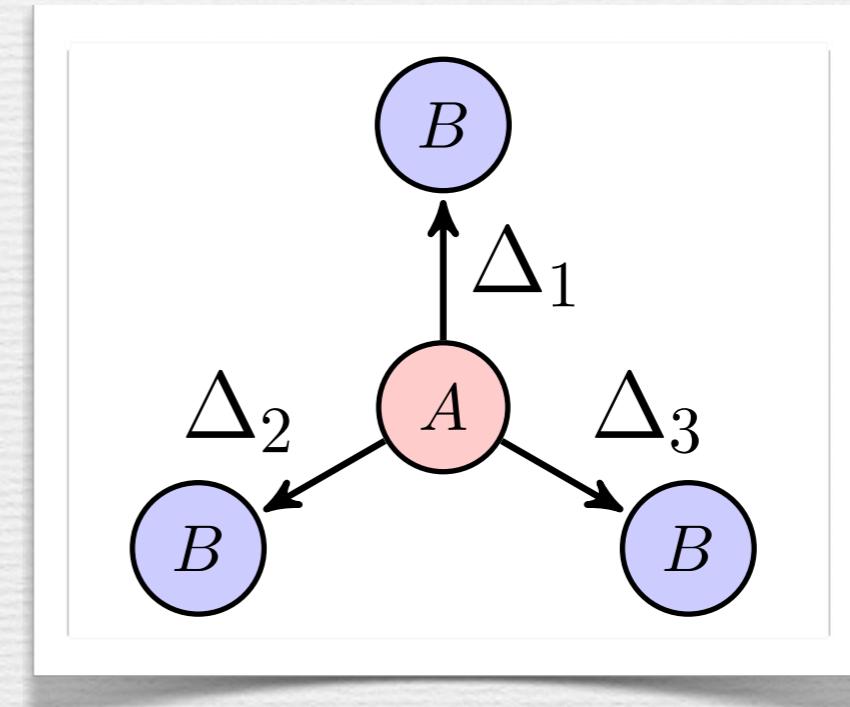
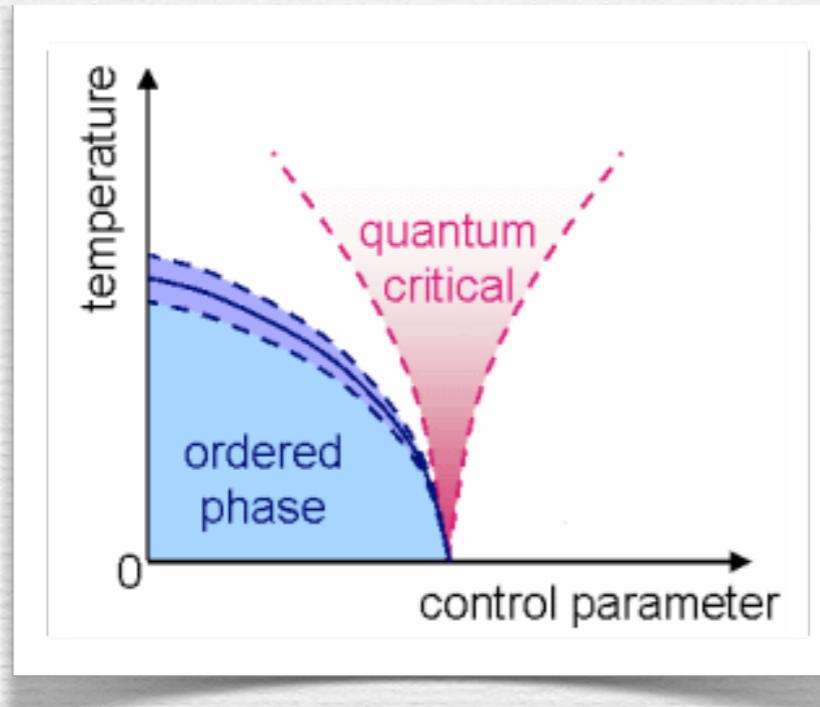


Spinless Fermions on a Honeycomb Lattice

From quantum criticality to topological superconductors

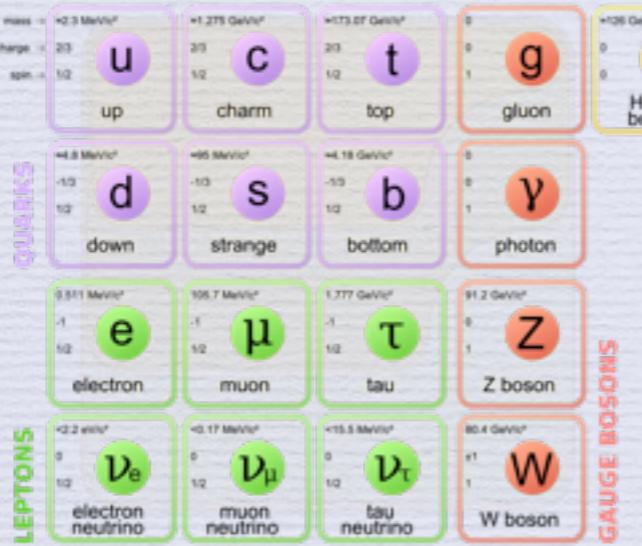


Lei Wang
ETH Zurich

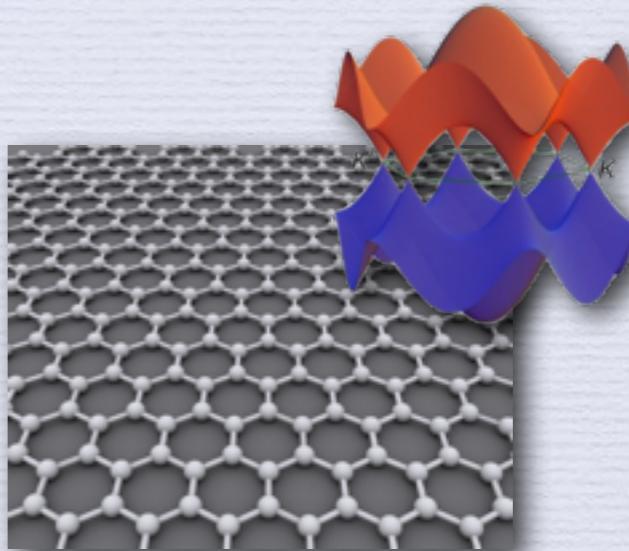
Collaborators
Philippe Corboz
Matthias Troyer

Dirac Fermions

Elementary Particles



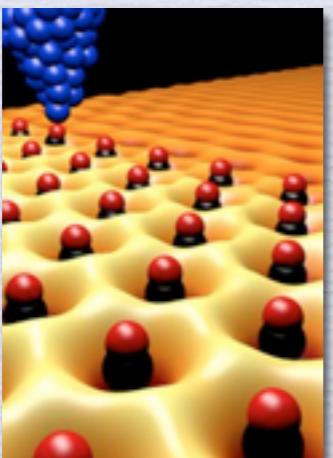
Graphene



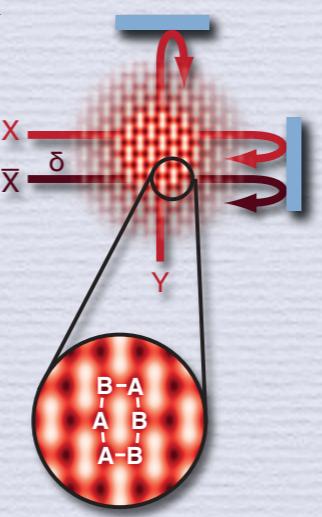
Novoselov et al, Zhang, et al, Nature, 2005

“Artificial graphene”

Gomes et al, Nature, 2012

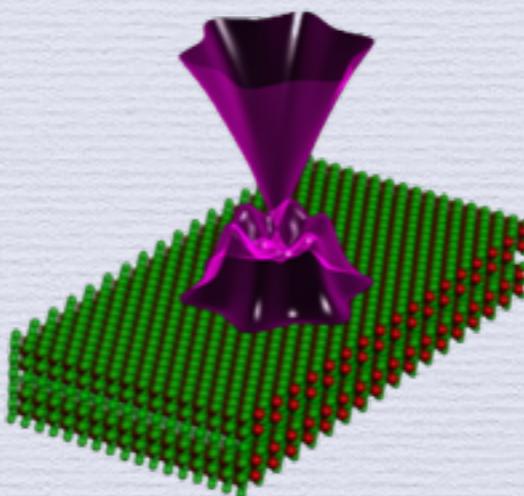


Tarruell et al, Nature, 2012

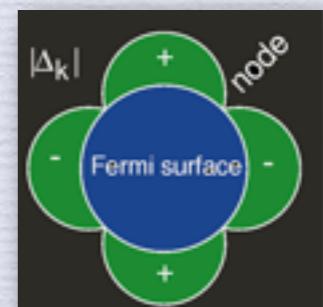


Many others...

Topological insulator



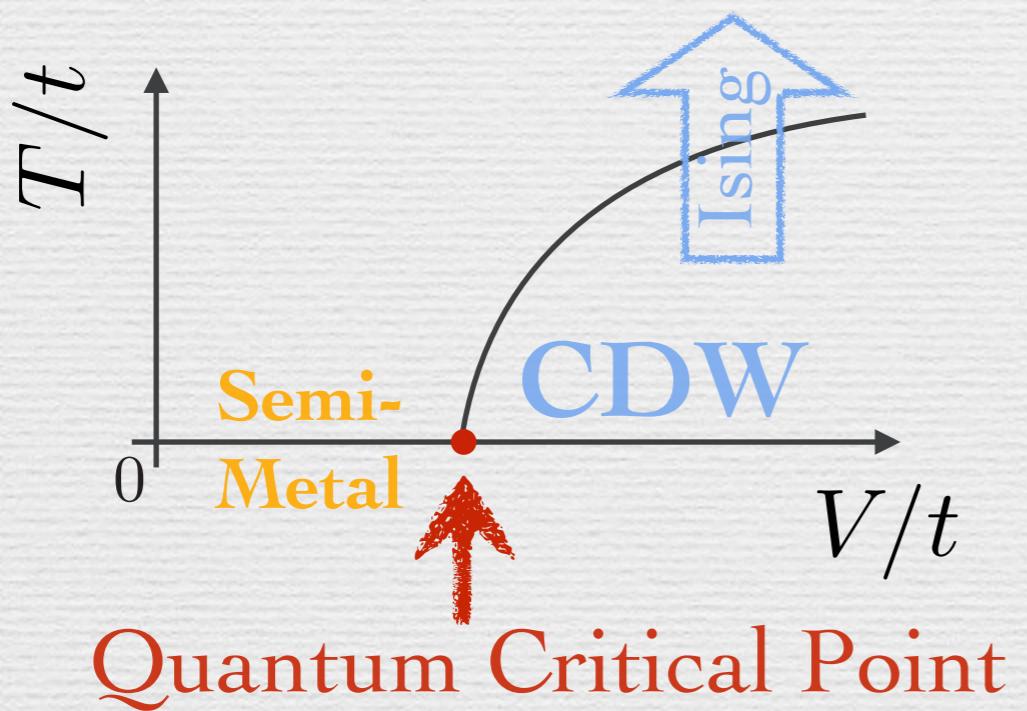
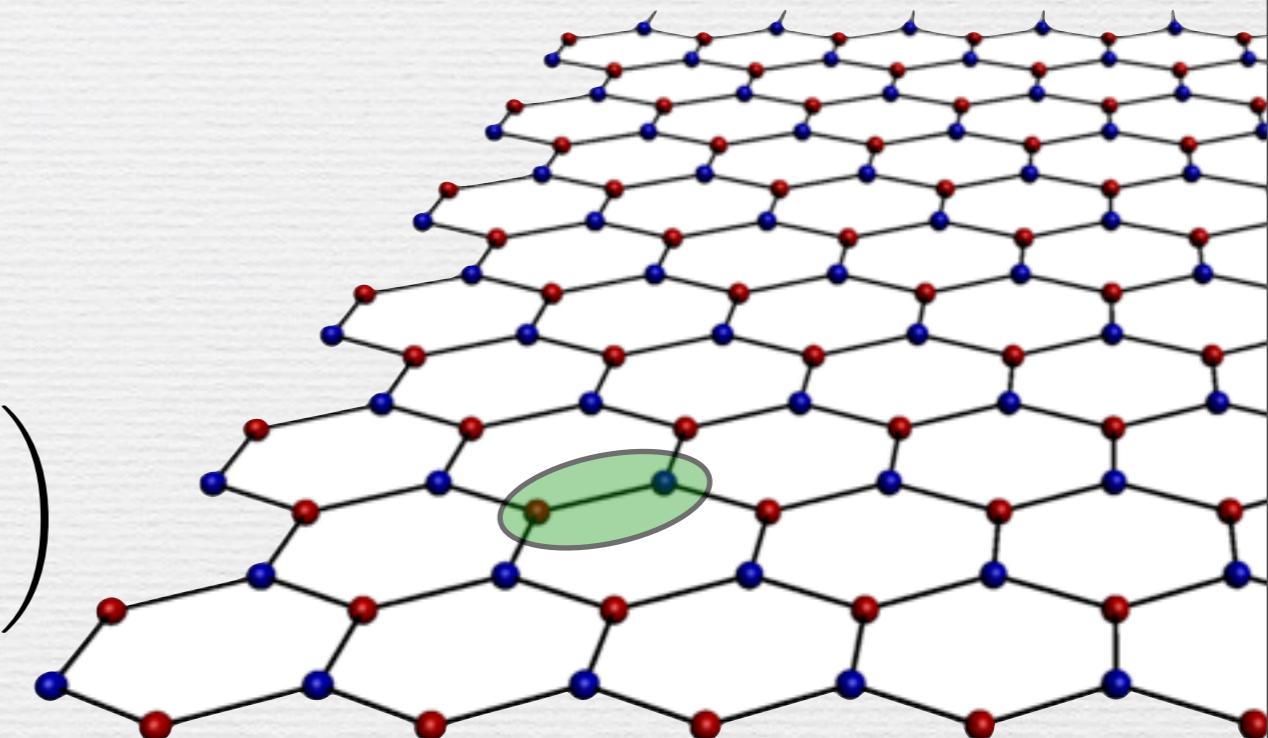
d-wave superconductor



Spinless fermions on a honeycomb lattice

$$\hat{H}_0 = -t \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \hat{c}_{\mathbf{i}}^\dagger \hat{c}_{\mathbf{j}} + h.c.$$

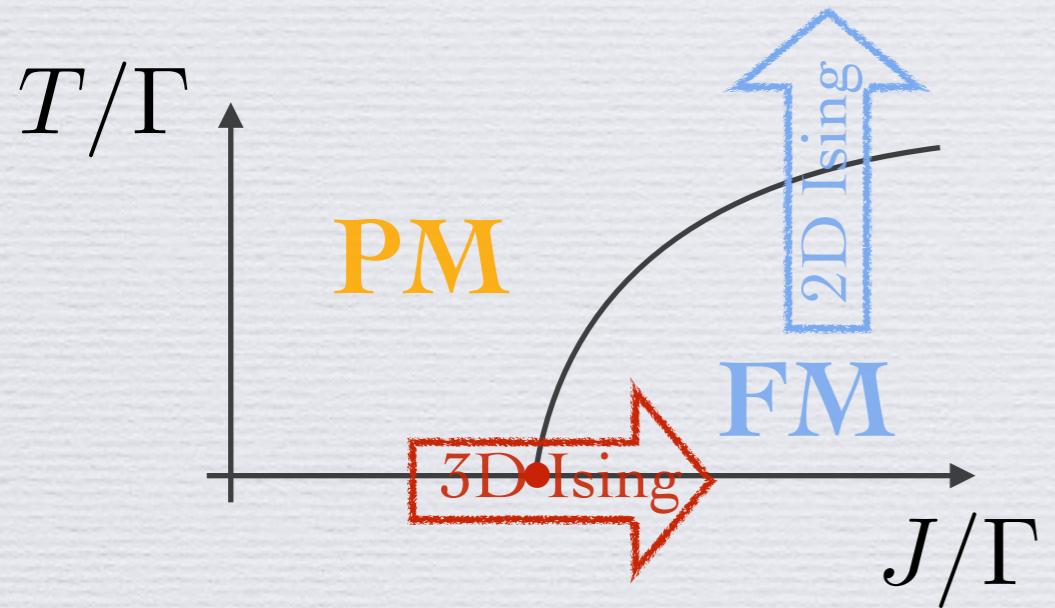
$$\hat{H}_1 = V \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \left(\hat{n}_{\mathbf{i}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{j}} - \frac{1}{2} \right)$$



- Where is the QCP ?
- What is the universality class ?
- What are the critical exponents ?

Quantum Critical Points

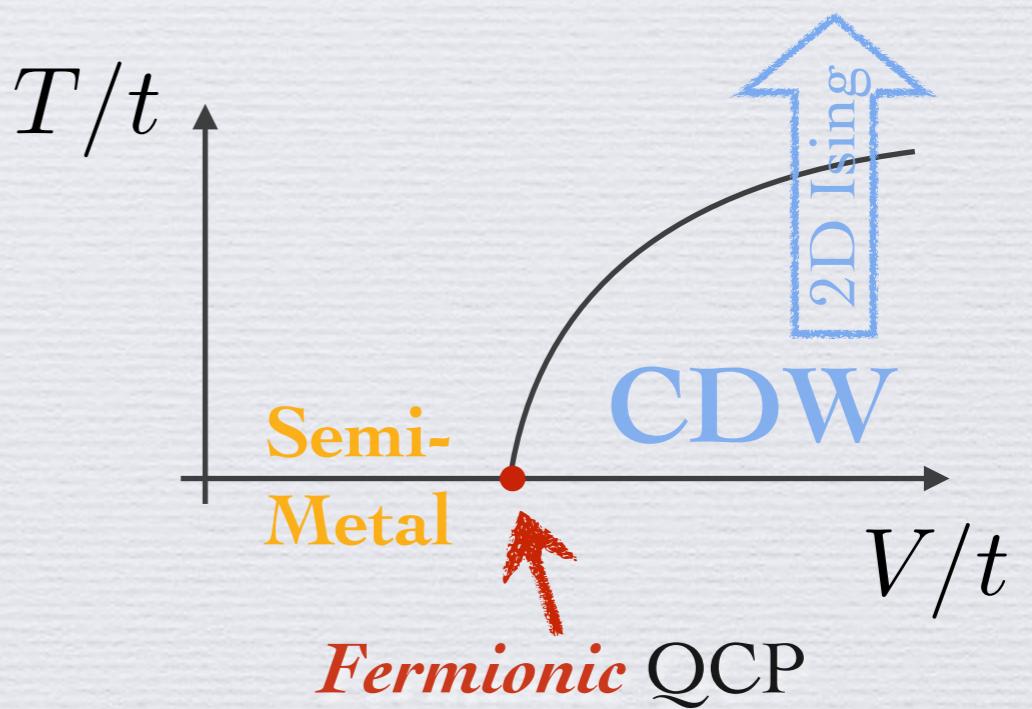
$$H_{\text{TFIM}} = -J \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \sigma_{\mathbf{i}}^z \sigma_{\mathbf{j}}^z + \Gamma \sum_{\mathbf{i}} \sigma_{\mathbf{i}}^x$$



Scalar ϕ^4 -theory

$$\mathcal{L}_\phi = \frac{1}{2}(\partial\phi)^2 - \frac{m^2}{2}\phi^2 - \frac{\lambda}{4!}\phi^4$$

$$H = -t \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} (\hat{c}_{\mathbf{i}}^\dagger \hat{c}_{\mathbf{j}} + h.c.) + V \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \left(\hat{n}_{\mathbf{i}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{j}} - \frac{1}{2} \right)$$



Gross-Neveu-Yukawa theory

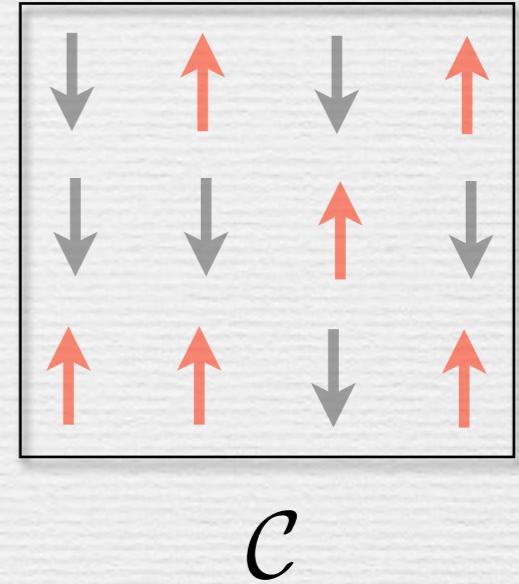
$$\mathcal{L} = \mathcal{L}_\phi + \mathcal{L}_\Psi + g\phi\bar{\Psi}\sigma^z\Psi$$

Sign problem in auxiliary field QMC

Blankenbecler, et al, PRD, 1981

$$Z = \sum_{\mathcal{C}} w(\mathcal{C})$$

- **No sign problem:** attractive Hubbard model with balanced filling



$$w(\mathcal{C}) = \det M_{\uparrow} \times \det M_{\downarrow}$$

$$= |\det M_{\uparrow}|^2 \geq 0$$

- How about spinless fermions ?

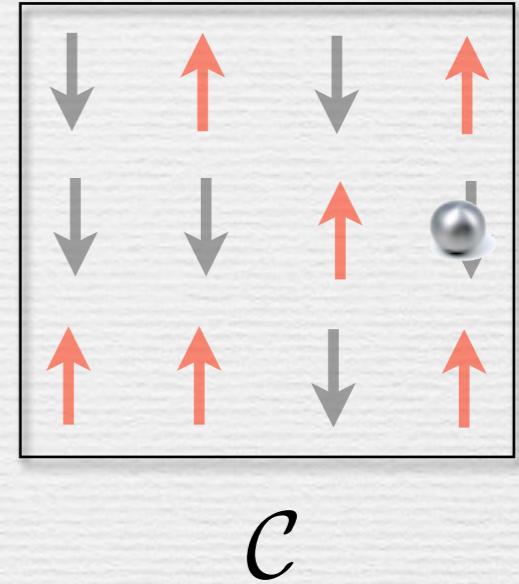
$$w(\mathcal{C}) = \det M$$

Sign problem in auxiliary field QMC

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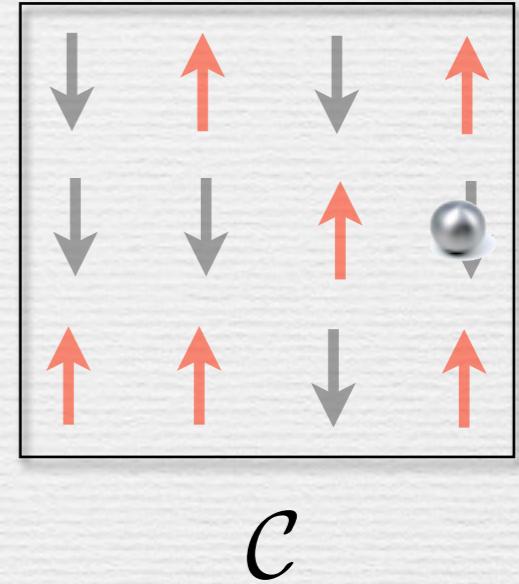
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Sign problem in auxiliary field QMC

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\mathcal{C}

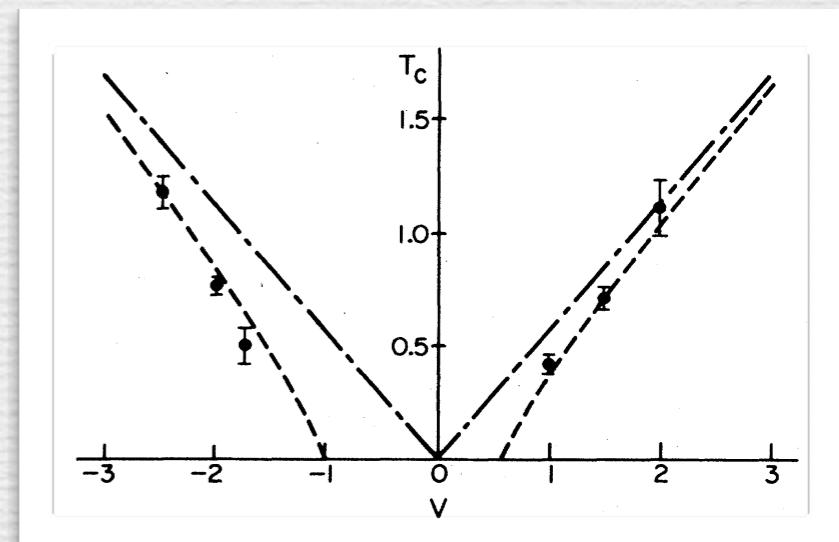
$$w(\mathcal{C}) = \det M_{\uparrow} \times \det M_{\downarrow}$$

$$= |\det M_{\uparrow}|^2 \geq 0$$

Scalapino, et al, PRB, 1984
Gubernatis, et al, PRB, 1985

- How about spinless fermions ?

$$w(\mathcal{C}) = \det M$$



up to 8×8 square lattice, $T=0.3t$

Determinant = Pfaffian²

For skew-symmetric matrices

Huffman and Chandrasekharan, PRB, 2014

$$M = -M^T$$

$$\det M = (\text{pf } M)^2 \geq 0 \quad \text{Muir, 1882}$$

Named after J. F. Pfaff (1765-1825), a teacher of Gauss

$$\text{pf} \begin{pmatrix} 0 & a & b & c \\ -a & 0 & d & e \\ -b & -d & 0 & f \\ -c & -e & -f & 0 \end{pmatrix} = af - be + cd$$



Johann Friedrich Pfaff

Is M skew-symmetric ?

No

$$w(\mathcal{C}) = \det(\mathbb{I} + B_{N_\tau} \dots B_2 B_1)$$

Yes

in **continuous-time** QMC ...

CTQMC

Rubtsov et al, PRB, 2005

Gull et al, RMP, 2011

$$Z = \text{Tr} \left[e^{-\beta \hat{H}_0} \mathcal{T} e^{-\int_0^\beta \hat{H}_1(\tau)} \right]$$

$$\hat{H}_0 = -t \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \hat{c}_{\mathbf{i}}^\dagger \hat{c}_{\mathbf{j}} + h.c.$$

$$\hat{H}_1 = V \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \left(\hat{n}_{\mathbf{i}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{j}} - \frac{1}{2} \right)$$

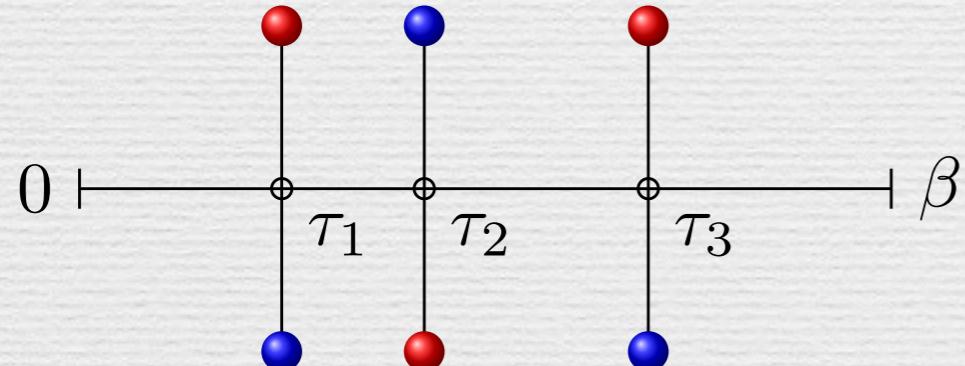
$$= \sum_{k=0}^{\infty} \int_0^{\beta} d\tau_1 \dots \int_{\tau_{k-1}}^{\beta} d\tau_k (-1)^k \text{Tr} \left[e^{-\beta \hat{H}_0} \hat{H}_1(\tau_k) \dots \hat{H}_1(\tau_1) \right]$$

$$= \sum_{\mathcal{C}} w(\mathcal{C})$$

cf. Nikolay's tutorial talk



$$w(\mathcal{C}) = (-V)^k \det(G)$$

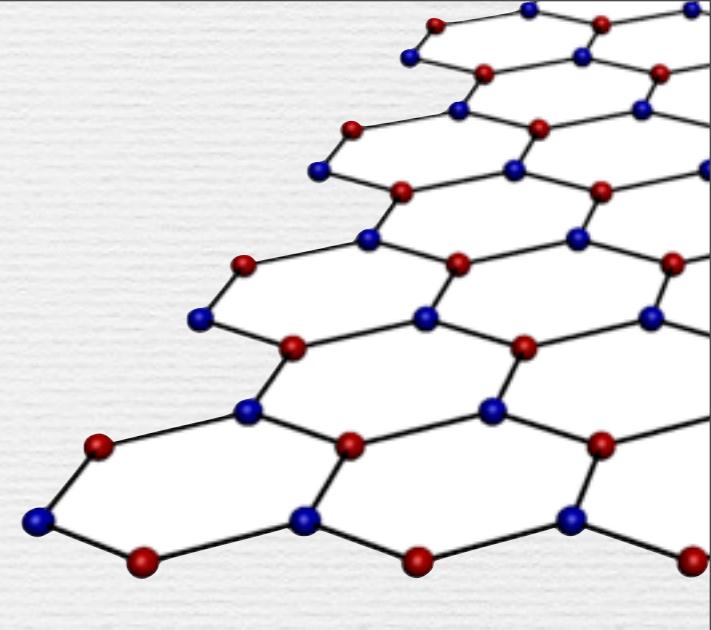


$$G = \begin{pmatrix} \text{Noninteracting} \\ \text{Green's functions} \end{pmatrix}_{2k \times 2k}$$

~~Sign Problem~~

Parity Matrix

$$D = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & \ddots & \\ & & & 1 & -1 \end{pmatrix}_{2k \times 2k}$$



Huffman and Chandrasekharan, PRB, 2014

$$G^T = -DGD$$



$$(GD)^T = -GD$$

$$w(\mathcal{C}) = (-V)^k \det(G)$$

$$= (-V)^k \det(D) \det(GD)$$

$$= V^k \text{pf}(GD)^2 \geq 0$$

*half-filling ensures diagonal element vanishes

Observables & Scaling Ansatz

$$M_2 = \frac{1}{N^2} \sum_{\mathbf{i}, \mathbf{j}} \eta_{\mathbf{i}} \eta_{\mathbf{j}} \left\langle \left(\hat{n}_{\mathbf{i}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{j}} - \frac{1}{2} \right) \right\rangle$$

$$M_4 = \frac{1}{N^4} \sum_{\mathbf{i}, \mathbf{j}, \mathbf{k}, \mathbf{l}} \eta_{\mathbf{i}} \eta_{\mathbf{j}} \eta_{\mathbf{k}} \eta_{\mathbf{l}} \left\langle \left(\hat{n}_{\mathbf{i}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{j}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{k}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{l}} - \frac{1}{2} \right) \right\rangle$$

± 1 for A(B) sublattice



$2L^2$ up to 450 sites

Observables & Scaling Ansatz

$$M_2 = \frac{1}{N^2} \sum_{\mathbf{i}, \mathbf{j}} \eta_{\mathbf{i}} \eta_{\mathbf{j}} \left\langle \left(\hat{n}_{\mathbf{i}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{j}} - \frac{1}{2} \right) \right\rangle$$

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Scalings ansatz close to the QCP

$$M_2 = L^{-z-\eta} \mathcal{F}[L^{1/\nu}(V - V_c), L^z/\beta]$$

$$M_4 = L^{-2z-2\eta} \mathcal{G}[L^{1/\nu}(V - V_c), L^z/\beta]$$

Observables & Scaling Ansatz

$$M_2 = \frac{1}{N^2} \sum_{\mathbf{i}, \mathbf{j}} \eta_{\mathbf{i}} \eta_{\mathbf{j}} \left\langle \left(\hat{n}_{\mathbf{i}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{j}} - \frac{1}{2} \right) \right\rangle$$

± 1 for A(B) sublattice

$$M_4 = \frac{1}{N^4} \sum_{\mathbf{i}, \mathbf{j}, \mathbf{k}, \mathbf{l}} \eta_{\mathbf{i}} \eta_{\mathbf{j}} \eta_{\mathbf{k}} \eta_{\mathbf{l}} \left\langle \left(\hat{n}_{\mathbf{i}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{j}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{k}} - \frac{1}{2} \right) \left(\hat{n}_{\mathbf{l}} - \frac{1}{2} \right) \right\rangle$$

2L² up to 450 sites

Scalings ansatz close to the QCP

relativistic invariance
 $z = 1$

$$M_2 = L^{-z-\eta} \mathcal{F}[L^{1/\nu}(V - V_c), L^z/\beta]$$

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Observables & Scaling Ansatz

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2L² up to 450 sites

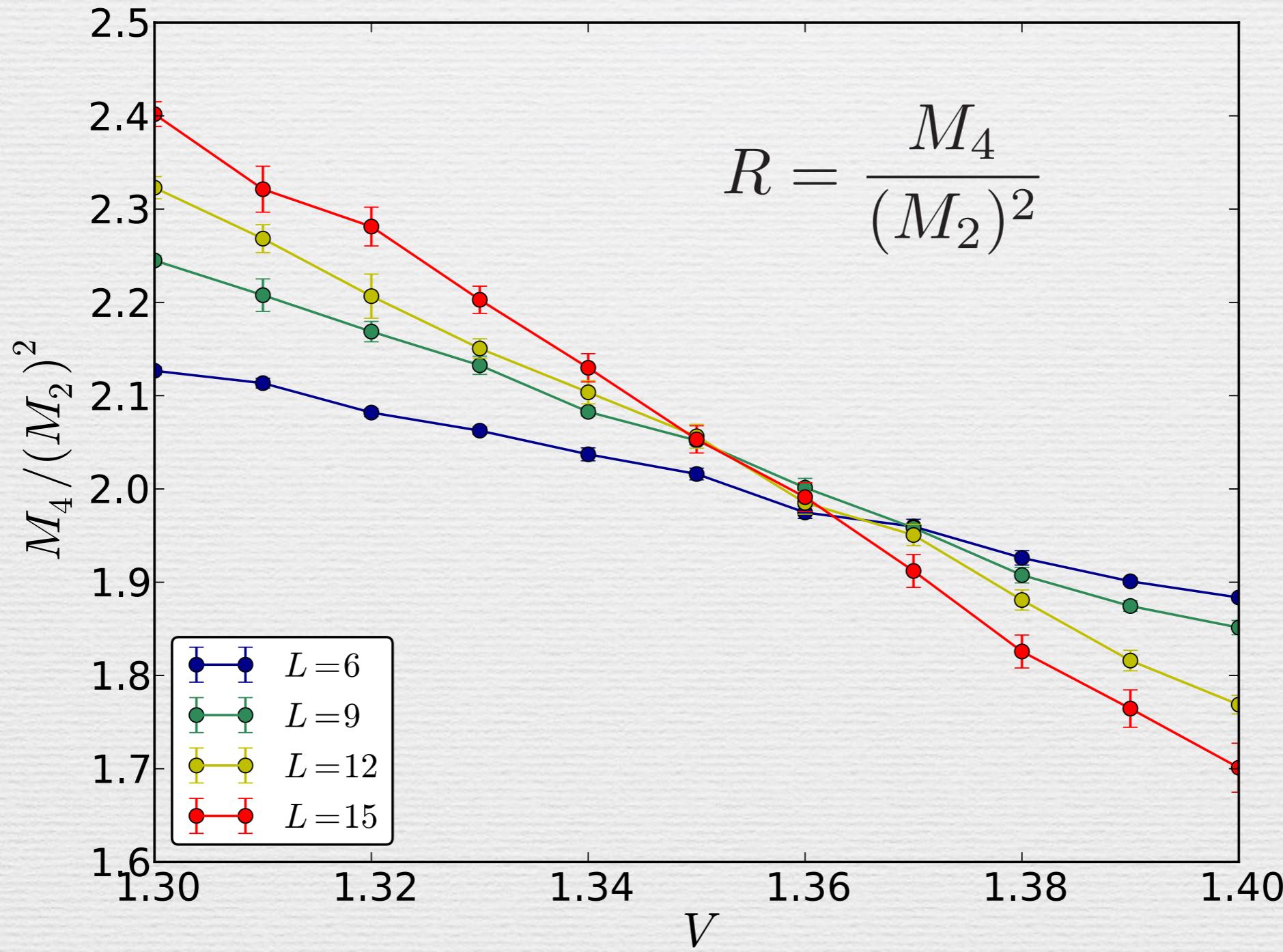
Scalings ansatz close to the QCP

relativistic invariance
 $z = 1$

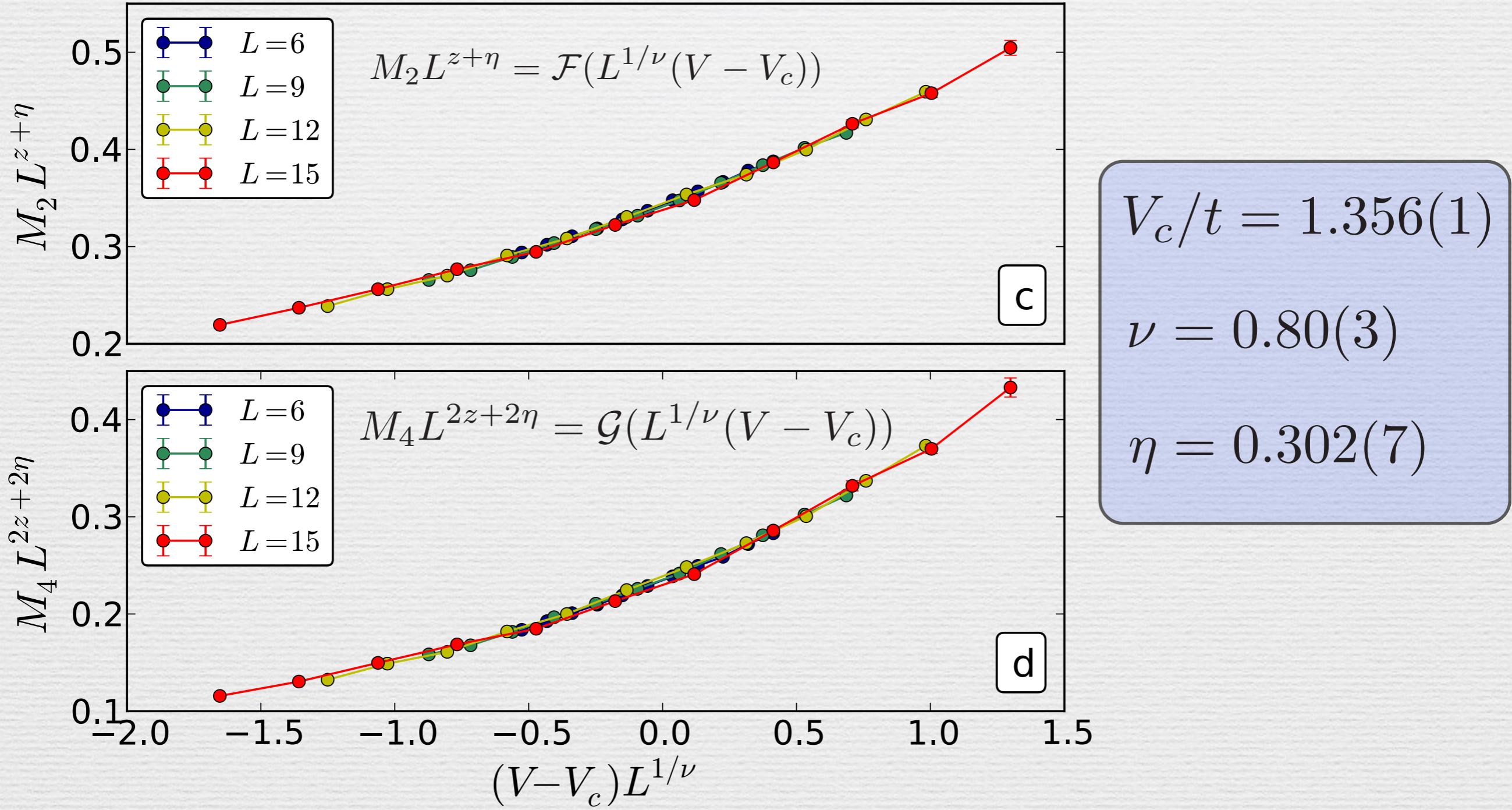
$$M_2 = L^{-z-\eta} \mathcal{F}[L^{1/\nu}(V - V_c), \cancel{L^z/\beta}]$$

$$M_4 = L^{-2z-2\eta} \mathcal{G}[L^{1/\nu}(V - V_c), \cancel{L^z/\beta}]$$

Binder Ratio



Data Collapse



* Errorbar from χ^2+1 analysis

Gross-Neveu-Yukawa Theory



ε -expansion

Rosenstein et al, PLB, 1993

$$\nu = 0.797$$

$$\eta = 0.502$$



“Exact” renormalization group

Rosa et al, PRL, 2001 Höfling et al, PRB, 2002

$$\nu = 0.738 \sim 0.927 \quad \eta = 0.525 \sim 0.635$$

Honeycomb

$$\nu = 0.80(3)$$

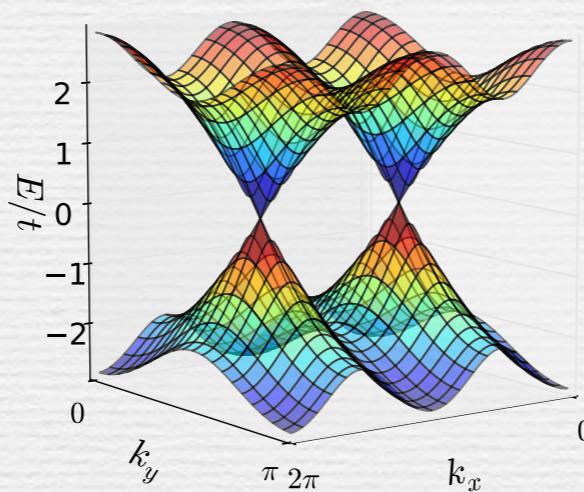
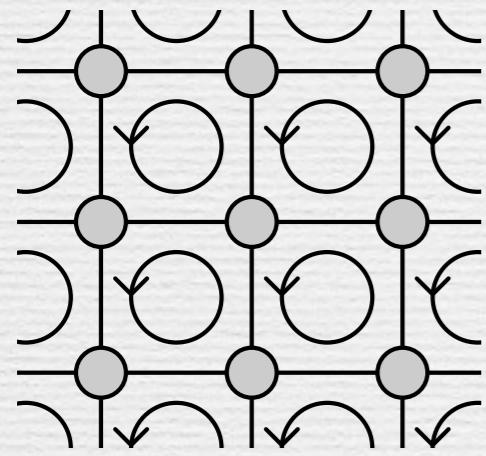
$$\eta = 0.302(7)$$

ν agrees

η does not

* Calculations based on 2-flavors of 2-component
Dirac fermions with the same chirality

Check-I: π -flux square lattice



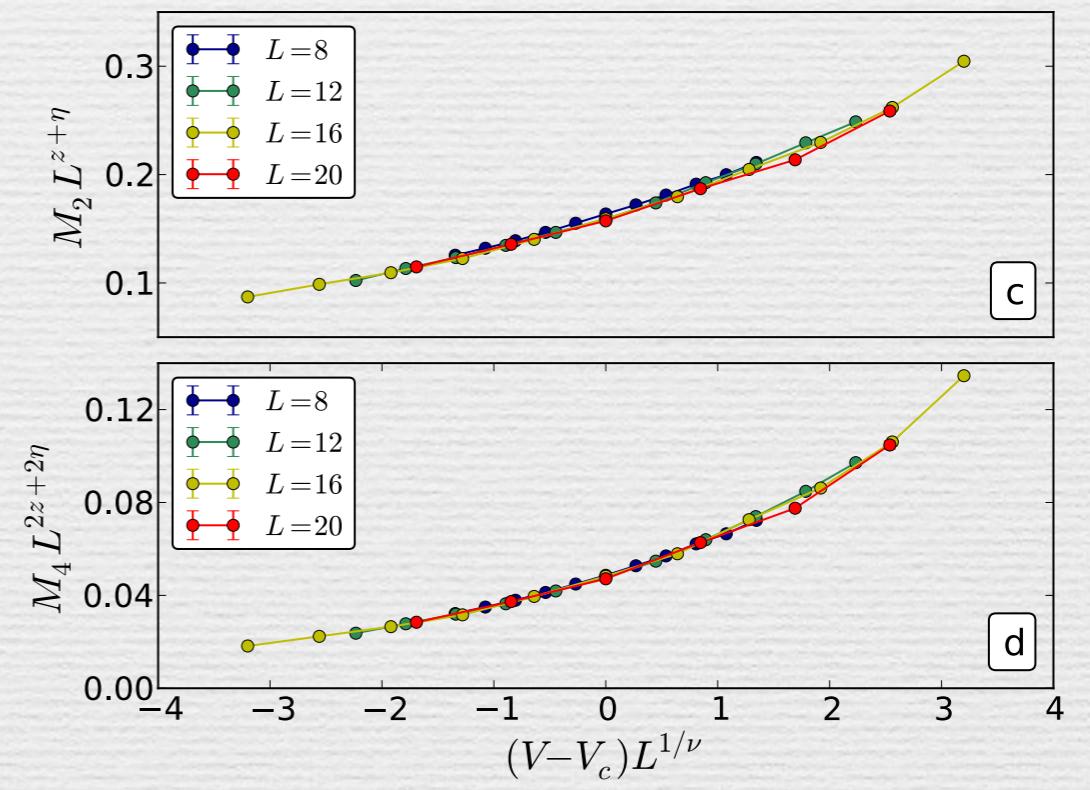
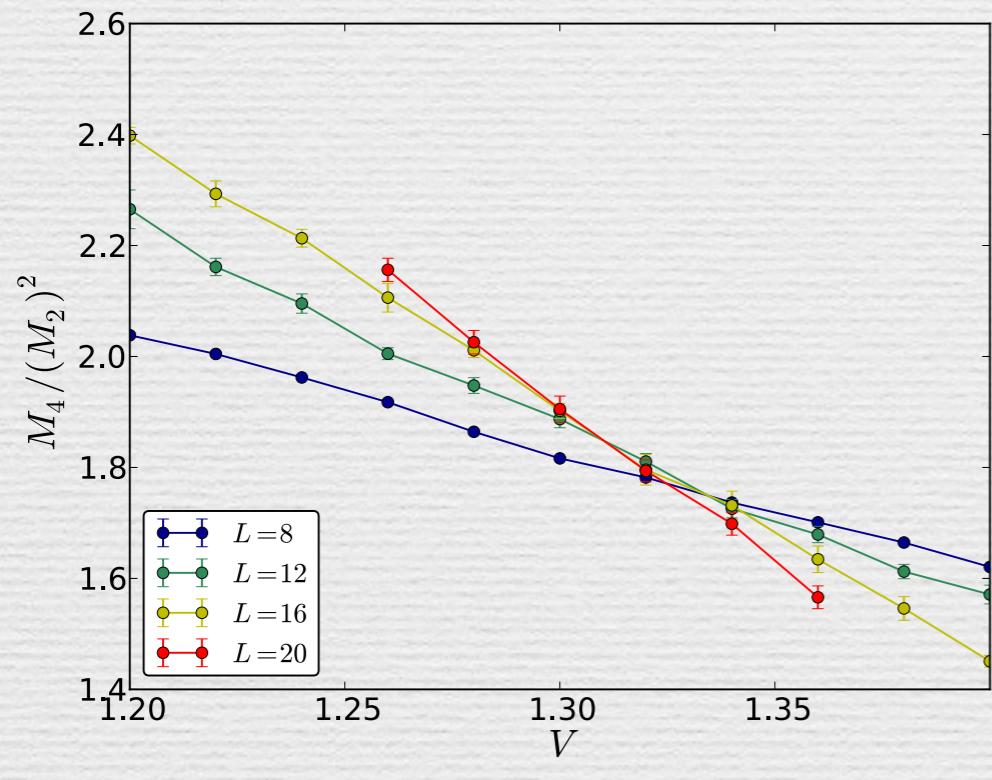
also features two Dirac points

π -flux lattice

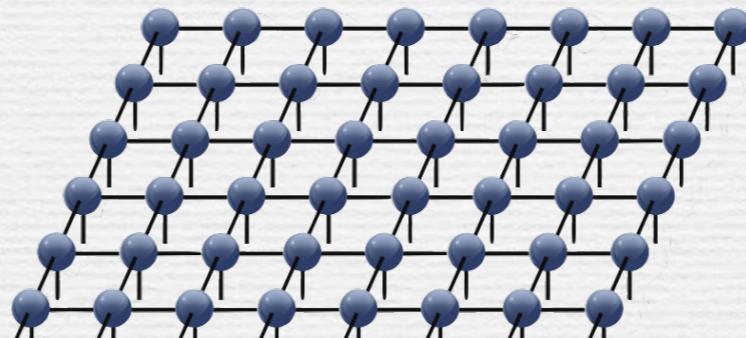
$$V_c/t = 1.304(2)$$

$$\nu = 0.80(6)$$

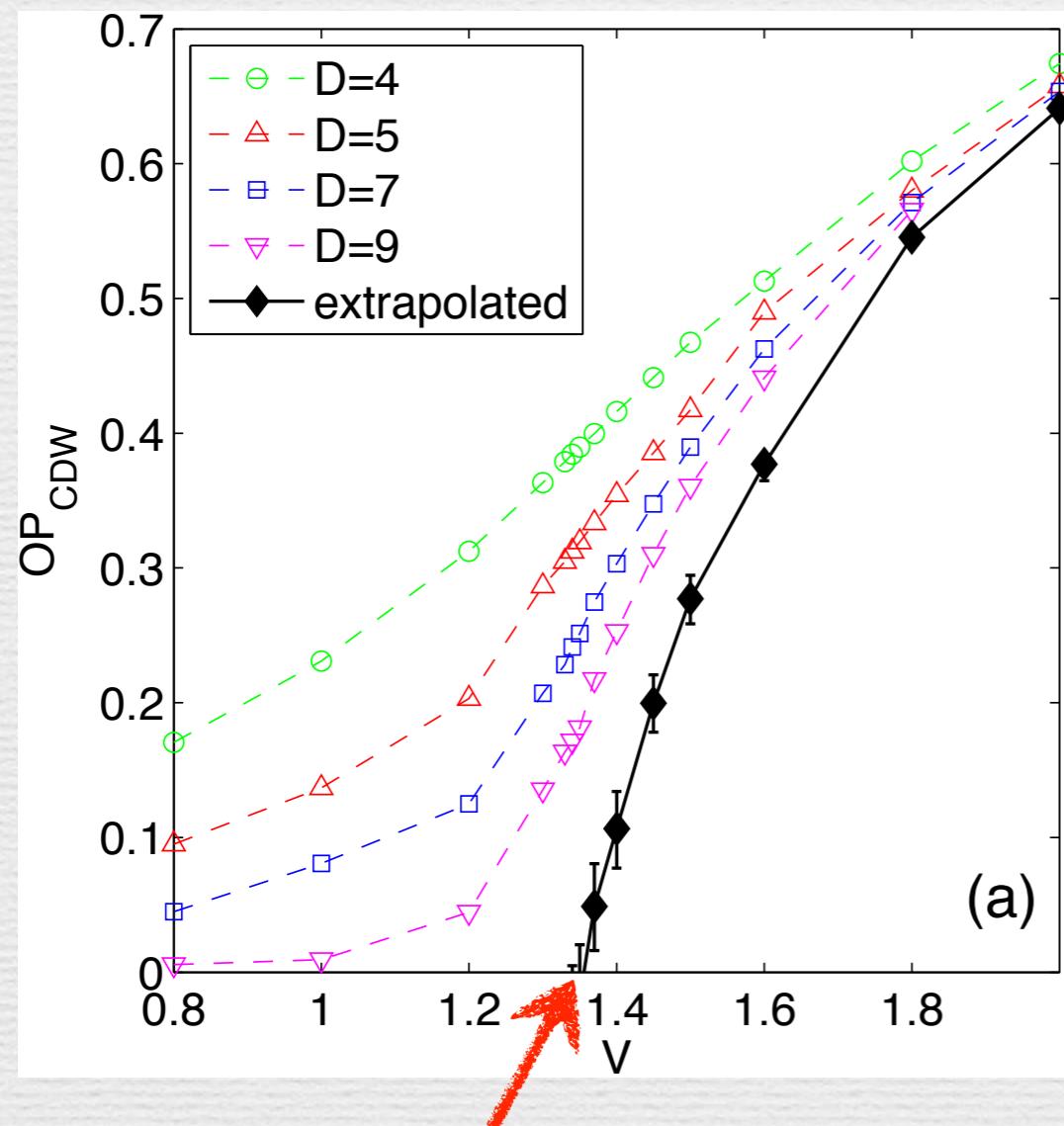
$$\eta = 0.318(8)$$



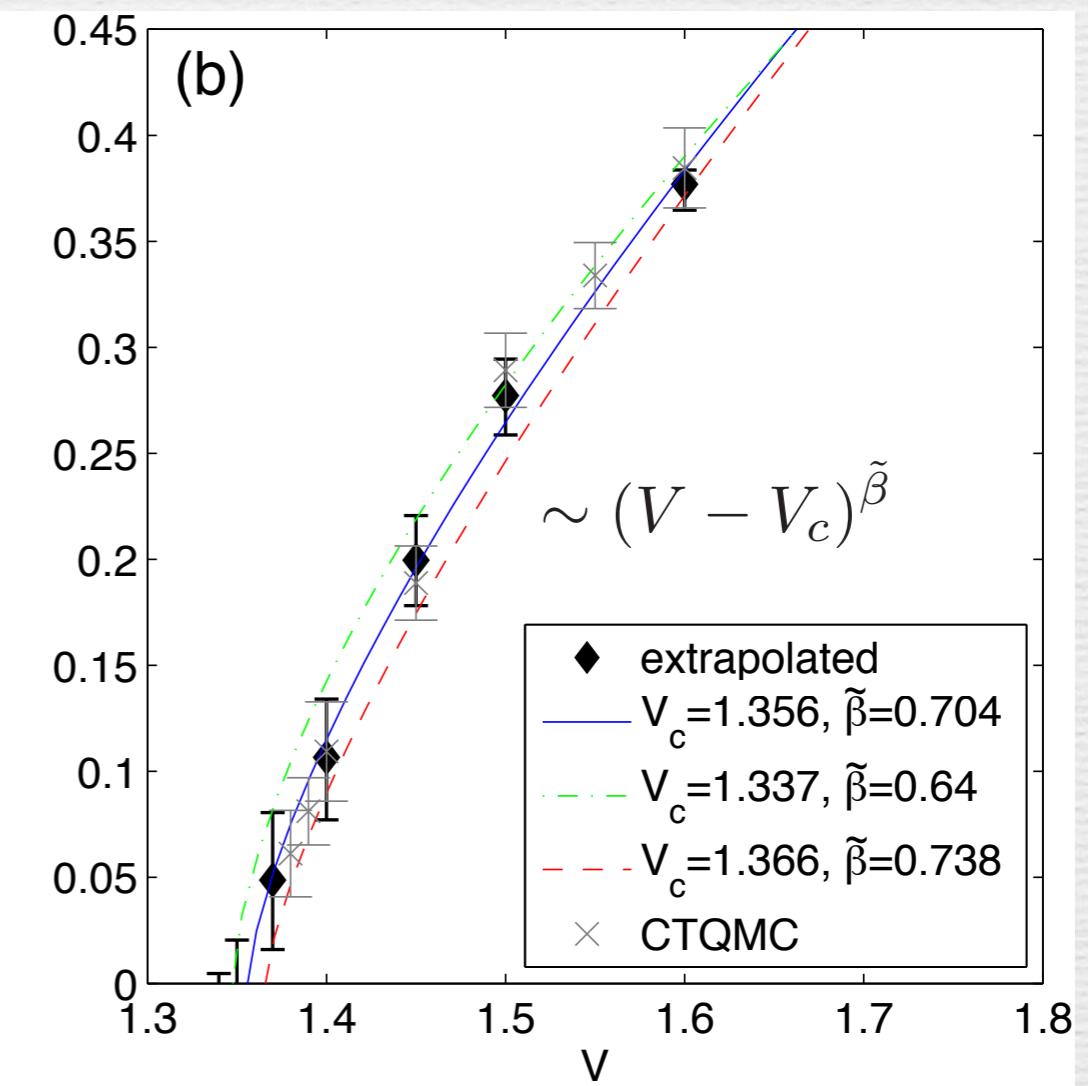
Check-II: iPEPS



Philippe Corboz
ETH → Amsterdam



$$V_c = 1.36(3)$$



CTQMC

$$\tilde{\beta} = \frac{\nu}{2}(z + \eta) = 0.52(3)$$

Summary-I

CTQMC

$$V_c/t = 1.356(1)$$

$$\nu = 0.80(3)$$

$$\eta = 0.302(7)$$

$$\tilde{\beta} = 0.52(3)$$

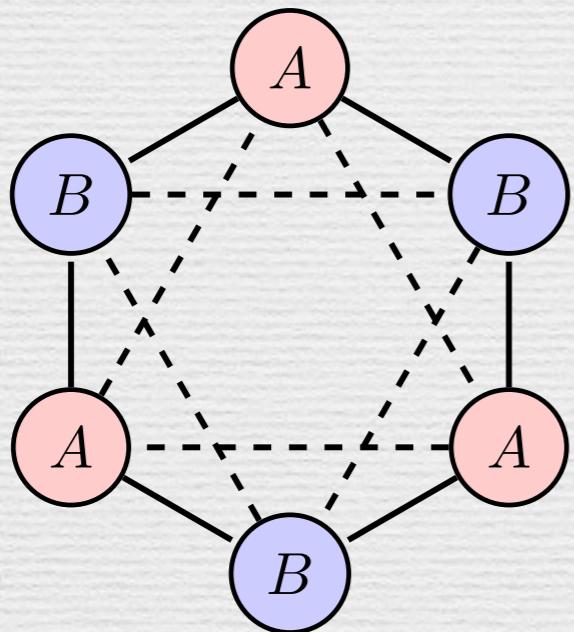
- Where is the QCP?
- What is the universality ?
- What are the critical exponents ?

To resolve the discrepancies we need
bigger systems and **more careful data analysis**

Where do we go from here ?

Half-filled, nearest-neighbor repulsion

Next-nearest-neighbor repulsion



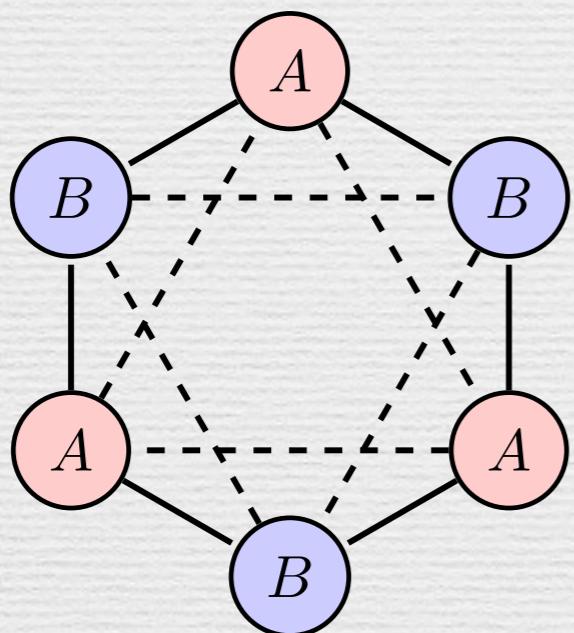
Doped attractive system



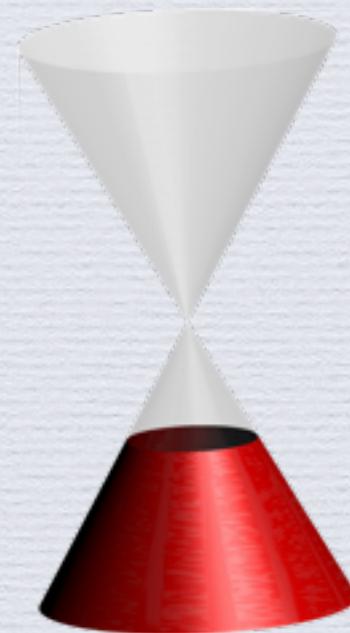
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Next-nearest-neighbor repulsion



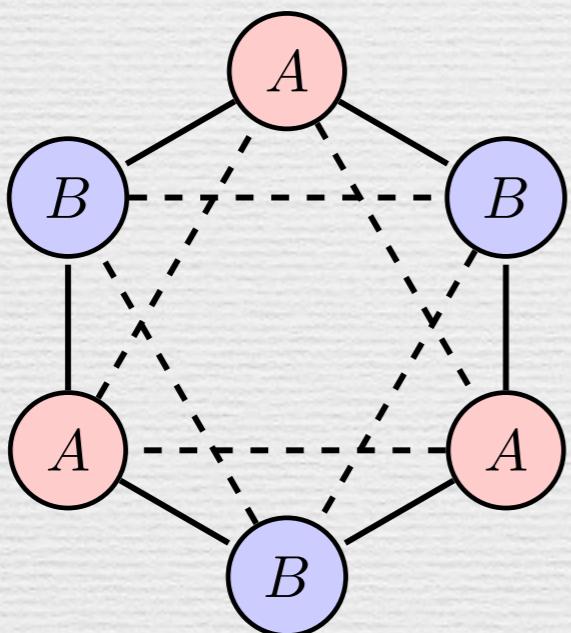
Doped attractive system



Where do we go from here ?

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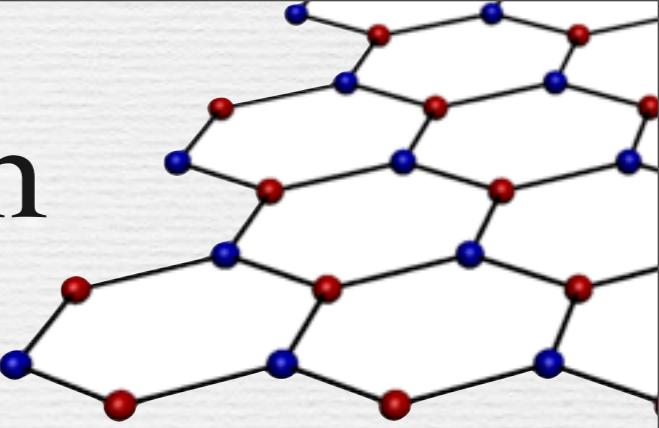


Doped attractive system



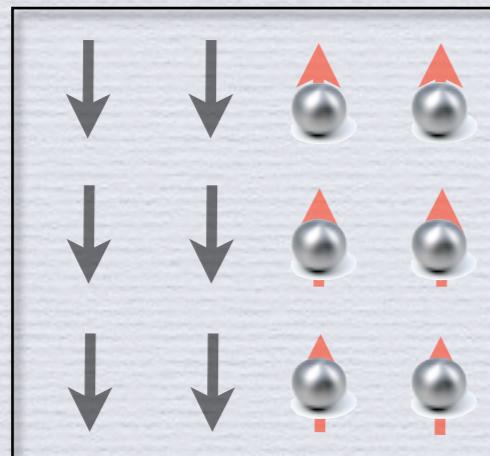
Doped attractive system

$$V < 0$$

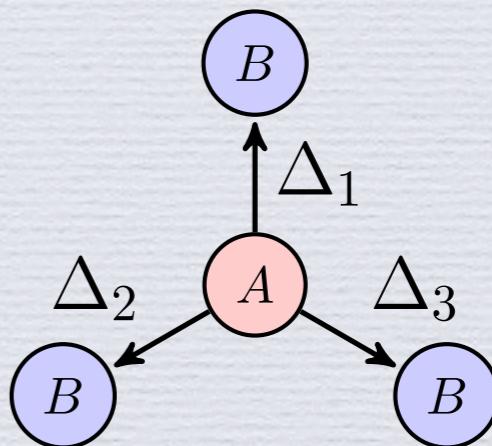


$$\hat{H} = -t \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} (\hat{c}_{\mathbf{i}}^\dagger \hat{c}_{\mathbf{j}} + h.c.) + V \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \hat{n}_{\mathbf{i}} \hat{n}_{\mathbf{j}} - \mu \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}}$$

Strong coupling
“Phase separation”



Weak-coupling
Superconductivity

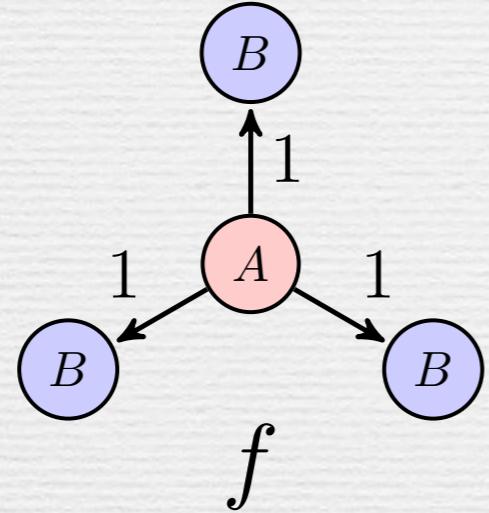


$$\Delta_\delta = \langle \hat{c}_{\mathbf{i} \in A} \hat{c}_{\mathbf{i} + \delta} \rangle$$

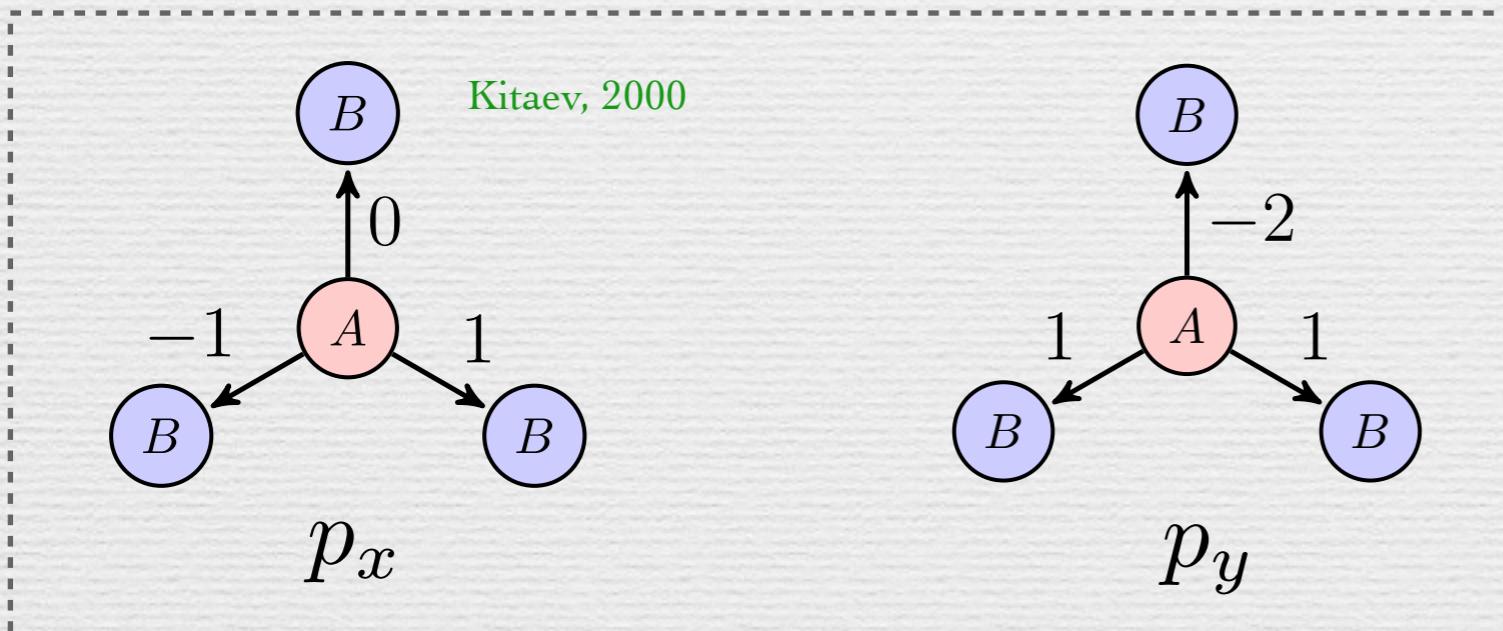
Pairing Symmetries

D_6	E	C_2	$2C_3$	$2C_6$	$3C'_2$	$3C''_2$
A_1	1	1	1	1	1	1
A_2	1	1	1	1	-1	-1
B_1	1	-1	1	-1	1	-1
B_2	1	-1	1	-1	-1	1
E_1	2	-2	-1	1	0	0
E_2	2	2	-1	-1	0	0

- 1-dim B_1 representation



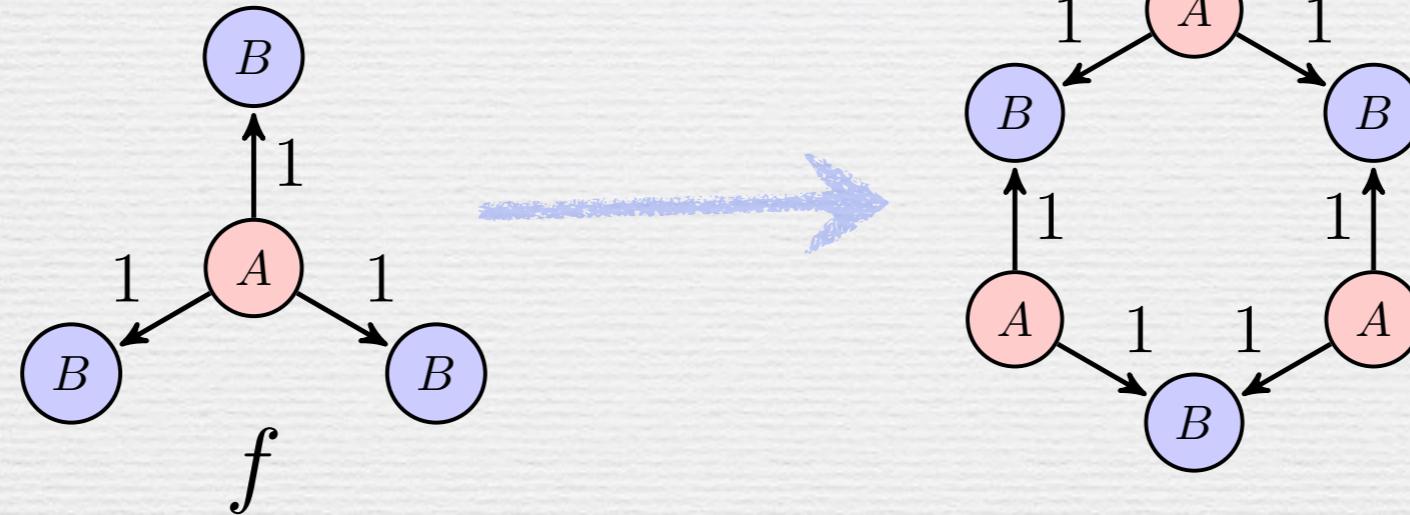
- 2-dim E_1 representation



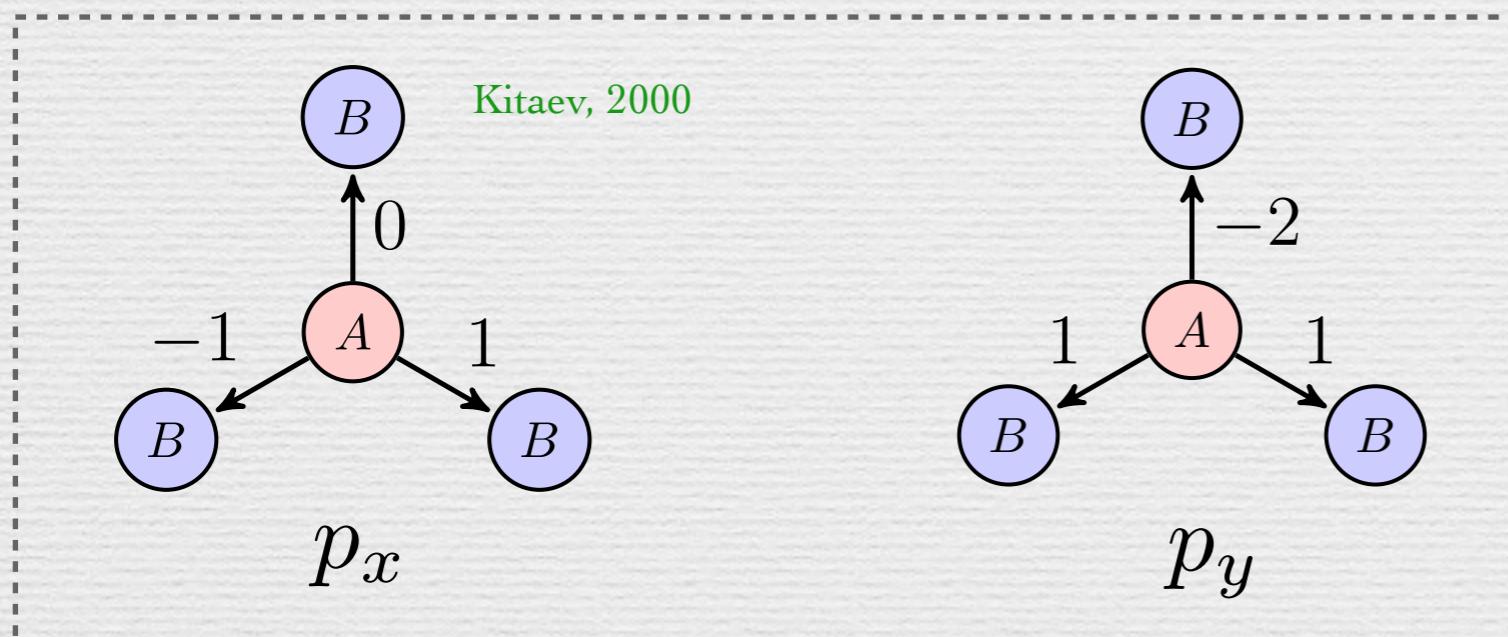
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A_2	1	1	1	1	-1	-1
B_1	1	-1	1	-1	1	-1
B_2	1	-1	1	-1	-1	1
E_1	2	-2	-1	1	0	0
E_2	2	2	-1	-1	0	0

• 1-dim B_1 representation



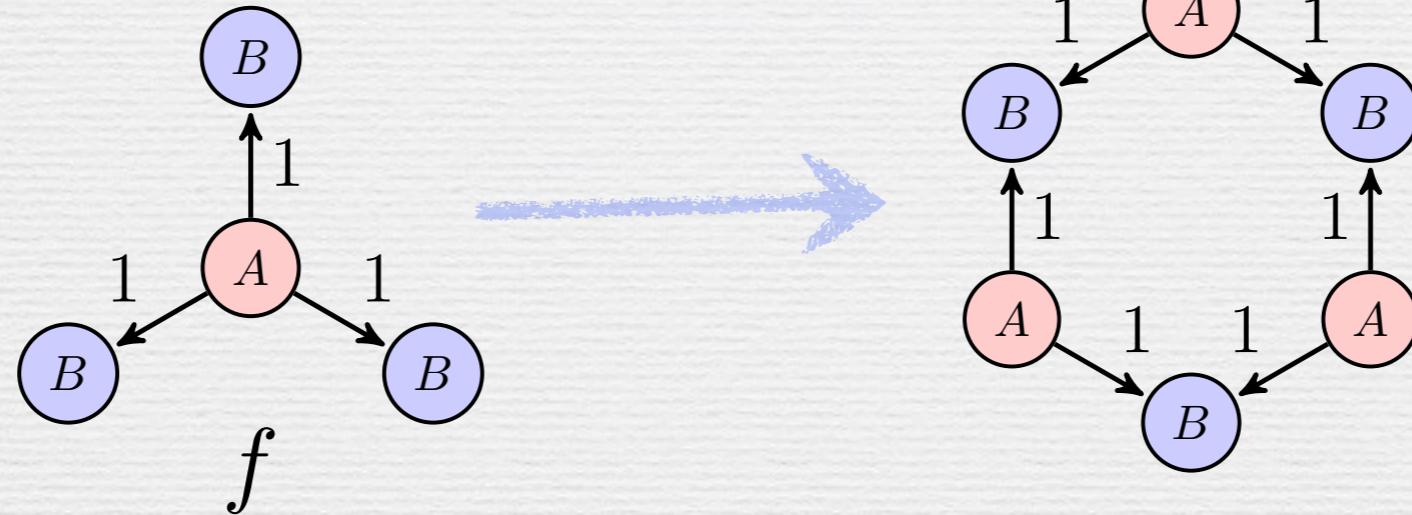
• 2-dim E_1 representation



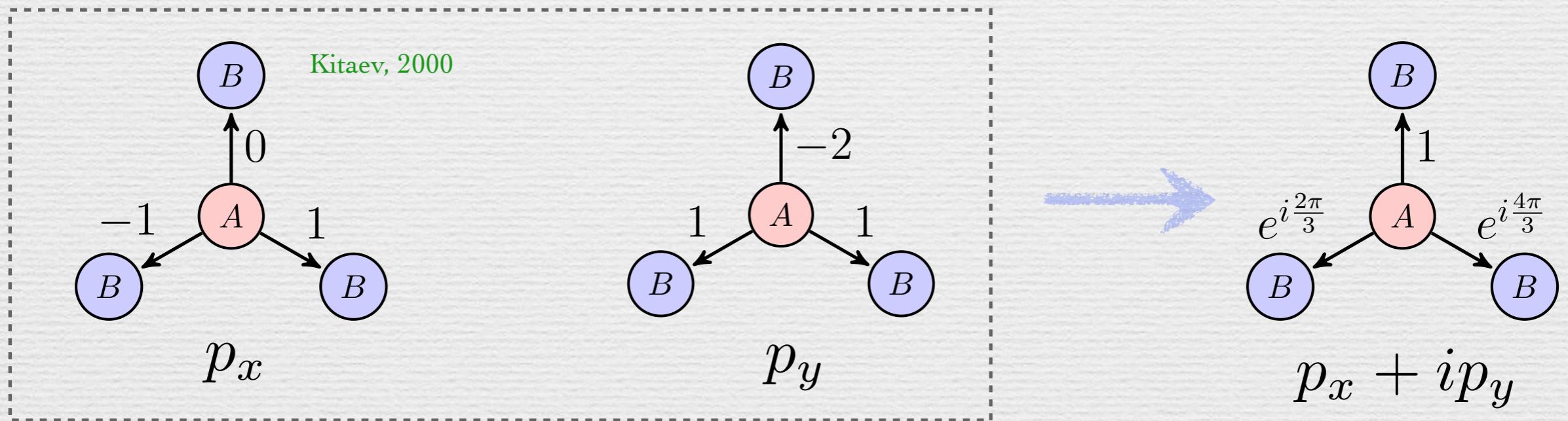
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B_1	1	-1	1	-1	1	-1
B_2	1	-1	1	-1	-1	1
E_1	2	-2	-1	1	0	0
E_2	2	2	-1	-1	0	0

• 1-dim B_1 representation



• 2-dim E_1 representation



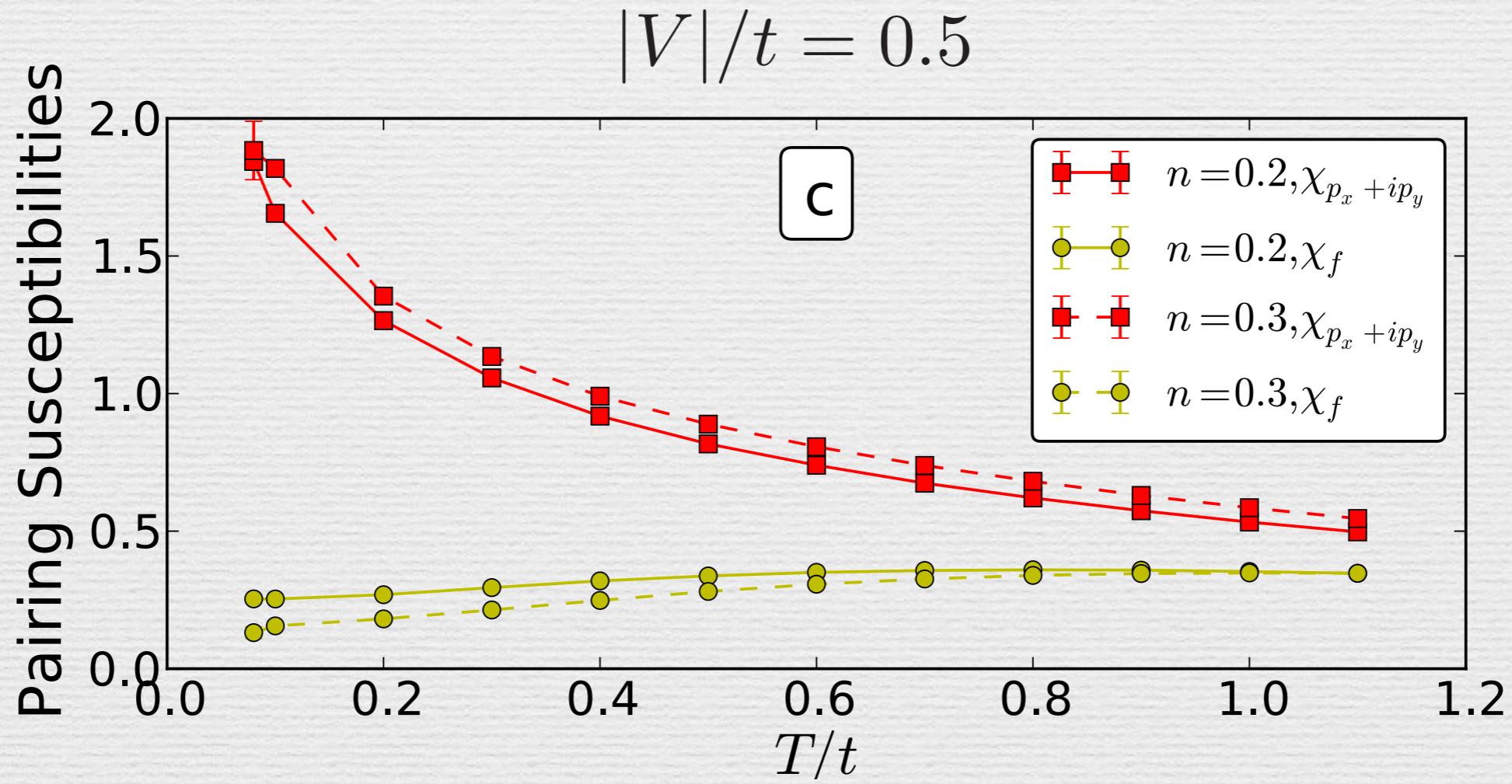
Pairing Susceptibilities

$$\chi_{\Gamma} = \int_0^{\beta} d\tau \langle \hat{\Delta}_{\Gamma}(\tau) \hat{\Delta}_{\Gamma}^{\dagger} \rangle$$

$$\hat{\Delta}_{\Gamma}(\tau) = \frac{1}{L^2} \sum_{\mathbf{i} \in A} \sum_{\delta} \mathcal{F}_{\Gamma}^{\delta} \hat{c}_{\mathbf{i}}(\tau) \hat{c}_{\mathbf{i}+\delta}(\tau)$$

$$\mathcal{F}_f = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\mathcal{F}_{p_x+ip_y} = \begin{pmatrix} 1 \\ e^{i2\pi/3} \\ e^{i4\pi/3} \end{pmatrix}$$



BdG Calculation

$$H_{\text{BdG}} =$$

$$\frac{1}{2} \sum_{\mathbf{k}} \left(\begin{array}{c} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \\ \hat{c}_{-\mathbf{k}A}^\dagger \\ \hat{c}_{-\mathbf{k}B}^\dagger \end{array} \right)^\dagger \left(\begin{array}{cccc} -\mu & z_{\mathbf{k}} & 0 & \Delta_{\mathbf{k}} \\ z_{\mathbf{k}}^* & -\mu & -\Delta_{-\mathbf{k}} & 0 \\ 0 & -\Delta_{-\mathbf{k}}^* & \mu & -z_{-\mathbf{k}}^* \\ \Delta_{\mathbf{k}}^* & 0 & -z_{-\mathbf{k}} & \mu \end{array} \right) \left(\begin{array}{c} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \\ \hat{c}_{-\mathbf{k}A}^\dagger \\ \hat{c}_{-\mathbf{k}B}^\dagger \end{array} \right)$$

BdG Calculation

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$$-t(1 + e^{-i\mathbf{k}\mathbf{a}_2} + e^{i\mathbf{k}(\mathbf{a}_1 - \mathbf{a}_2)})$$



BdG Calculation

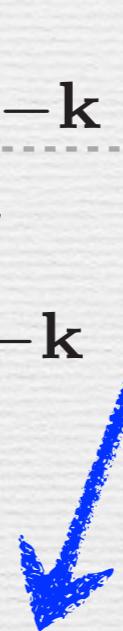
$$H_{\text{BdG}} =$$

$$\frac{1}{2} \sum_{\mathbf{k}} \left(\begin{array}{c} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \\ \hat{c}_{-\mathbf{k}A}^\dagger \\ \hat{c}_{-\mathbf{k}B}^\dagger \end{array} \right)^\dagger \left(\begin{array}{cccc} -\mu & z_{\mathbf{k}} & 0 & \Delta_{\mathbf{k}} \\ z_{\mathbf{k}}^* & -\mu & -\Delta_{-\mathbf{k}} & 0 \\ 0 & -\Delta_{-\mathbf{k}}^* & \mu & -z_{-\mathbf{k}}^* \\ \Delta_{\mathbf{k}}^* & 0 & -z_{-\mathbf{k}} & \mu \end{array} \right) \left(\begin{array}{c} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \\ \hat{c}_{-\mathbf{k}A}^\dagger \\ \hat{c}_{-\mathbf{k}B}^\dagger \end{array} \right)$$

$$-t(1 + e^{-i\mathbf{k}\mathbf{a}_2} + e^{i\mathbf{k}(\mathbf{a}_1 - \mathbf{a}_2)})$$



$$-V(\Delta_1 + \Delta_2 e^{-i\mathbf{k}\mathbf{a}_2} + \Delta_3 e^{i\mathbf{k}(\mathbf{a}_1 - \mathbf{a}_2)})$$

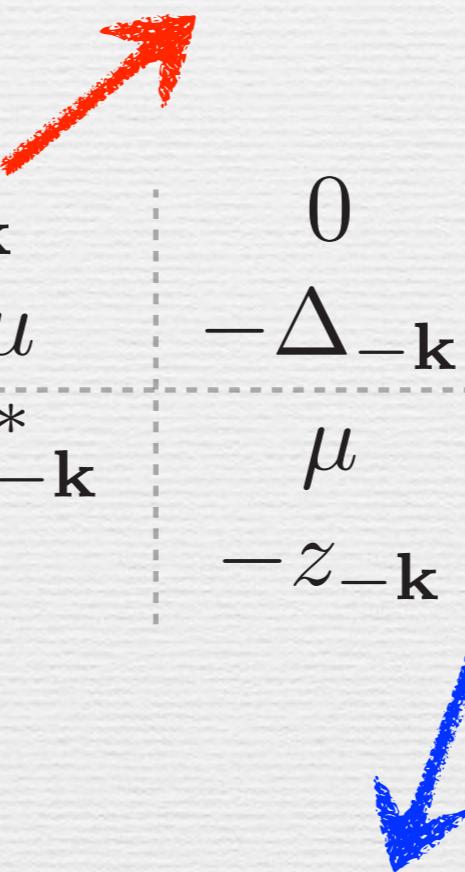


BdG Calculation

$$H_{\text{BdG}} =$$

$$\frac{1}{2} \sum_{\mathbf{k}} \left(\begin{array}{c} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \\ \hat{c}_{-\mathbf{k}A}^\dagger \\ \hat{c}_{-\mathbf{k}B}^\dagger \end{array} \right)^\dagger \left(\begin{array}{cccc} -\mu & z_{\mathbf{k}} & 0 & \Delta_{\mathbf{k}} \\ z_{\mathbf{k}}^* & -\mu & -\Delta_{-\mathbf{k}} & 0 \\ 0 & -\Delta_{-\mathbf{k}}^* & \mu & -z_{-\mathbf{k}}^* \\ \Delta_{\mathbf{k}}^* & 0 & -z_{-\mathbf{k}} & \mu \end{array} \right) \left(\begin{array}{c} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \\ \hat{c}_{-\mathbf{k}A}^\dagger \\ \hat{c}_{-\mathbf{k}B}^\dagger \end{array} \right)$$

$$-t(1 + e^{-i\mathbf{k}\mathbf{a}_2} + e^{i\mathbf{k}(\mathbf{a}_1 - \mathbf{a}_2)})$$

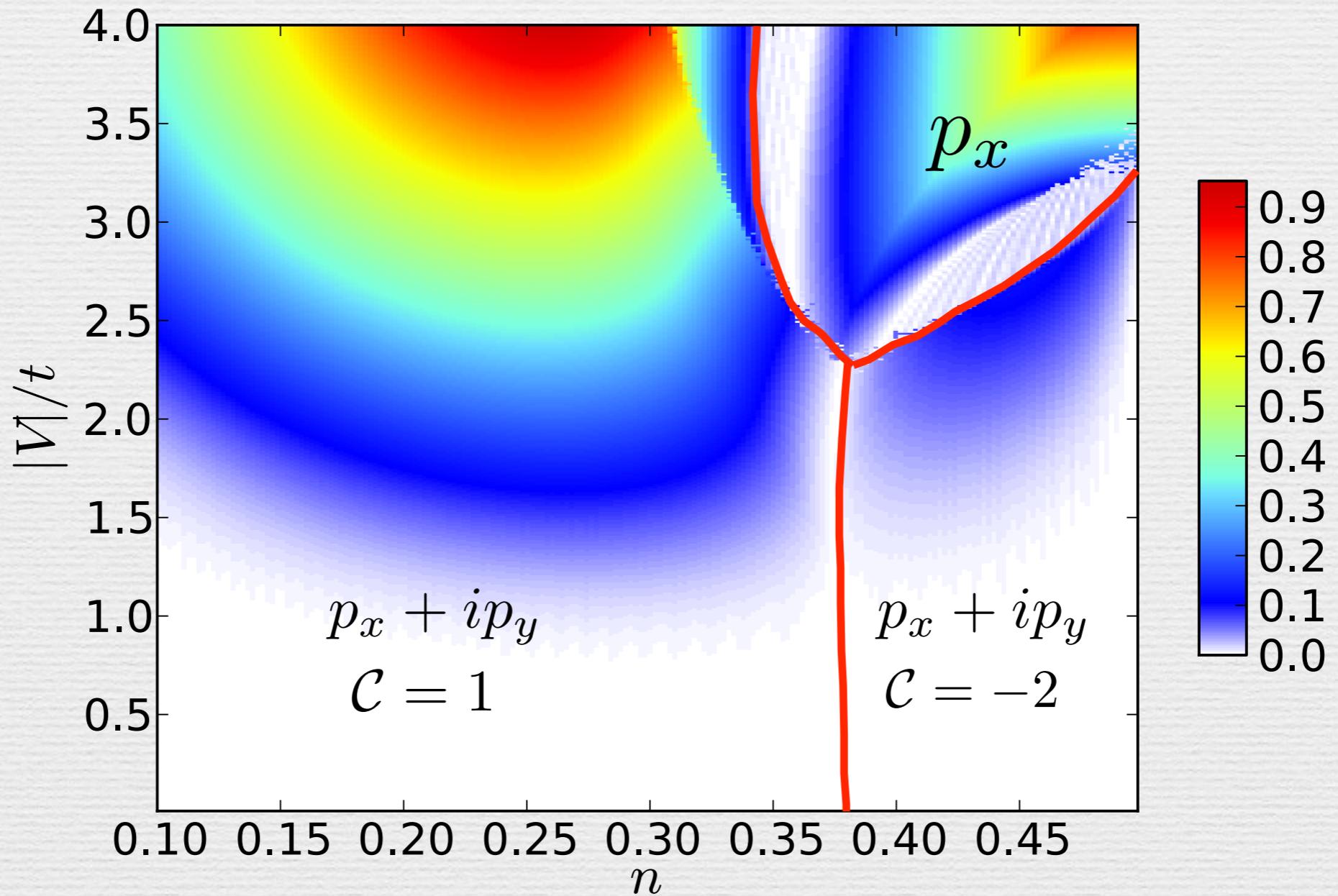


$$-V(\Delta_1 + \Delta_2 e^{-i\mathbf{k}\mathbf{a}_2} + \Delta_3 e^{i\mathbf{k}(\mathbf{a}_1 - \mathbf{a}_2)})$$



Start with **random guesses**, iterate until convergence

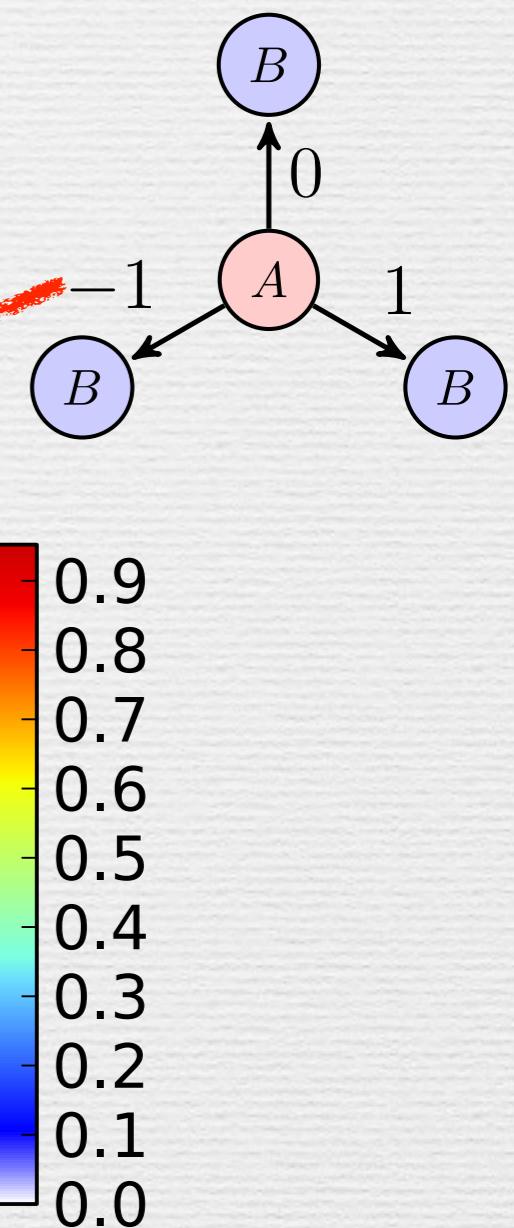
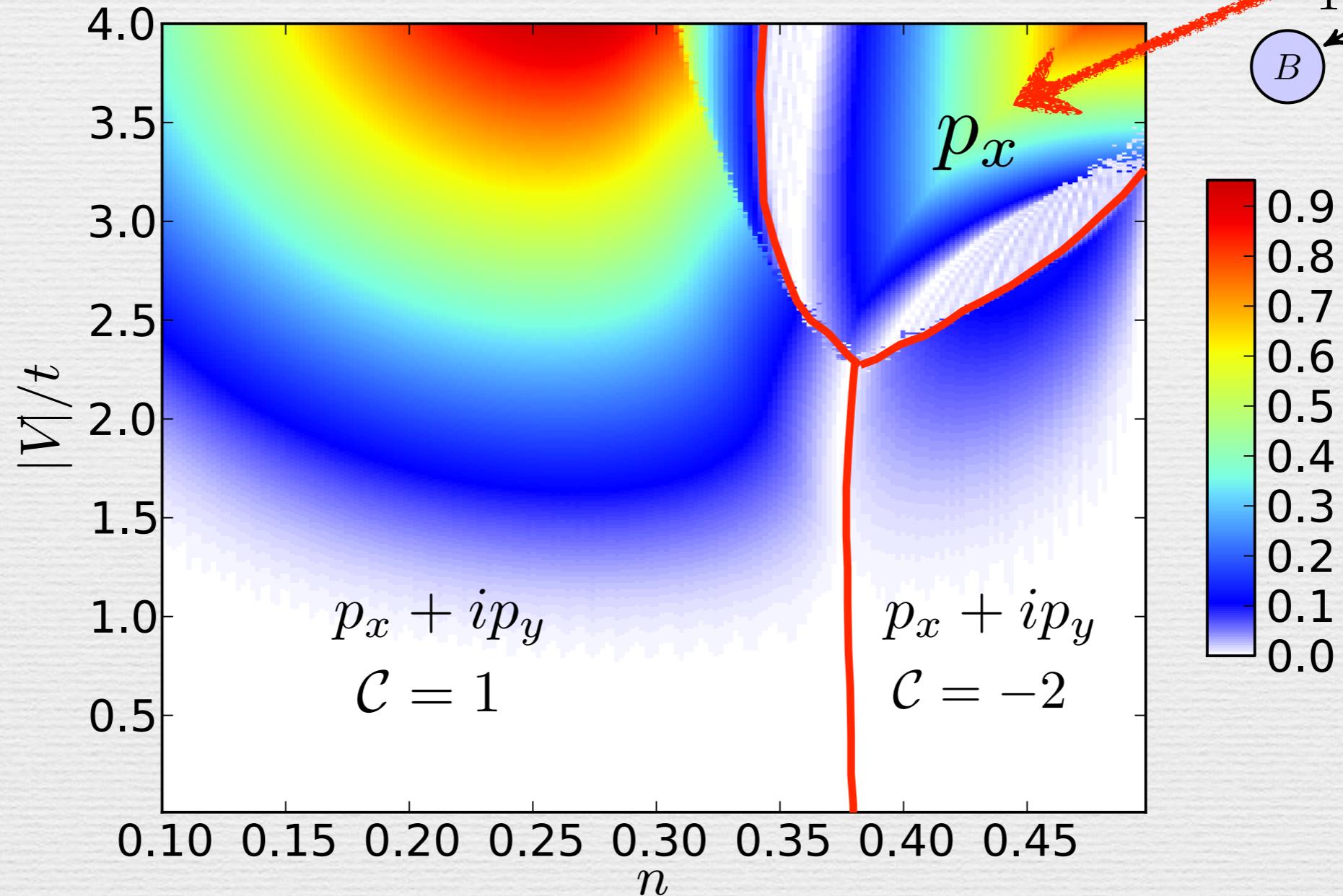
BdG phase diagram



*color indicates size of superconducting gap

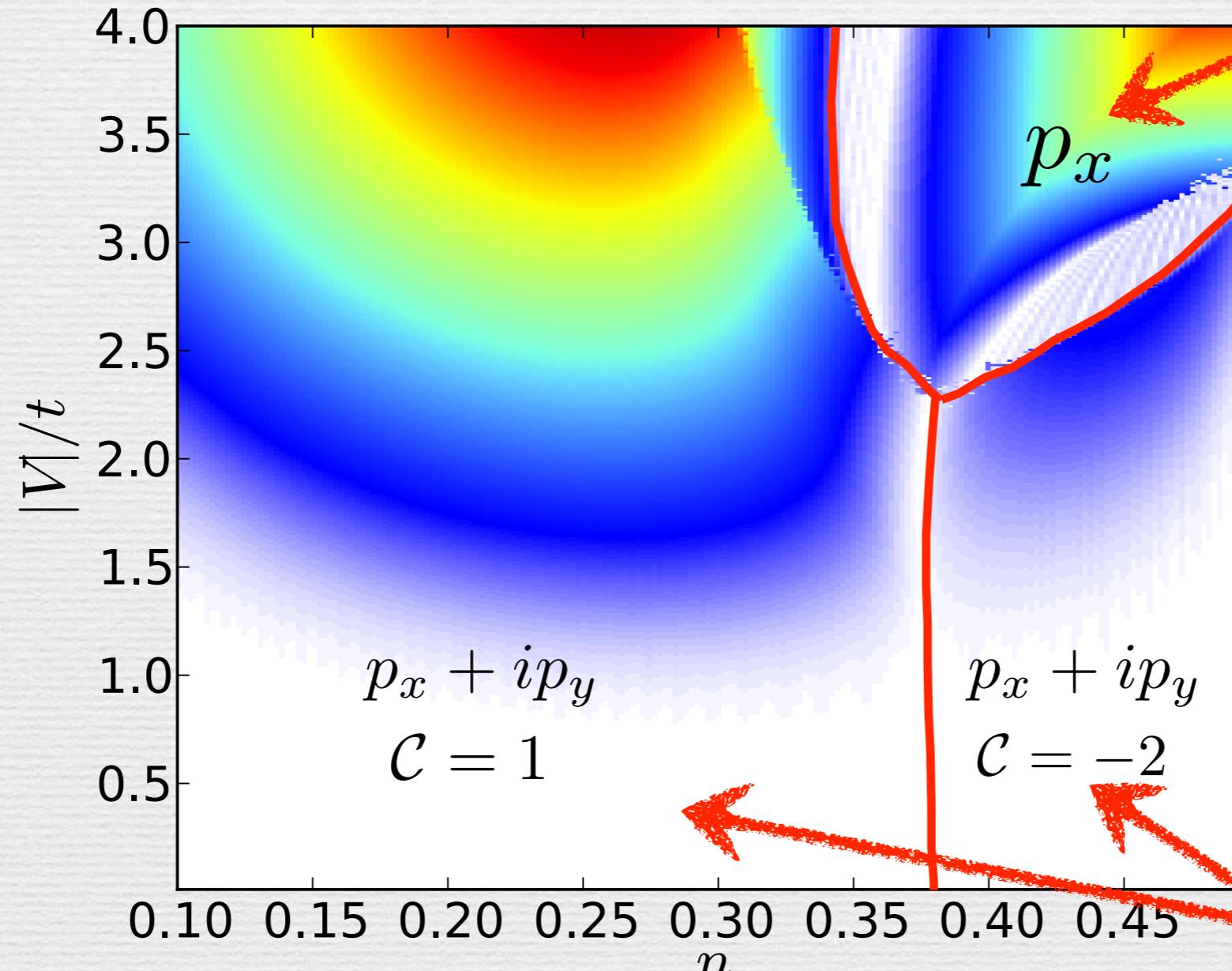
BdG phase diagram

Kitaev, 2000

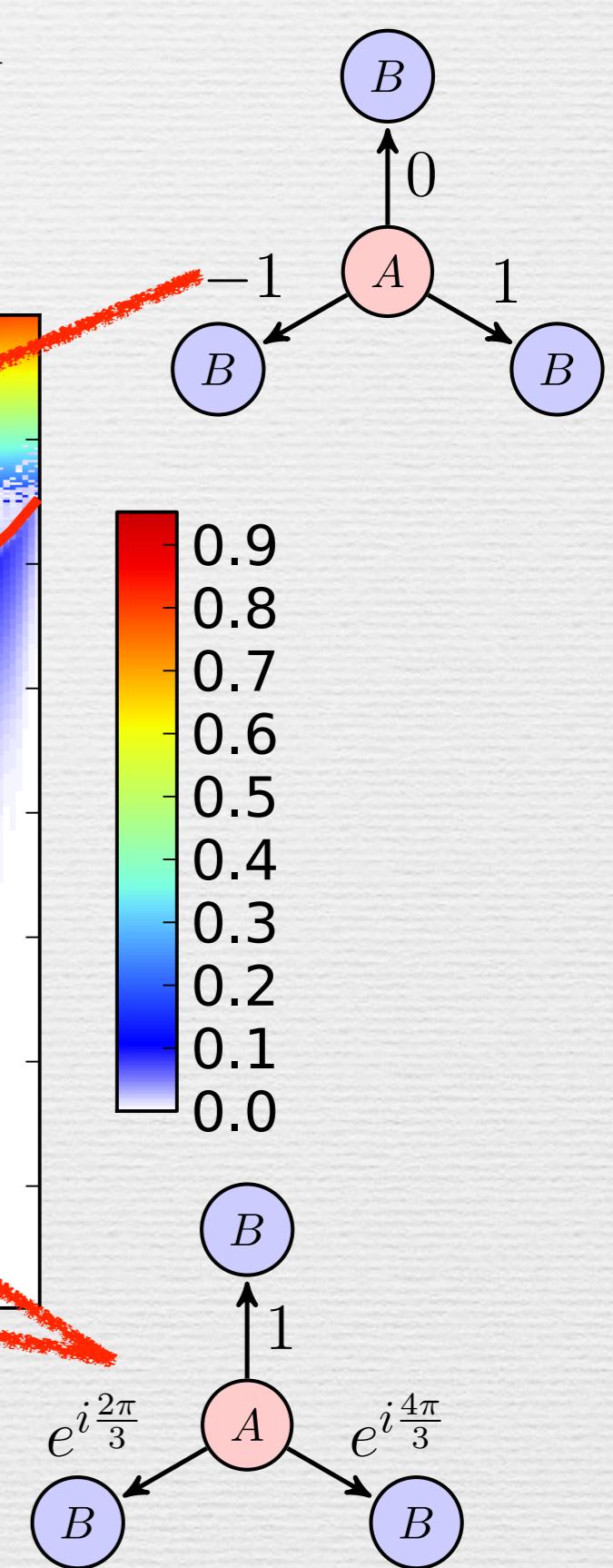


*color indicates size of superconducting gap

BdG phase diagram



Kitaev, 2000

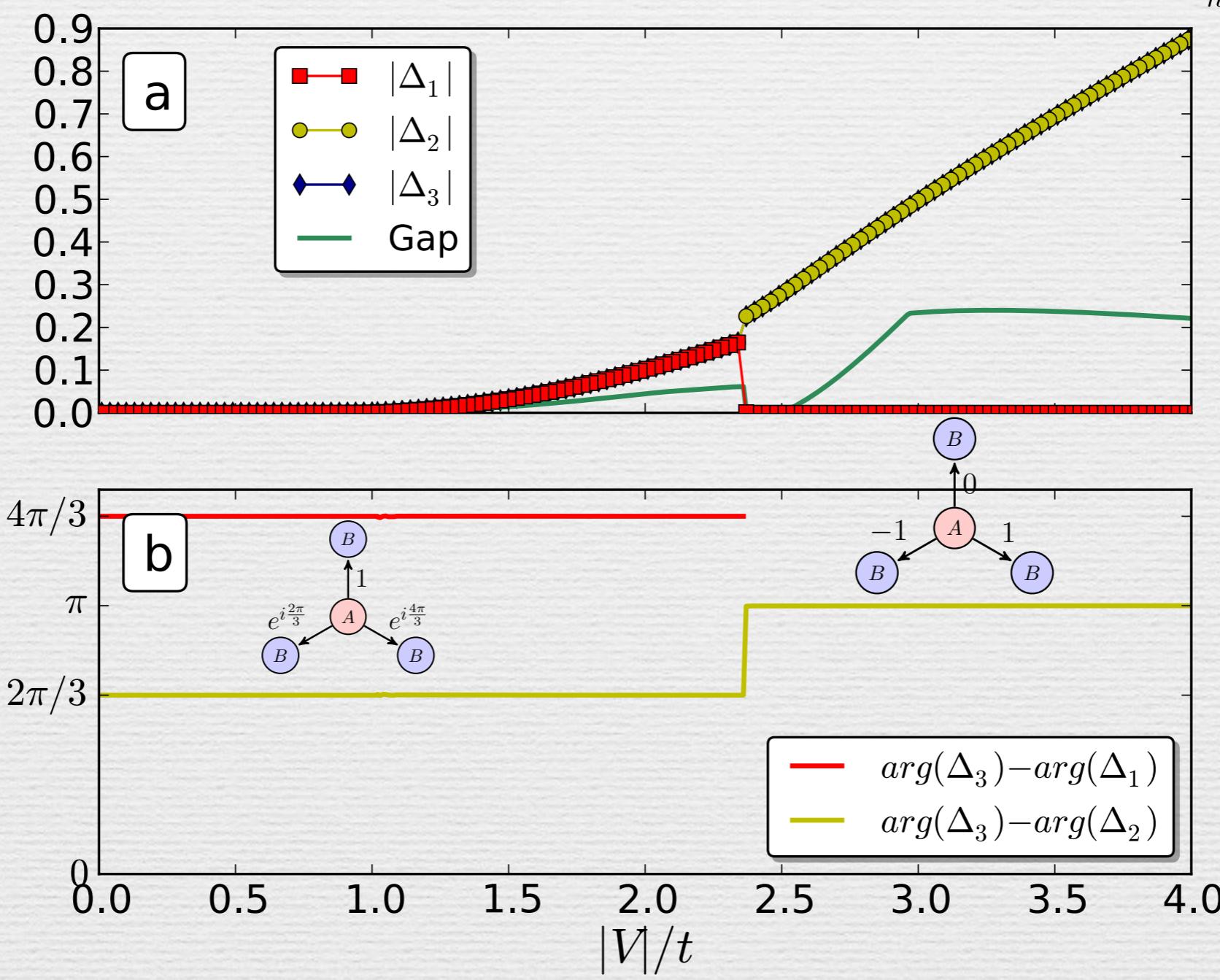
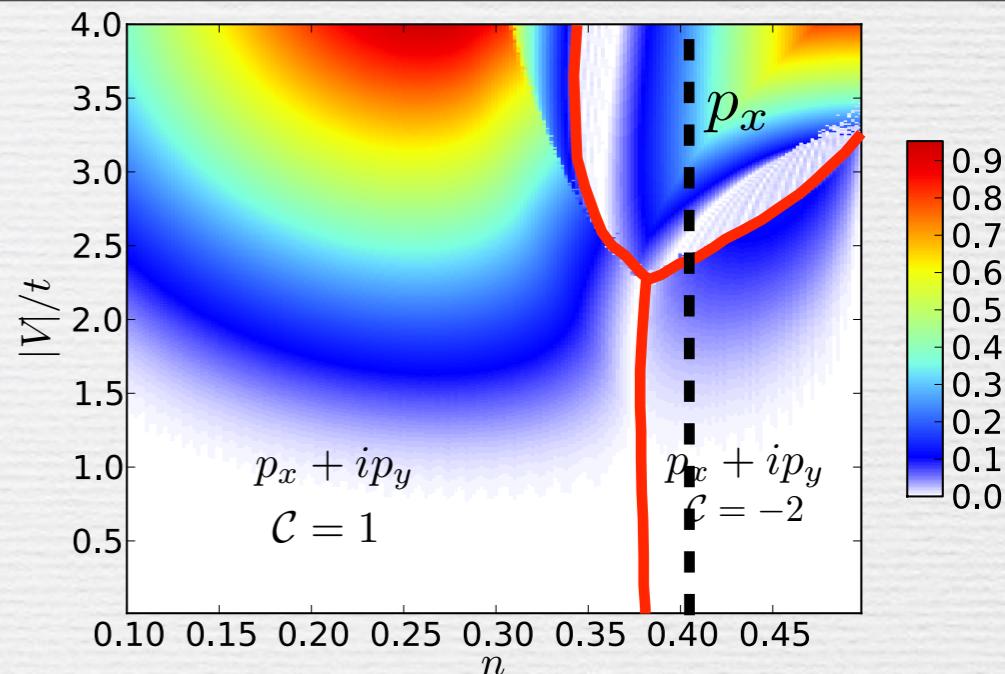


Read and Green, PRB, 2000

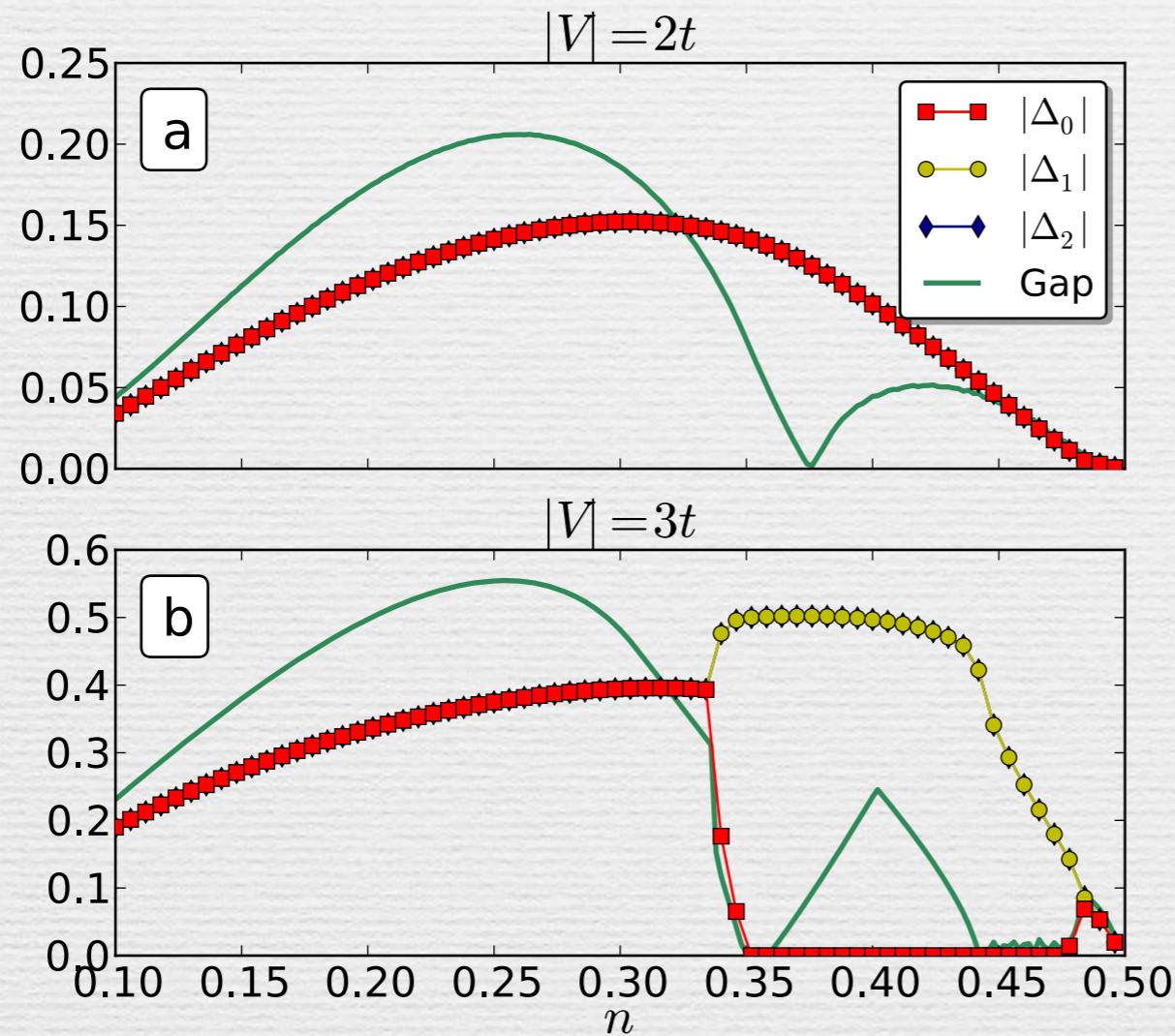
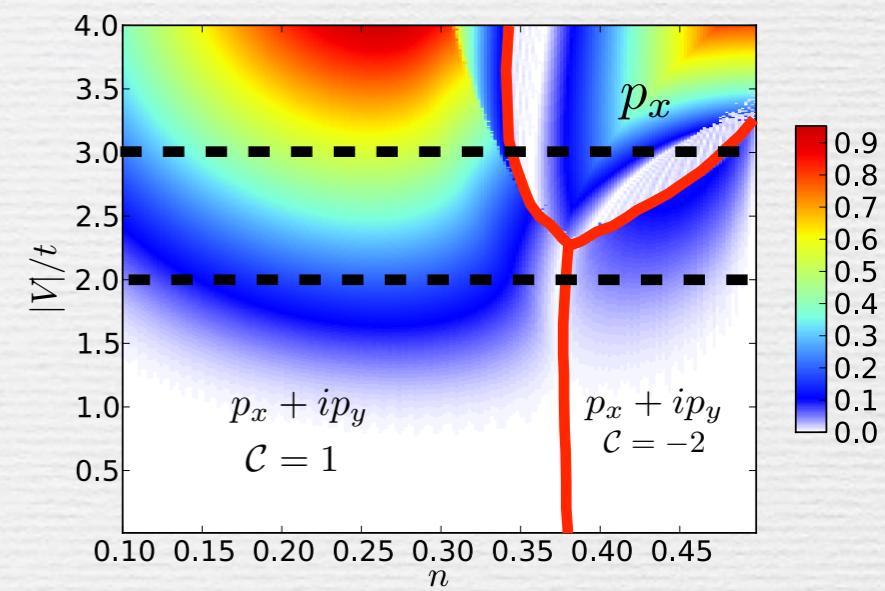
*color indicates size of superconducting gap

Scan V

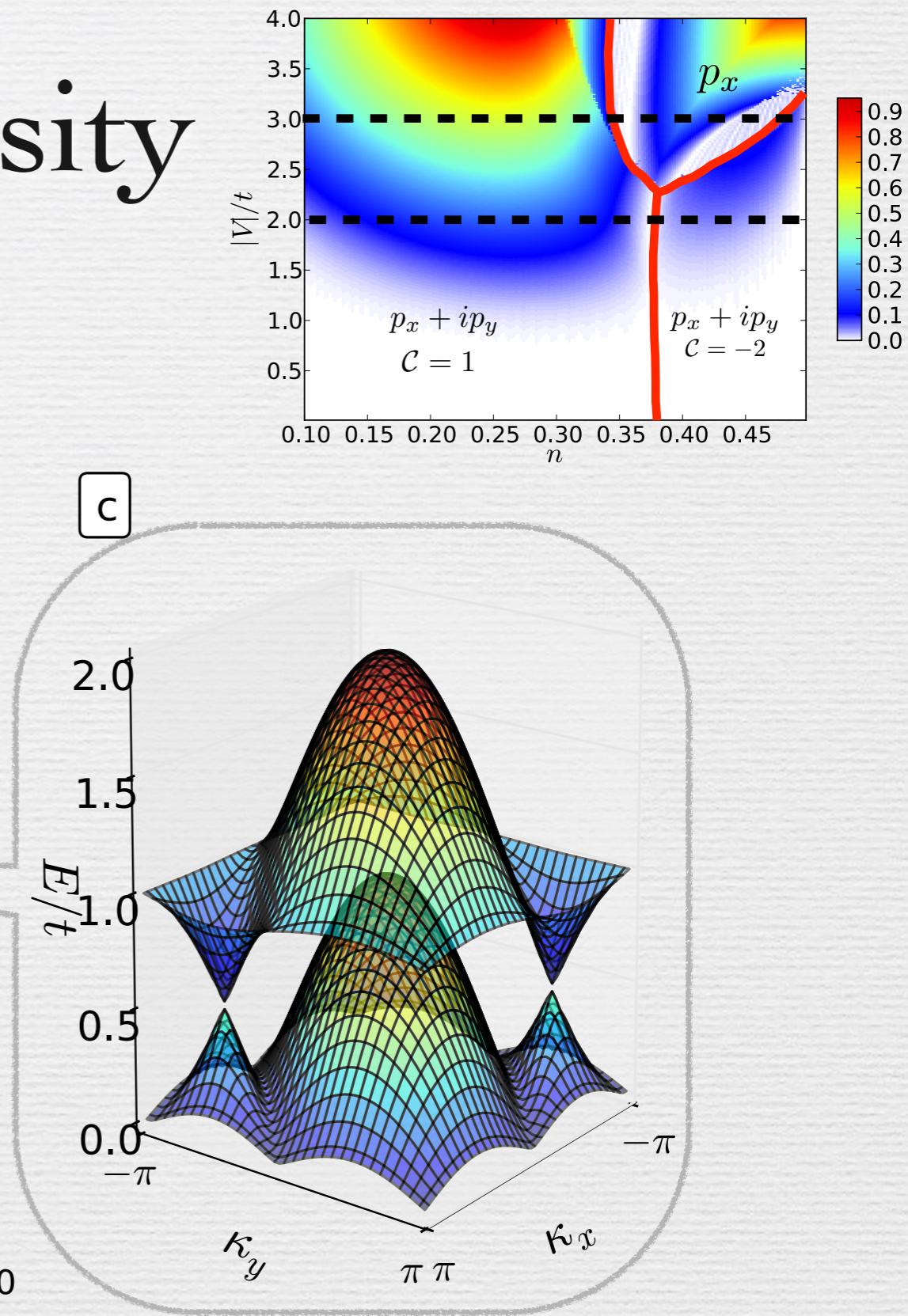
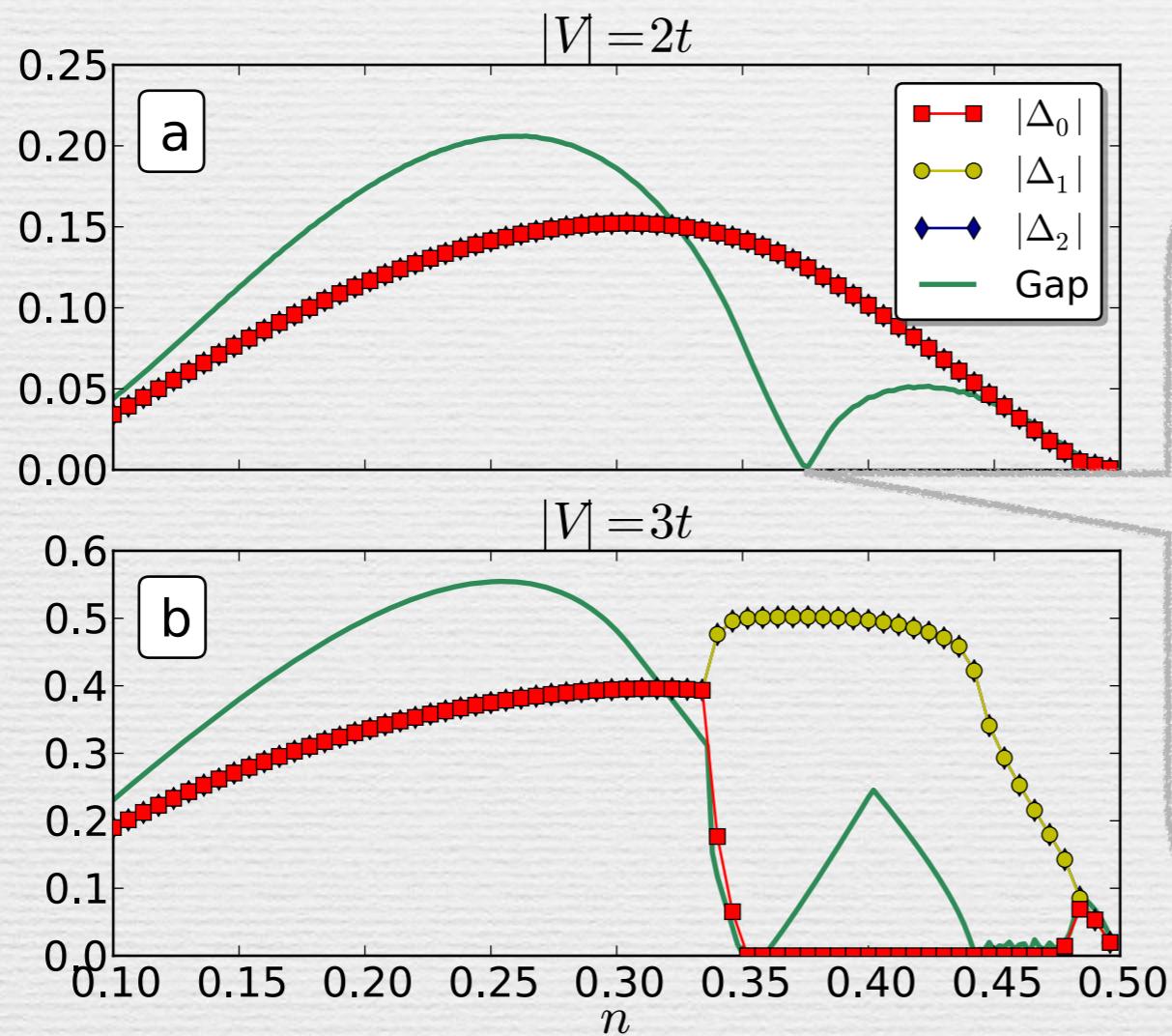
$n = 0.4$



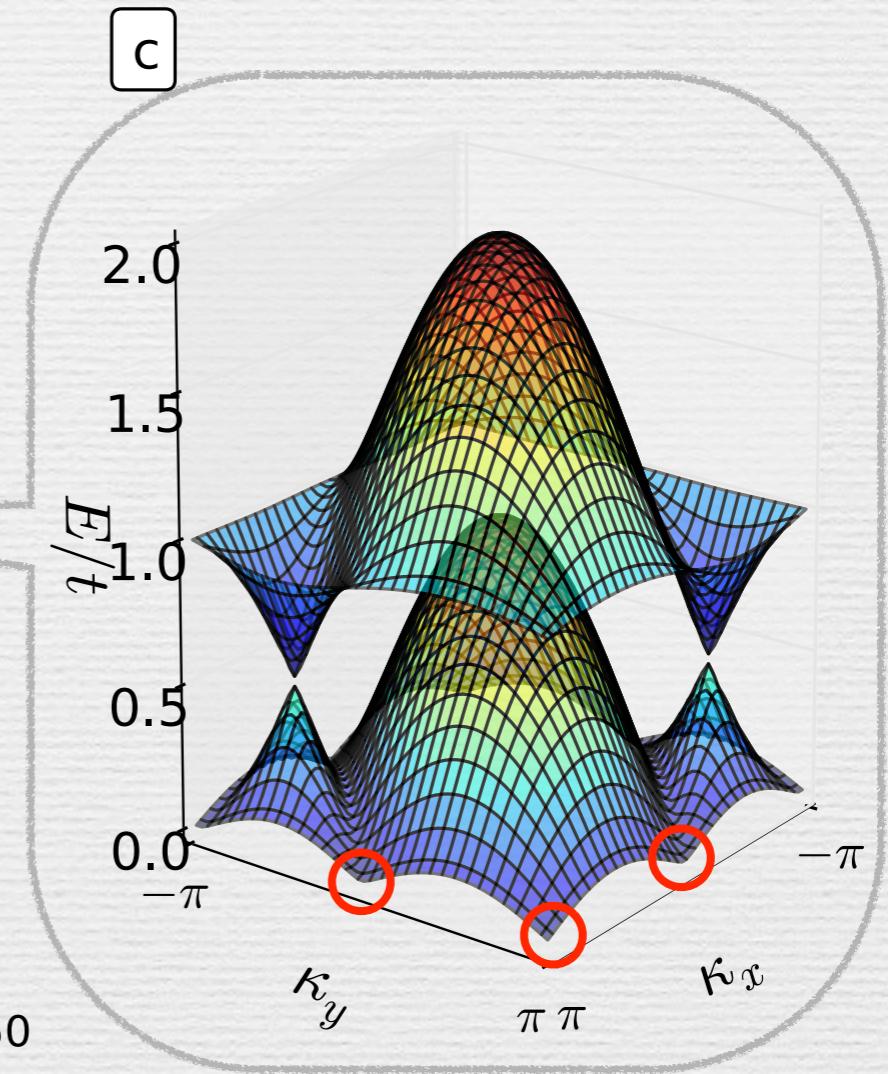
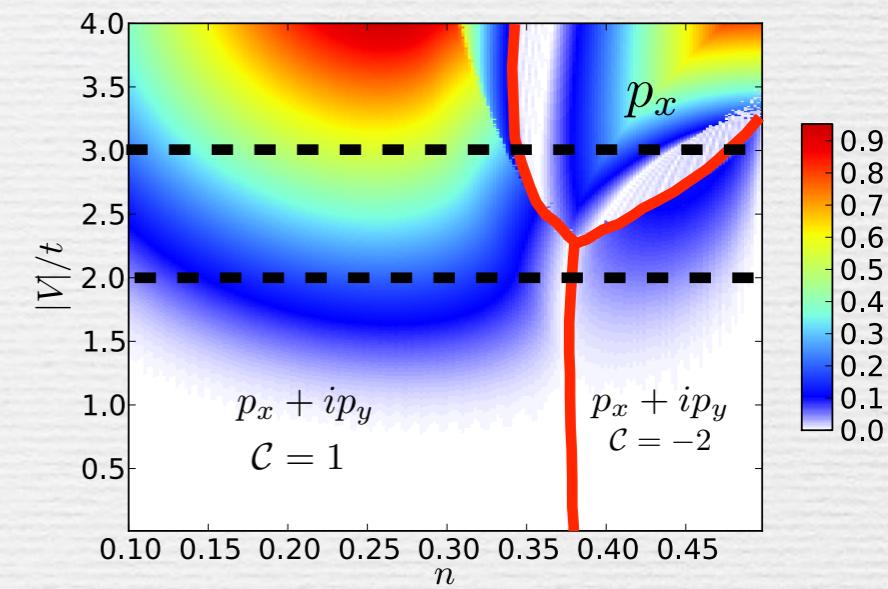
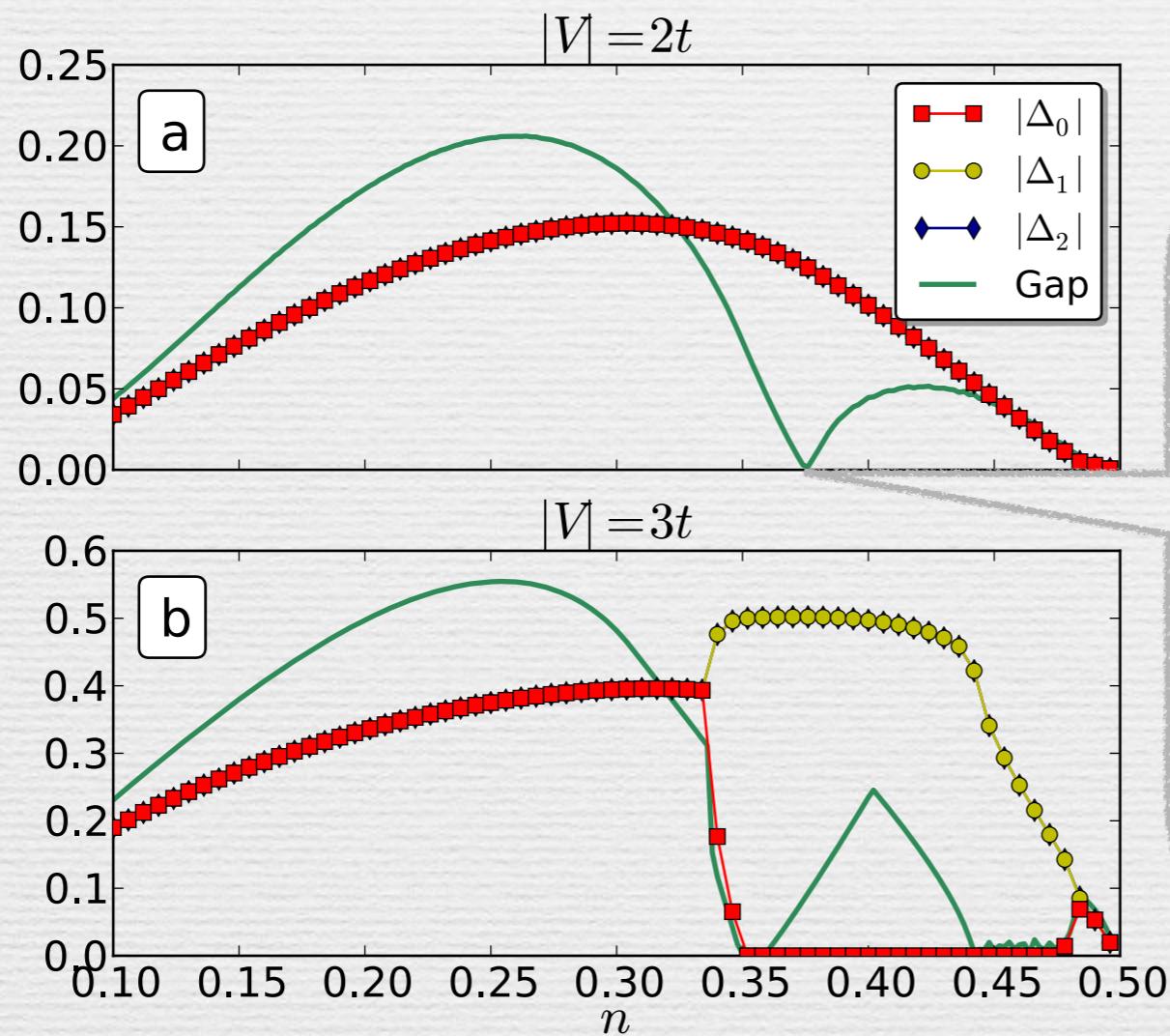
Scan density



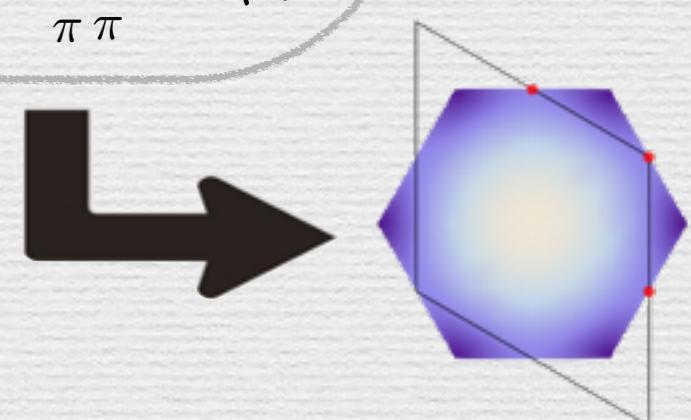
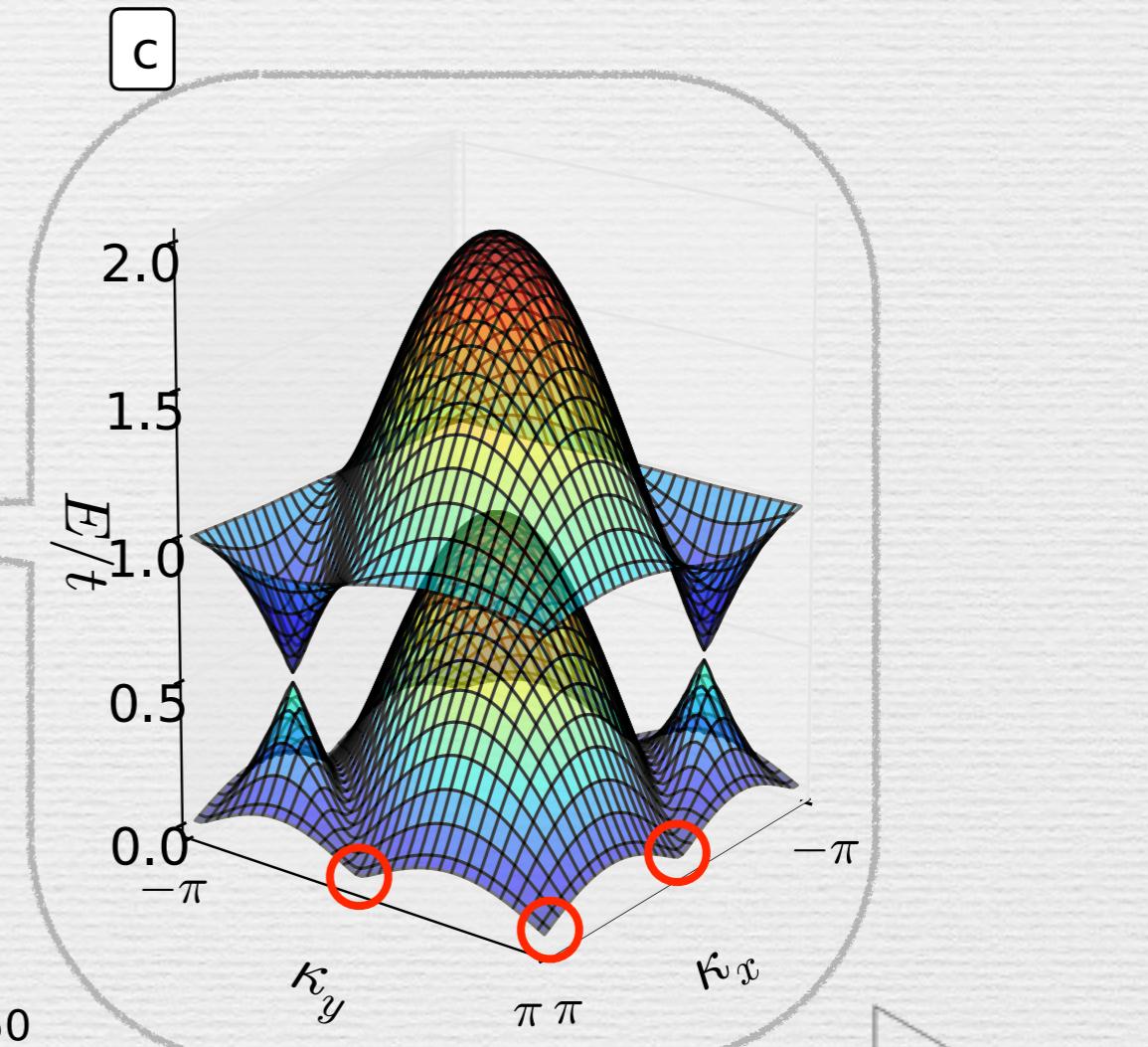
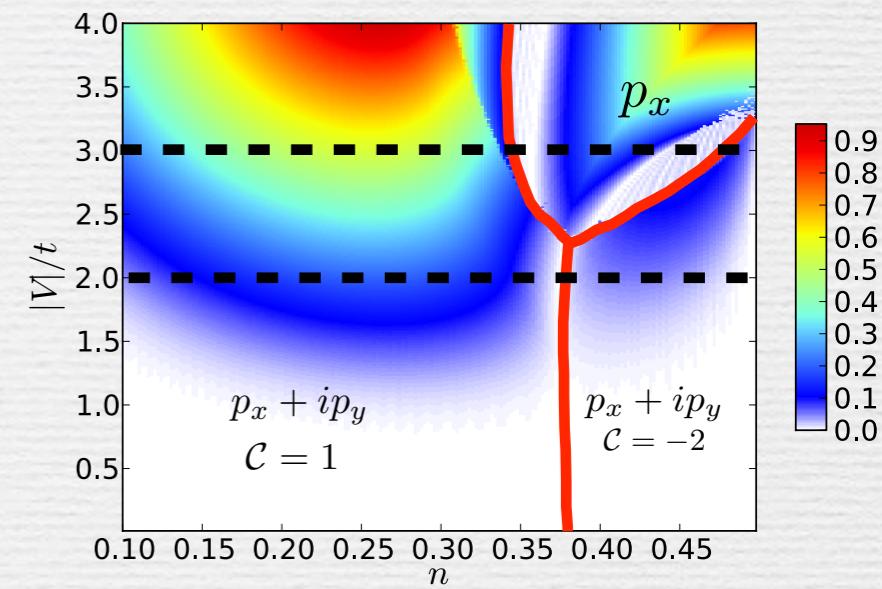
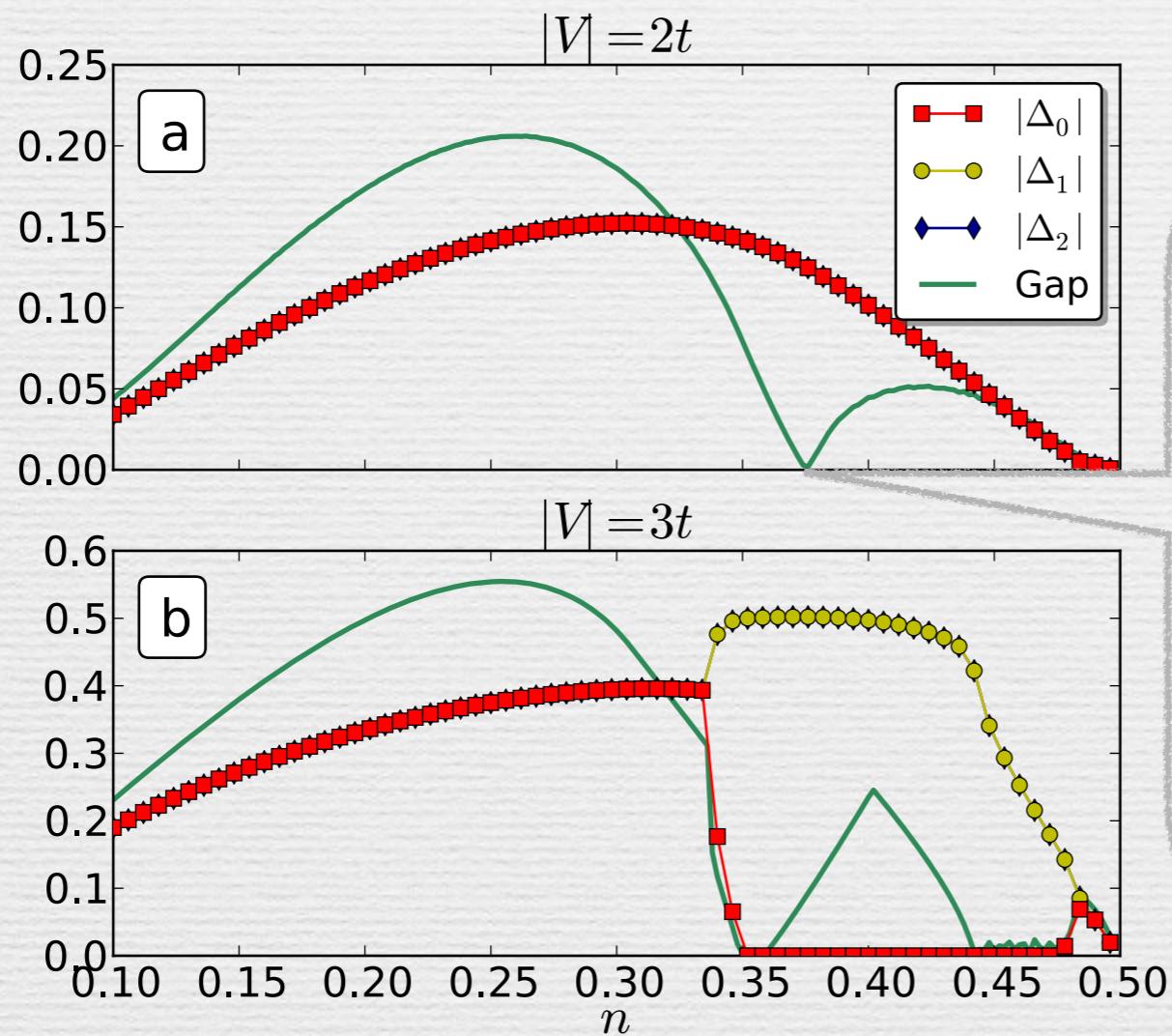
Scan density



Scan density



Scan density



Topological Phase Transition and Dirac Fermions

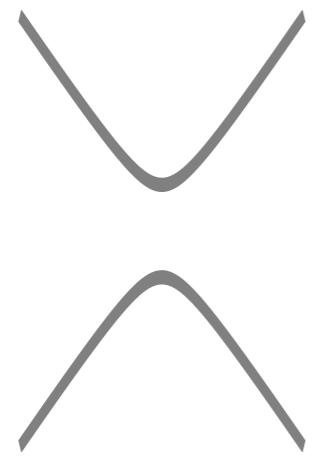
Chern number of a Dirac fermion

$$\mathcal{C} = \frac{\text{sgn}(m)}{2}$$

Oshikawa, PRB, 1994

Ludwig et al, PRB, 1994

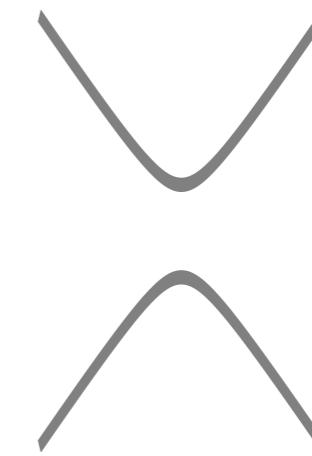
$$m > 0$$



$$m = 0$$

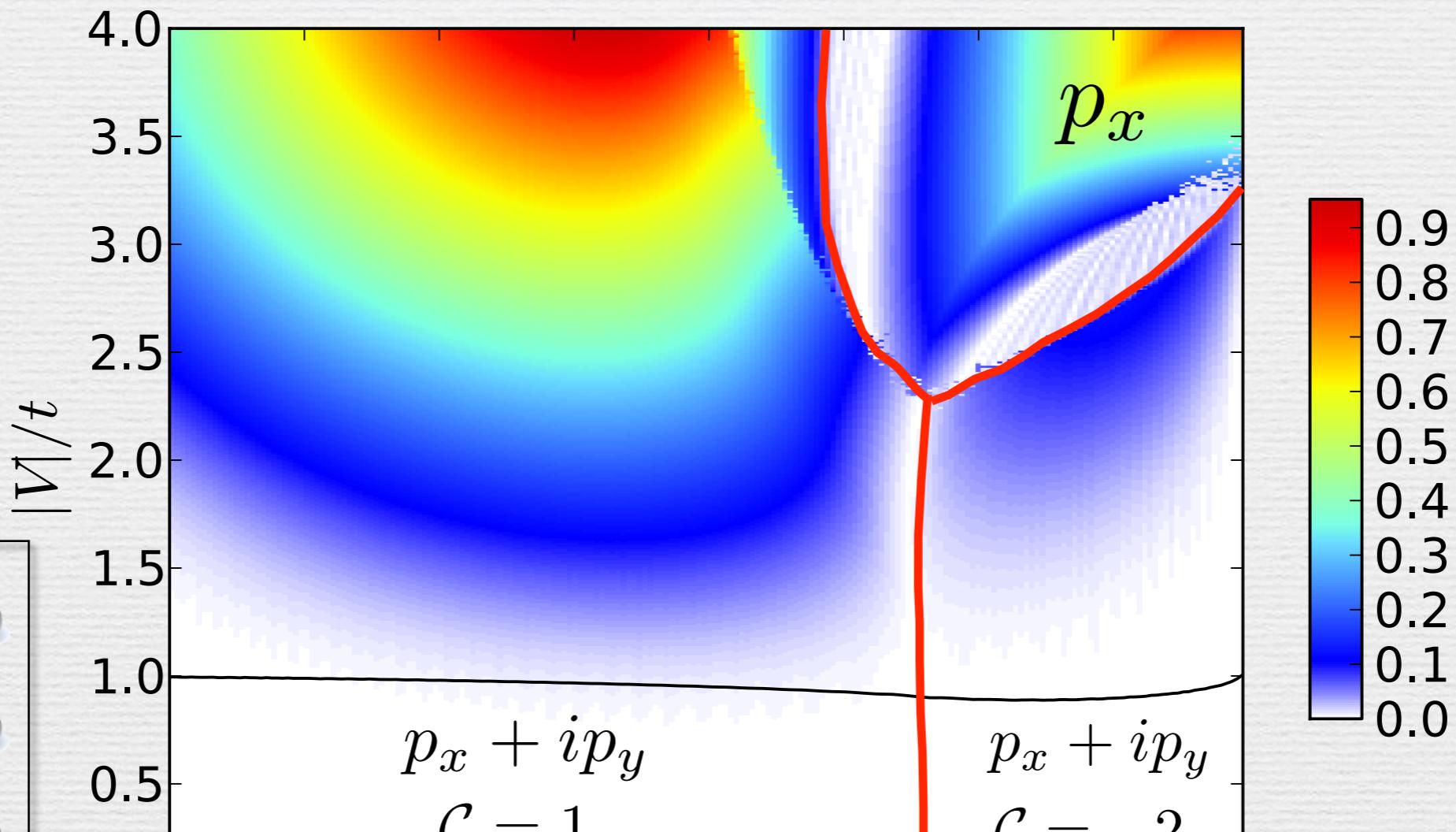


$$m < 0$$



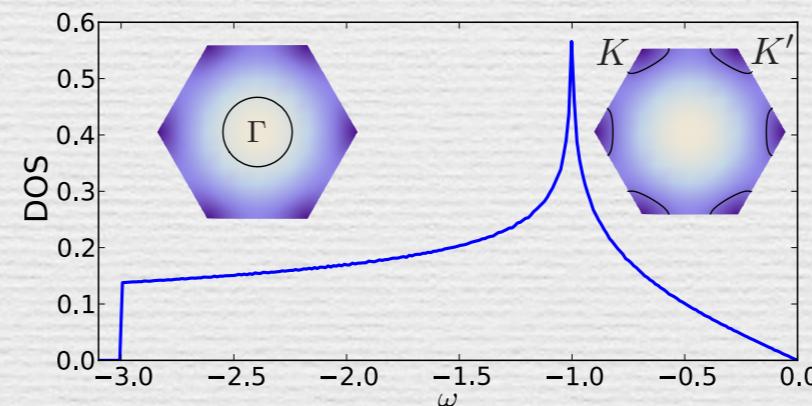
$$\Delta\mathcal{C} = \# \text{ of Dirac points}$$

Phase diagram, again



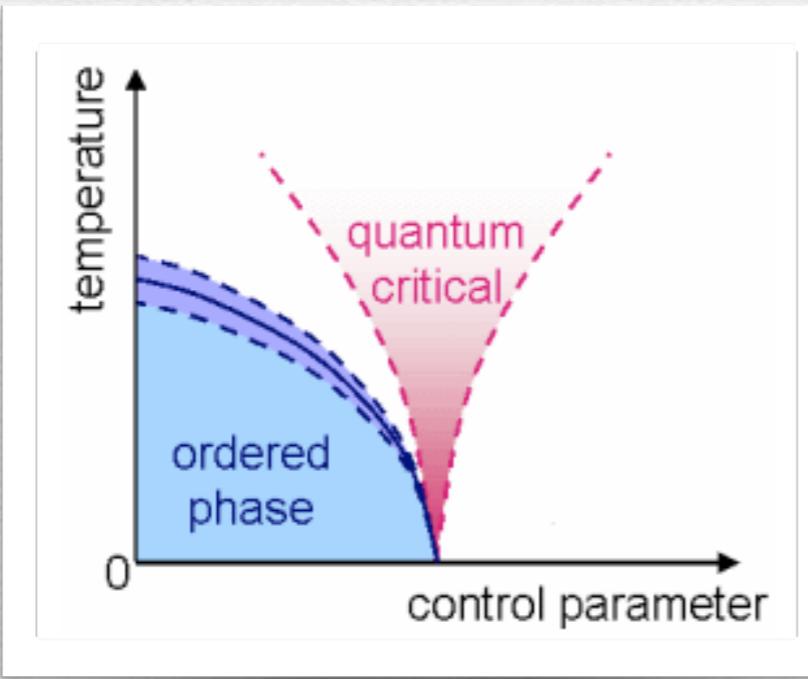
A general “theorem”, Cheng, Sun,
Galitski and Das Sarma, PRB, 2010

Grassmann Tensor RG, Gu, PRB, 2013

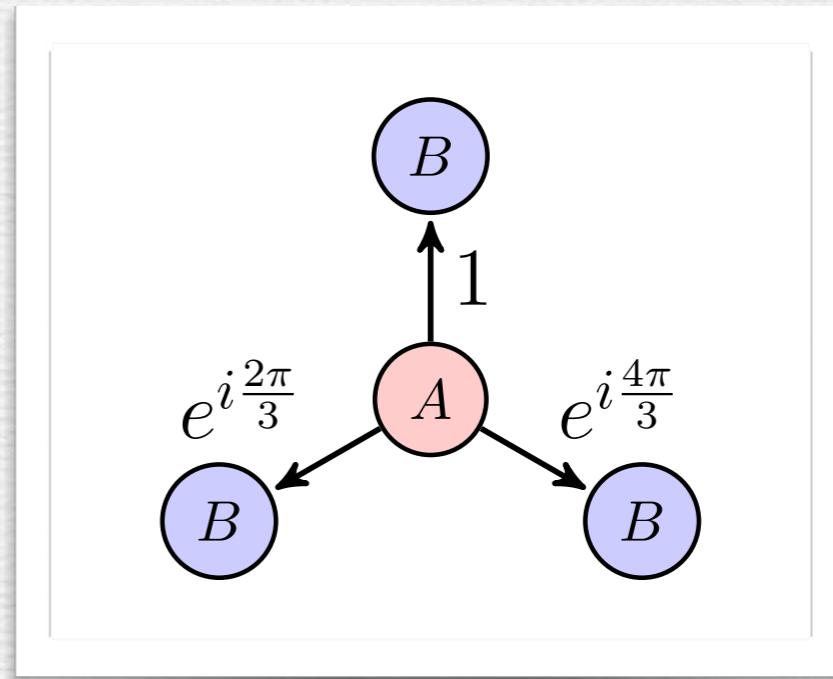


Summary-II

Fermionic Quantum Critical Point



Topological Superconductors



- 📌 Rich physics in a very simple model
- 📌 Hopefully **realizable in experiment** given its simple form

Thank you!