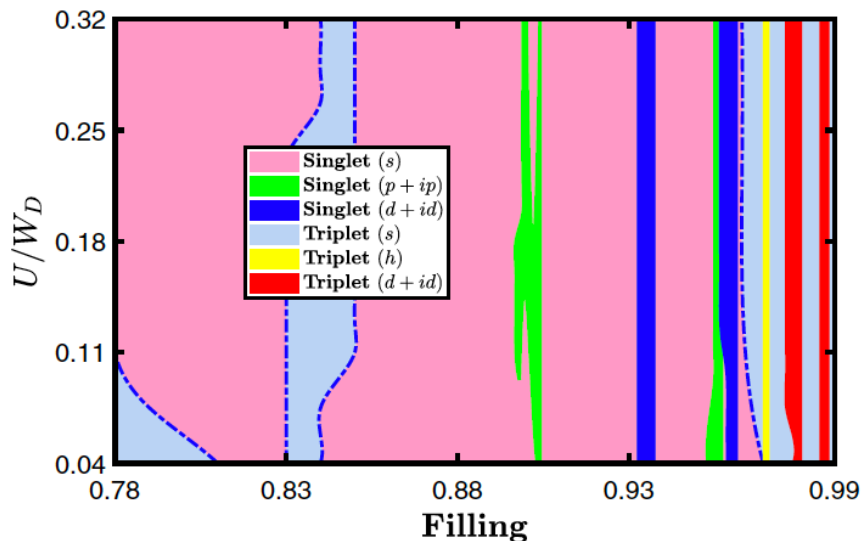
*Electrons self-organize into
a pattern compatible with
the quasiperiodicity!*

Are any other exotic pairings possible?

Kohn-Luttinger Mechanism Driven Exotic Topological Superconductivity on the Penrose Lattice

Ye Cao,¹ Yongyou Zhang¹, Yu-Bo Liu,¹ Cheng-Cheng Liu,¹ Wei-Qiang Chen,^{2,3,4} and Fan Yang^{1,*}

- Anisotropic and/or spin-triplet pairings
- Superconductivity from repulsive U
- Kohn-Luttinger mechanism without Fermi surface
- Topological superconductivity
- Spontaneous vortices without magnetic field



Angular momentum of absolute coordinate,
NOT a relative one of a pair

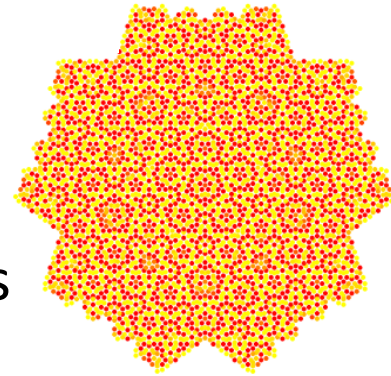


Both spin-singlet and triplet are possible
for each orbital pairing.

Summary

- Order parameter shows various spatial patterns, depending on the spatial extent of Cooper pairs.
- Weak-coupling SC with unusual extended Cooper pairs

SS, N. Takemori, A. Koga and R. Arita, PRB **95**, 024509 (2017).



- Deviation from the BCS universal properties

N. Takemori, R. Arita and SS, PRB **102**, 115108 (2020).

- FFLO-like SC at high magnetic field

SS and R. Arita, Phys. Rev. Research **1**, 022002(R) (2019).

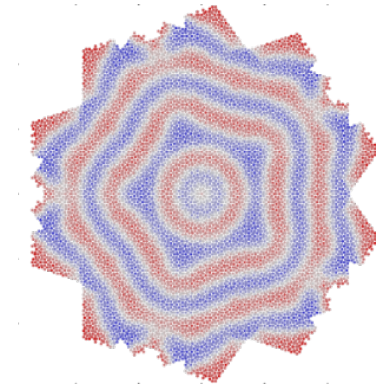
- Anisotropic SC

Y. Cao *et al.*, PRL **125**, 017002 (2020).

- Topological SC

I. C. Fulga *et al.*, PRL **116**, 257002 (2016).

R. Ghadimi *et al.*, arXiv:2006.06952



QC can be a novel platform of exotic SC!