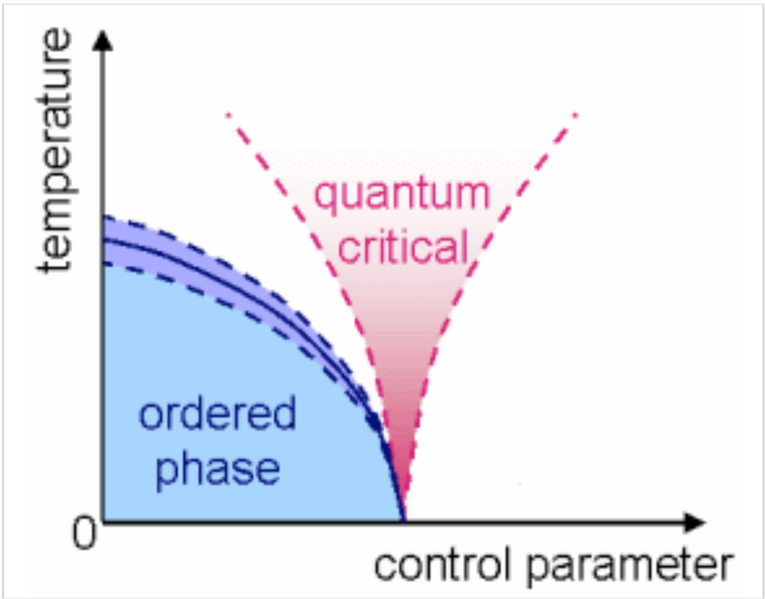
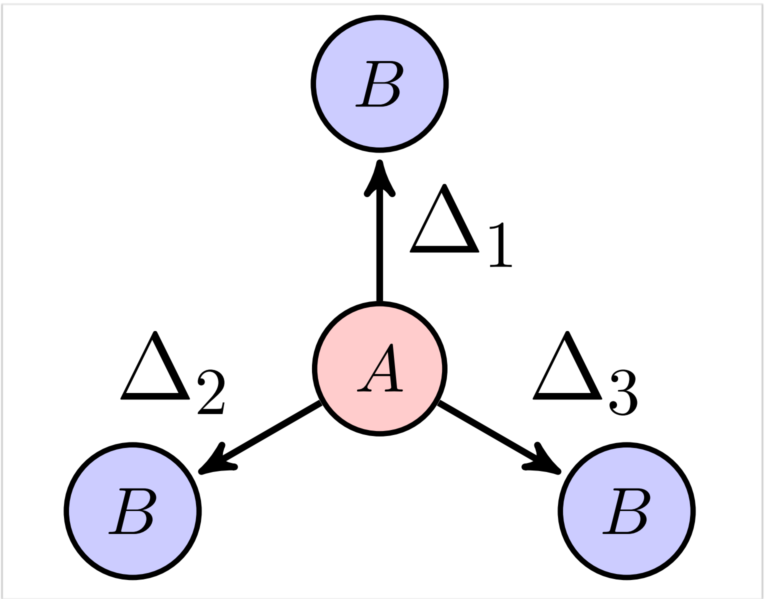
Spinless Fermions on a Honeycomb Lattice

From quantum criticality to topological superconductors





Lei Wang

ETH Zurich

LW, Corboz and Troyer,1407.0029

LW and Troyer, 1407.0707

LW and Troyer, to appear

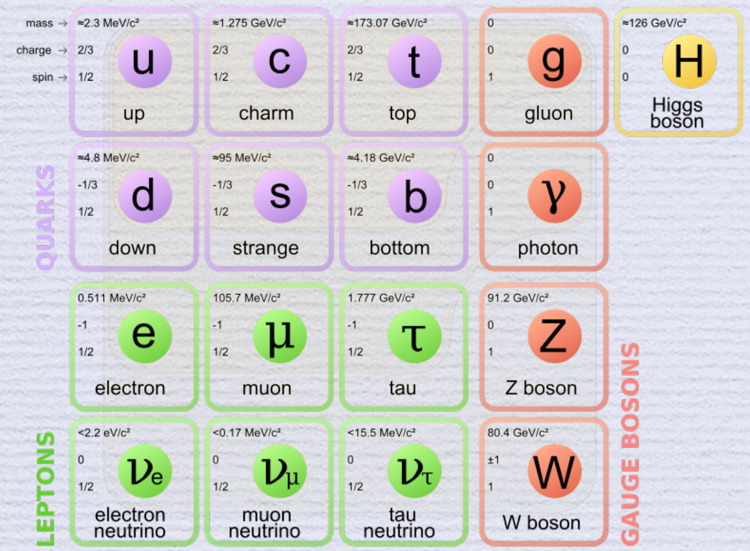
Collaborators

Philippe Corboz

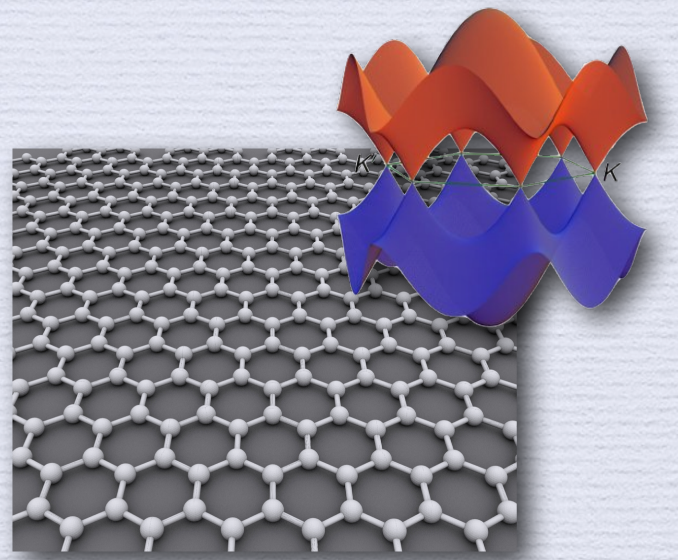
Matthias Troyer

Dirac Fermions

Elementary Particles



Graphene

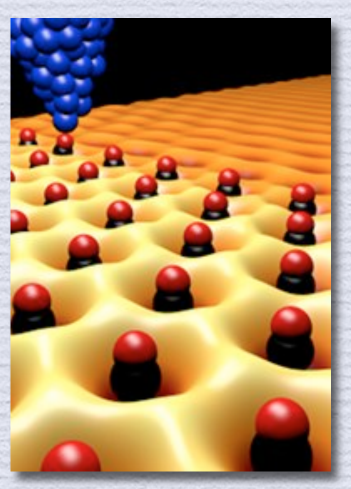


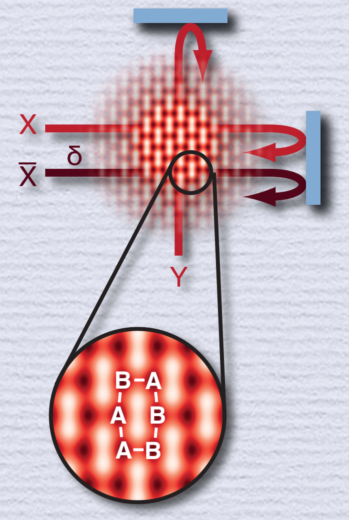
Novoselov et al, Zhang, et al, Nature, 2005

"Artificial graphene"

Gomes et al, Nature, 2012

Tarruell et al, Nature, 2012

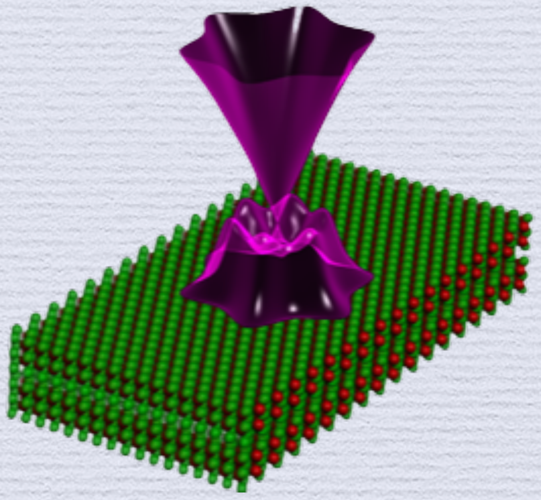


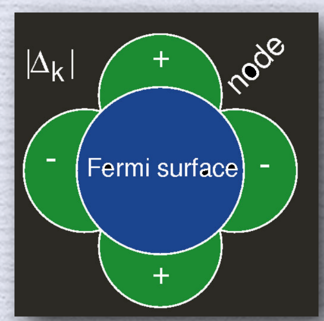


Many others...

Topological insulator

d-wave superconductor

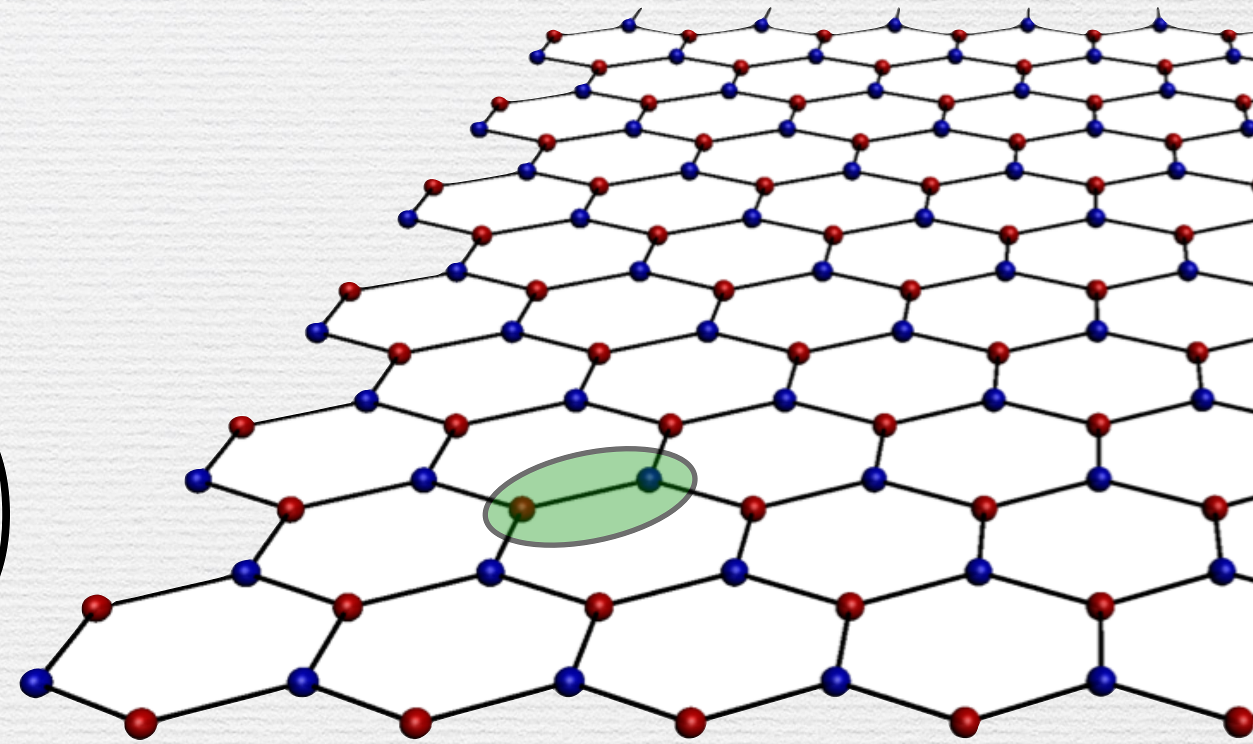


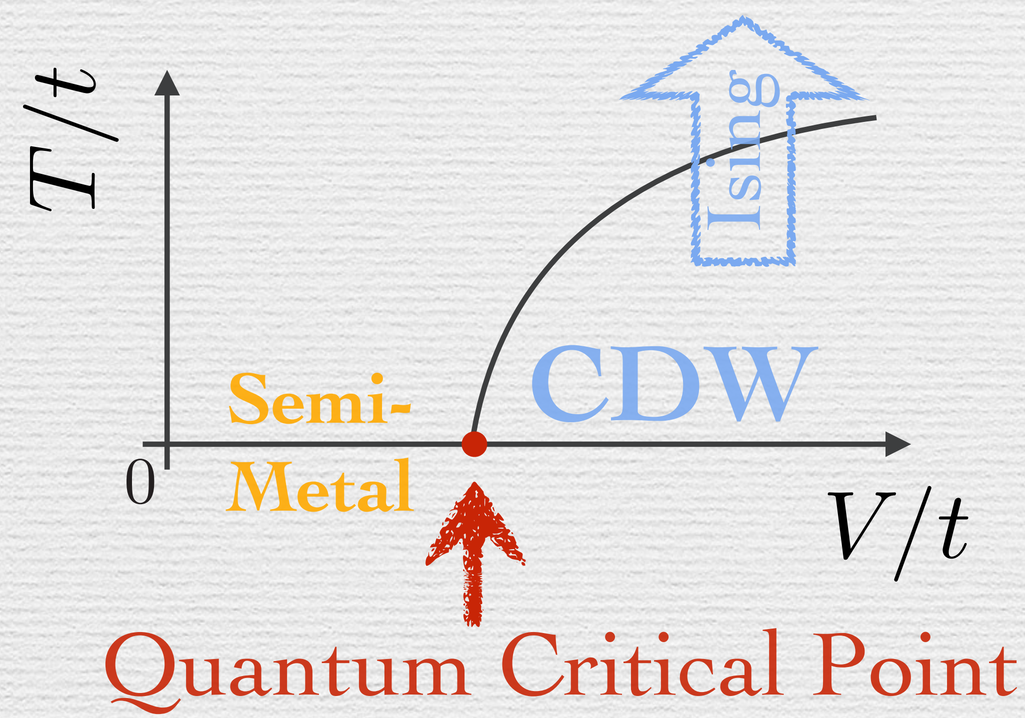


Spinless fermions on a honeycomb lattice

$$\hat{H}_0 = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \left(\hat{c}_{\mathbf{i}}^{\dagger} \hat{c}_{\mathbf{j}} + \hat{c}_{\mathbf{j}}^{\dagger} \hat{c}_{\mathbf{i}} \right)$$

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





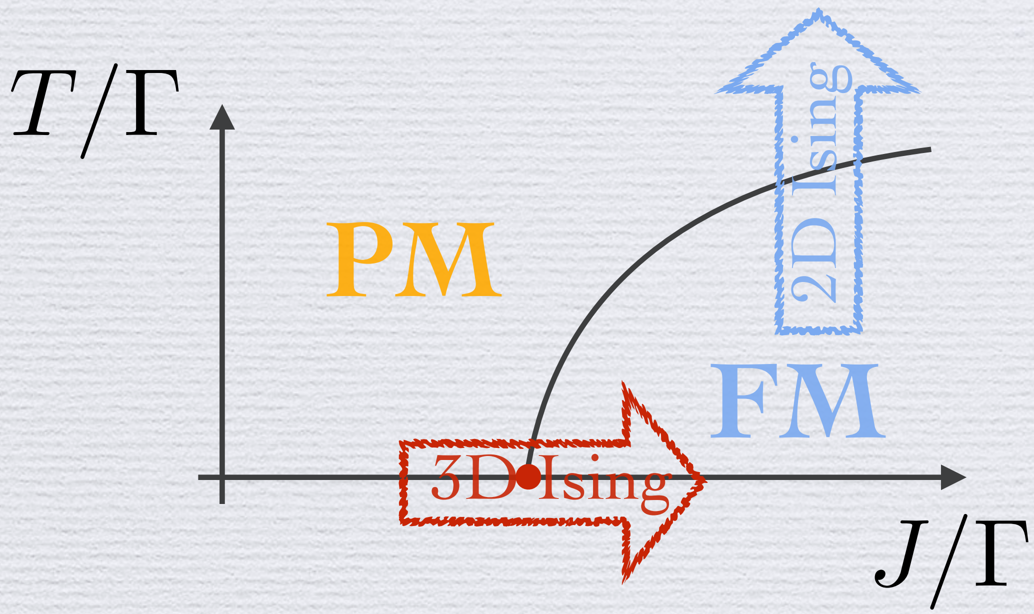
- Where is the QCP ?
- What is the universality class ?
- What are the critical exponents ?

cf. Studies of Hubbard model

Sorella, et al, EPL, 1992
Paiva, et al, PRB, 2005
Meng, et al, Nature, 2010
Sorella, et al, Sci.Rep., 2012
Assaad, et al, PRX, 2013

Quantum Critical Points

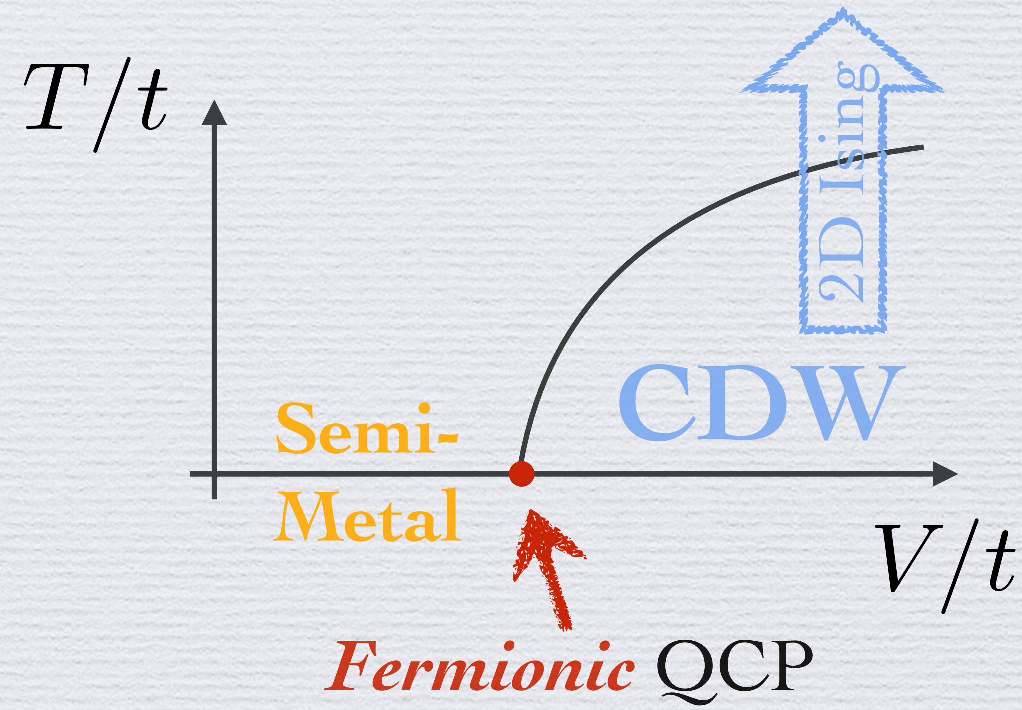
$$H_{\text{TFIM}} = -J \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \sigma_{\mathbf{i}}^z \sigma_{\mathbf{j}}^z + \Gamma \sum_{\mathbf{i}} \sigma_{\mathbf{i}}^x$$



Scalar ϕ⁴-theory

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

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



Gross-Neveu-Yukawa theory

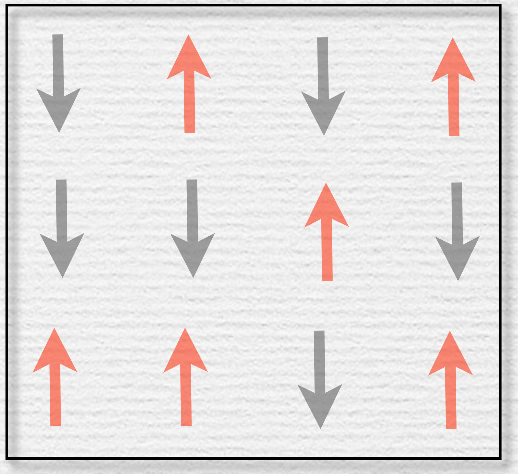
$$\mathcal{L} = \mathcal{L}_\phi + \mathcal{L}_\Psi + g\phi\bar{\Psi}\sigma^z\Psi$$

Sign problem in auxiliary field QMC

Blankenbecler et al, PRD, 1981

Assaad et al, Lect. Notes Phys. 2008

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



$\mathcal{C}$

- 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 ?

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

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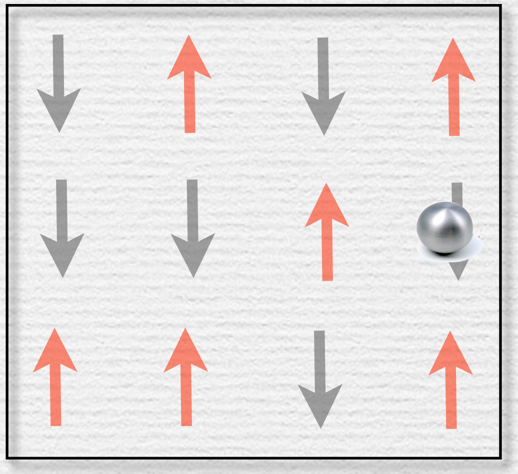

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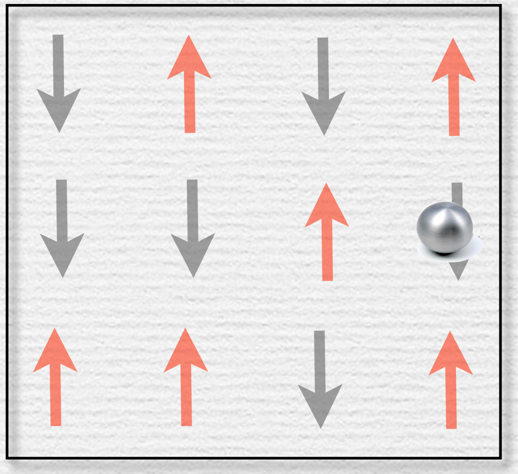

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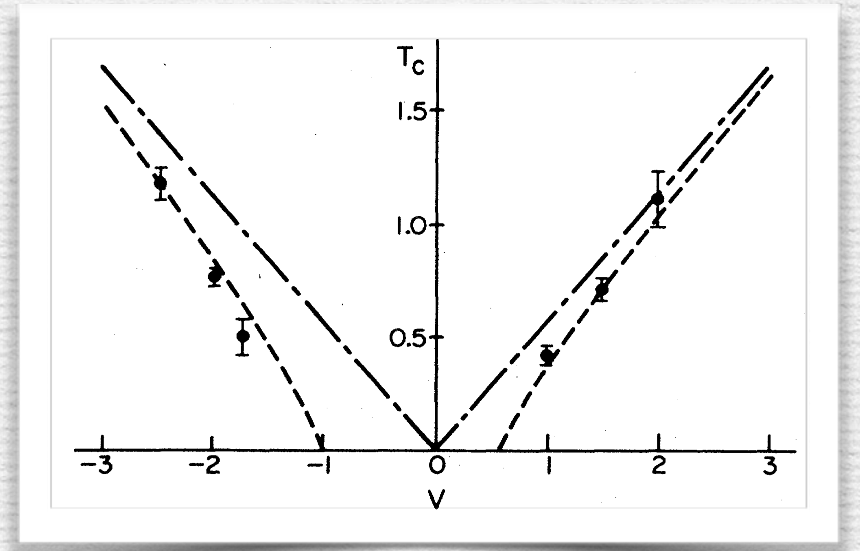
Scalapino et al, PRB, 1984

Gubernatis et al, PRB, 1985



up to 8×8 square lattice, T=0.3t

- How about spinless fermions ?

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

Determinant = Pfaffian^2

For skew-symmetric matrices Huffman and Chandrasekharan, PRB, 2014

$$M = -M^T$$

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

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

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

Johann Friedrich Pfaff

Is M skew-symmetric ?

No

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

Yes

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

CTQMC

Rubtsov et al, PRB,2005

Gull et al, RMP, 2011

$$\hat{H}_0 = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \left(\hat{c}^\dagger_{\mathbf{i}} \hat{c}_{\mathbf{j}} + \hat{c}^\dagger_{\mathbf{j}} \hat{c}_{\mathbf{i}} \right)$$

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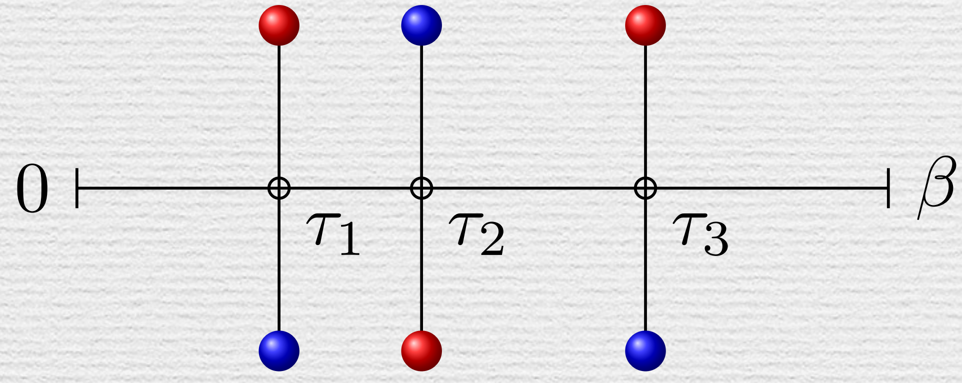
$$Z = \mathrm{Tr}\left[e^{-\beta \hat{H}_0} \mathcal{T} e^{-\int_0^\beta \hat{H}_1(\tau)} \right]$$

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

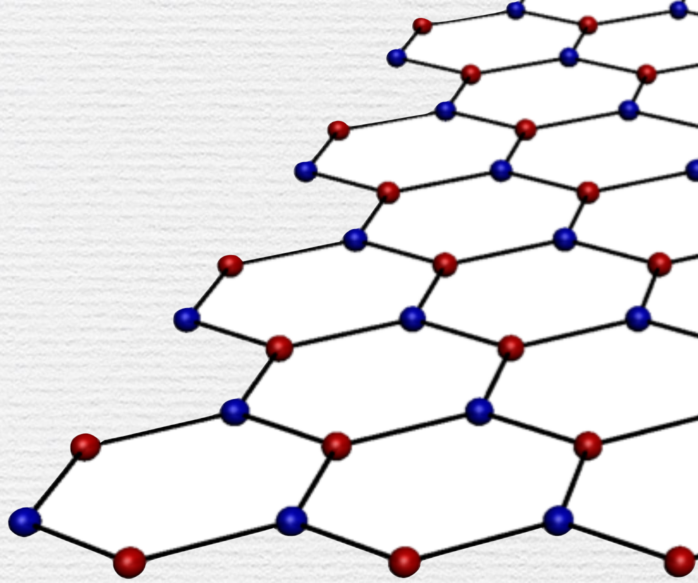
$$\sim \sum_{\mathcal{C}} w(\mathcal{C})$$

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



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

~~Sign Problem~~



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

Huffman and Chandrasekharan, PRB, 2014

$G^T = -DGD$ → $(GD)^T = -GD$

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

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

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

*half-filling ensures diagonal element vanishes

Observables & Scaling Ansatz

± 1 for A(B) sublattice

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

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

$2L^2$ up to 450 sites

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Scalings ansatz close to the QCP

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

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

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Scalings ansatz close to the QCP

relativistic invariance

$z = 1$

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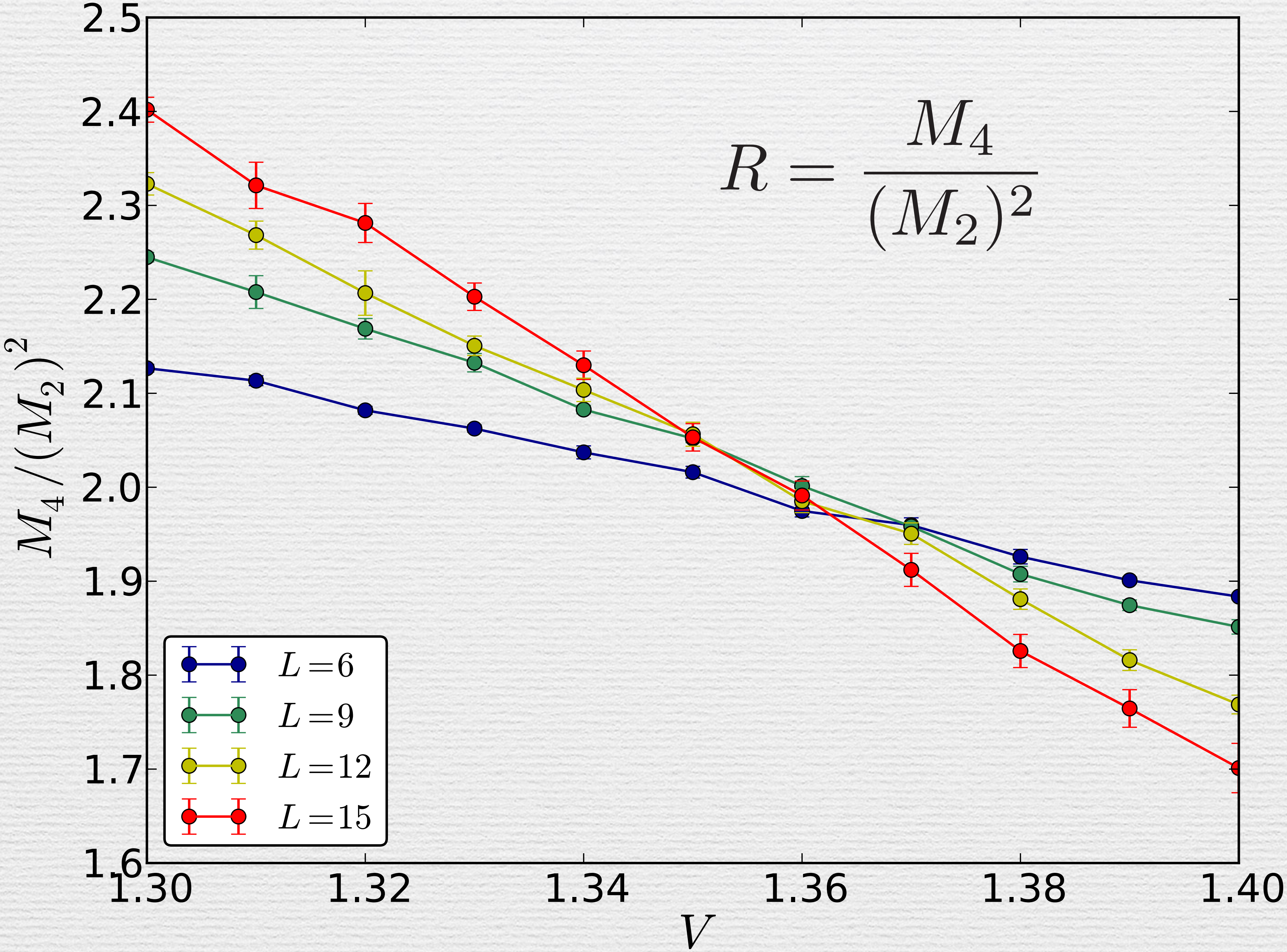
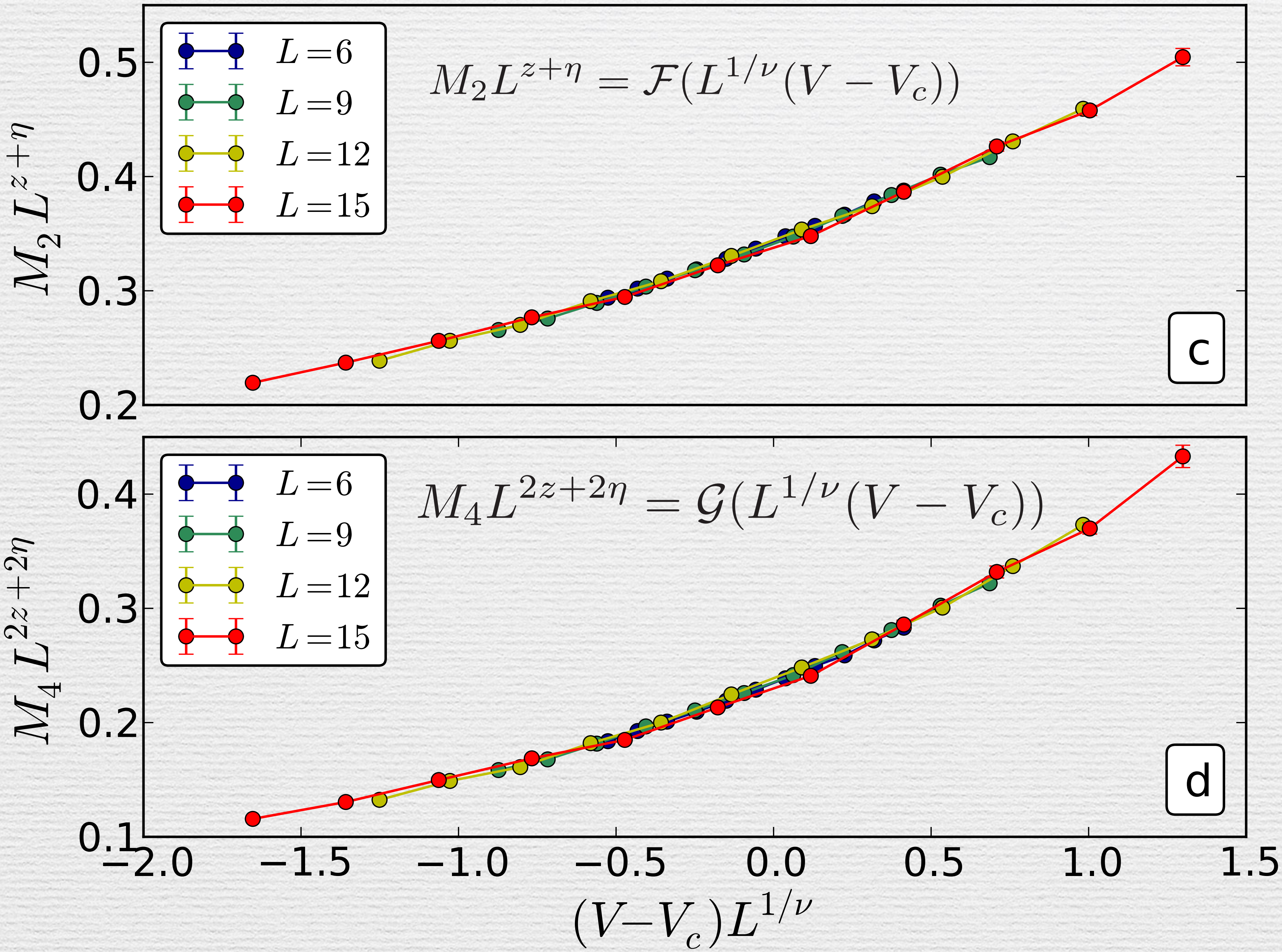
Binder Ratio



Data Collapse



$V_c/t = 1.356(1)$

$\nu = 0.80(3)$

$\eta = 0.302(7)$

* Errorbar from $\chi^2 + 1$ analysis

Gross-Neveu-Yukawa Theory

- ε-expansion Rosenstein et al, PLB, 1993

$$\nu = 0.797 \qquad \eta = 0.502$$

- functional renormalization group Rosa et al, PRL,2001 Höfling et al, PRB, 2002

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

Honeycom

$$\nu = 0.80(3)$$

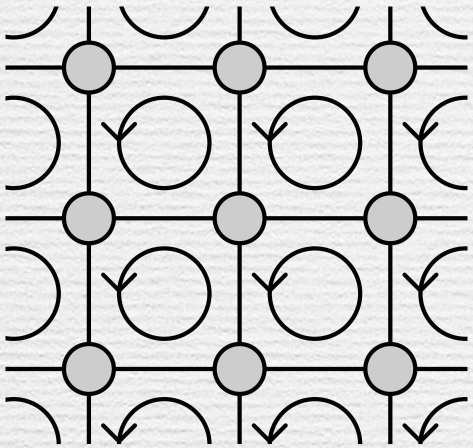
$$\eta = 0.302(7)$$

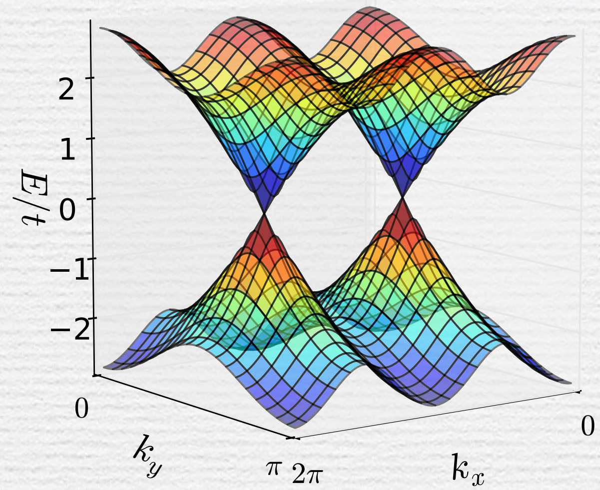
ν agrees

η does not

* Field theory calculations are based on 2-flavors of 2-component Dirac fermions with same chirality

Check-I: π-flux square lattice





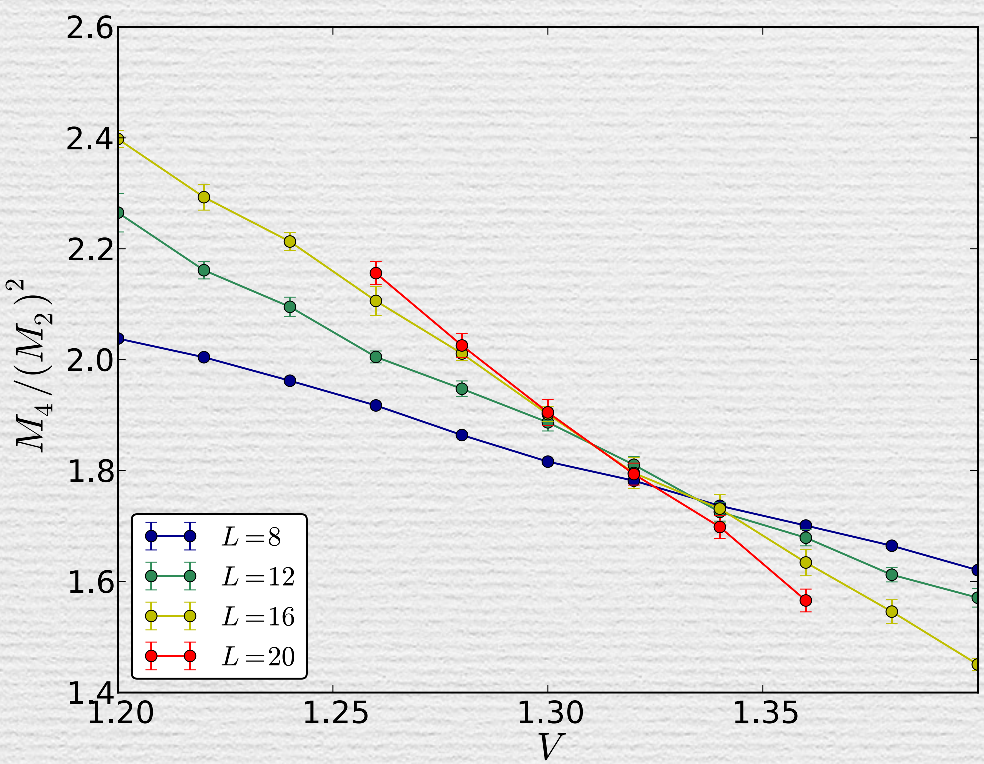
also features two Dirac points

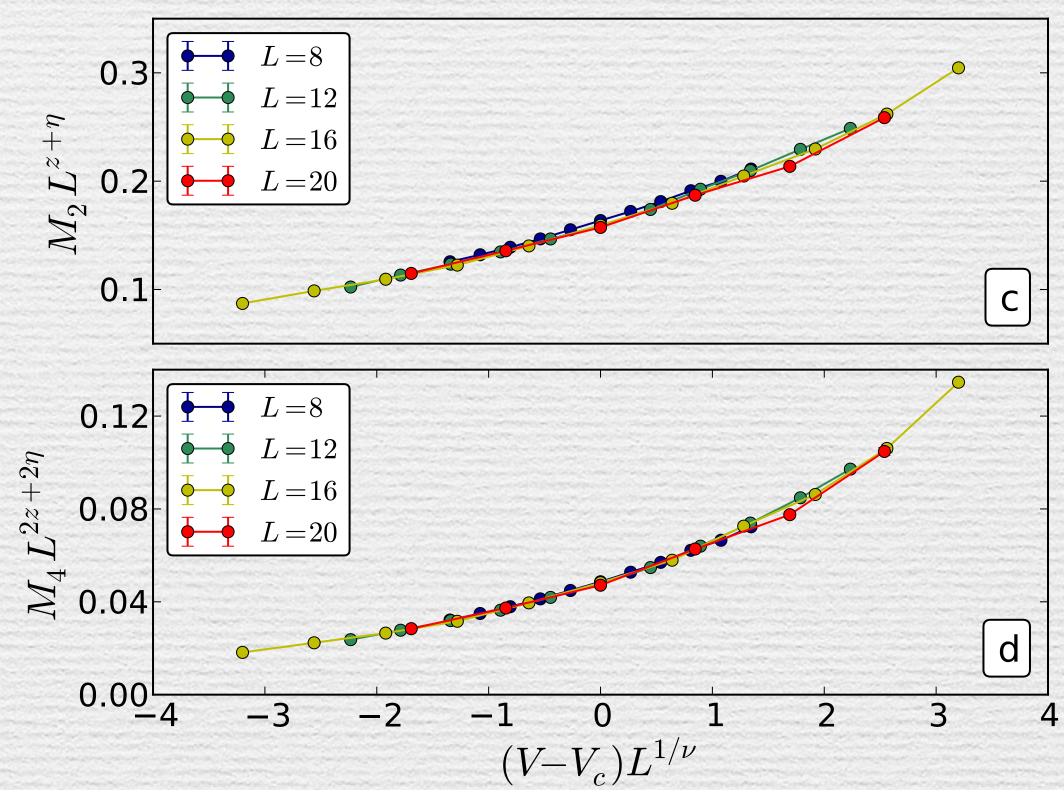
π-flux lattice

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

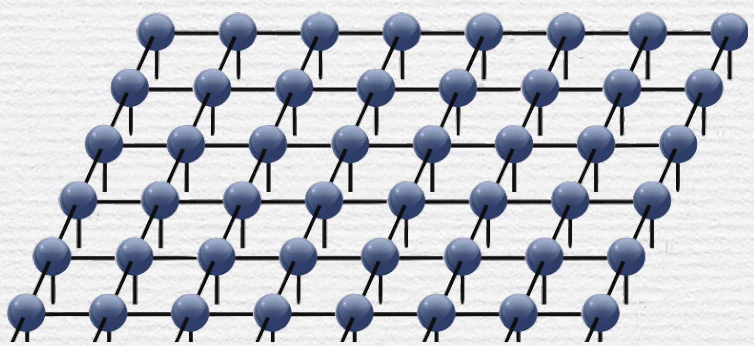
$$\nu = 0.80(6)$$

$$\eta = 0.318(8)$$

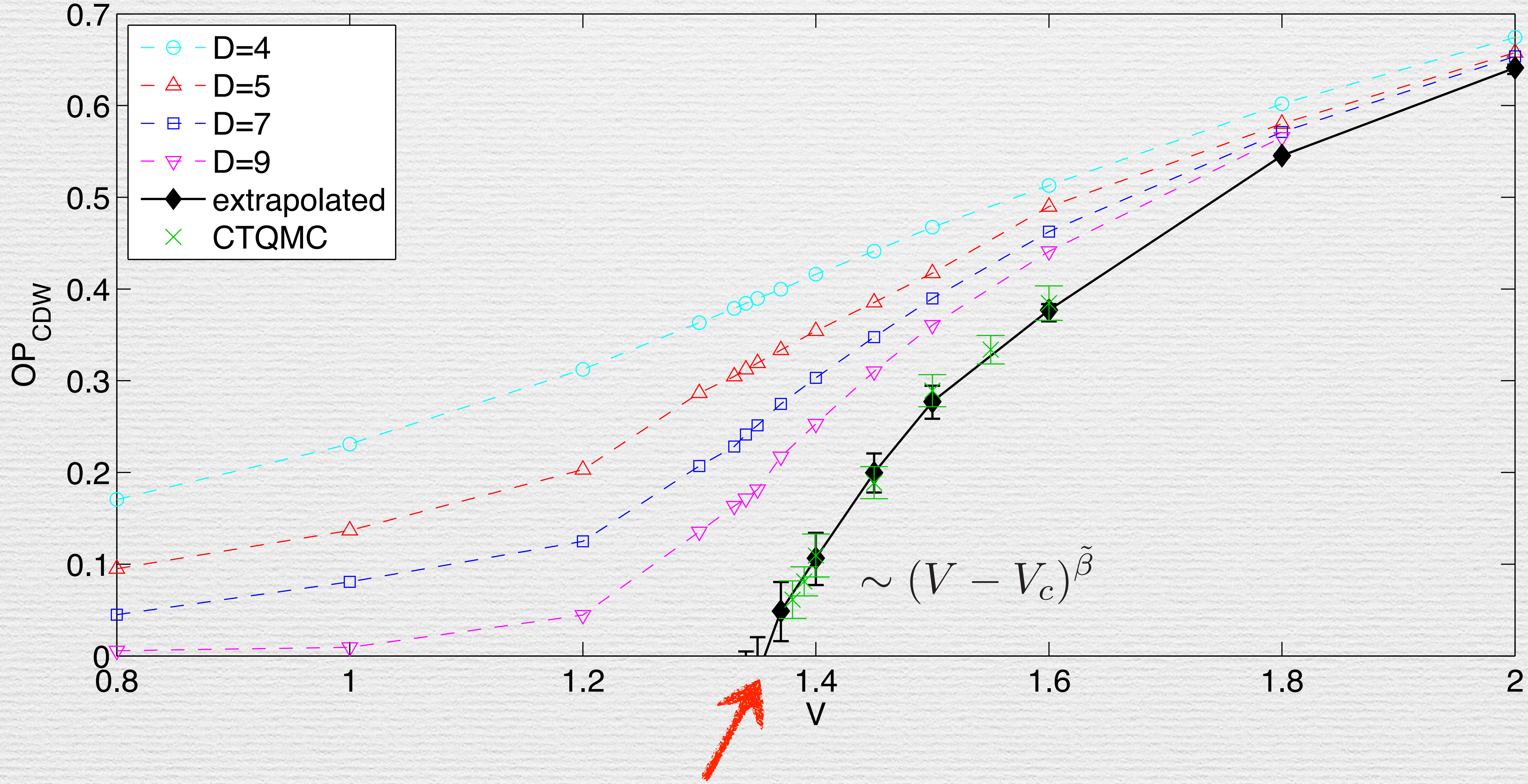




Check-II: iPEPS

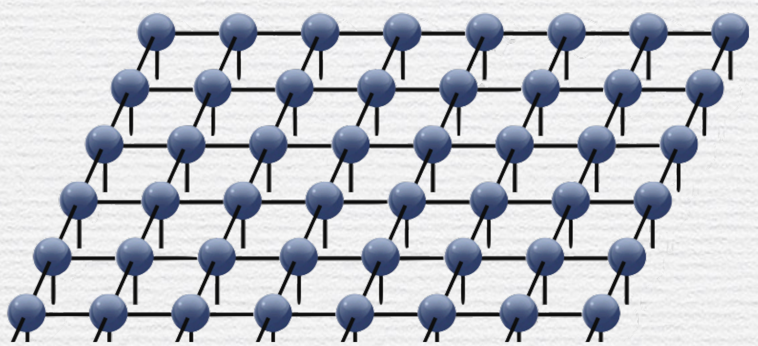


Philippe Corboz
ETH→Amsterdam



$V_c = 1.36(3)$

Check-II: iPEPS



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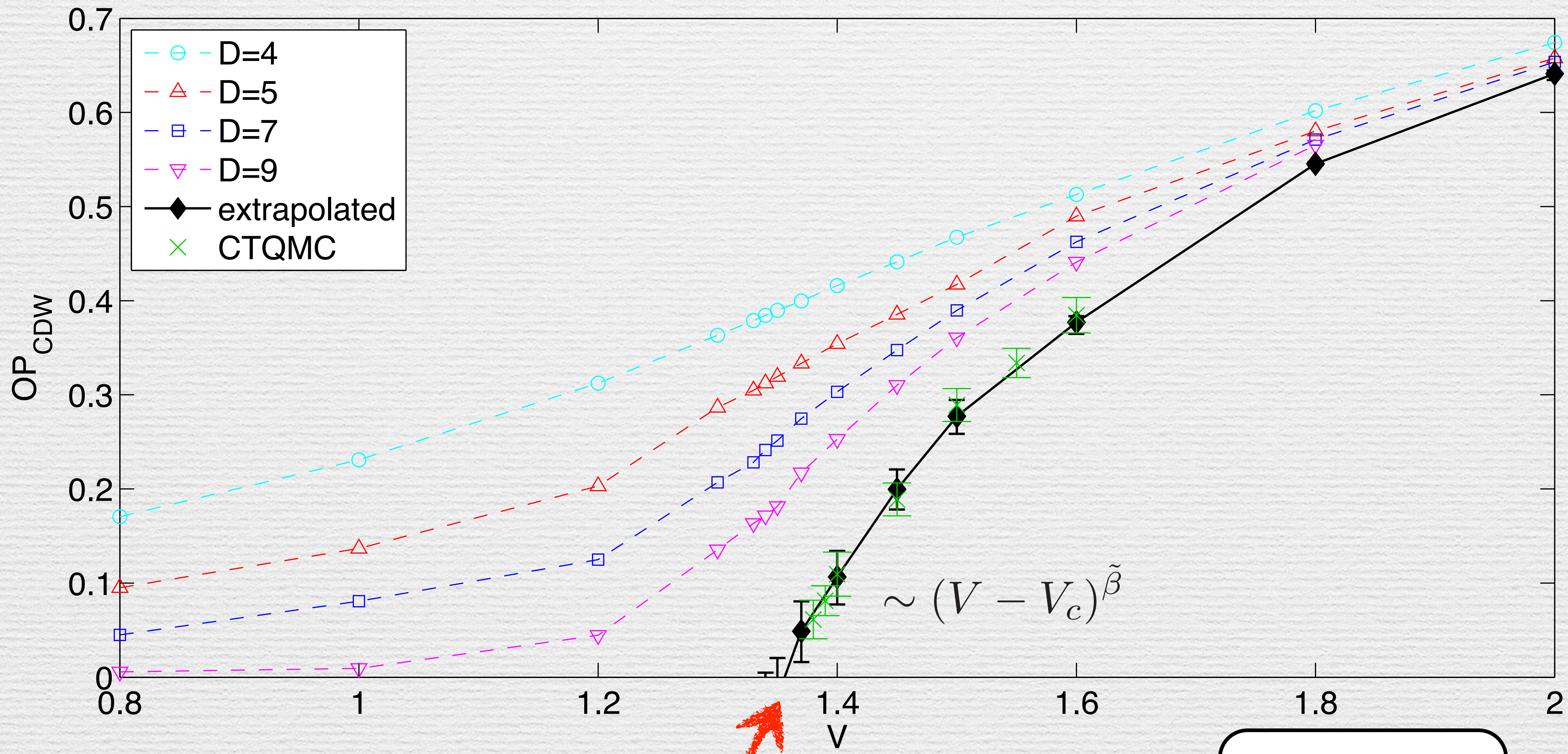


$$V_c = 1.36(3)$$

CTQMC

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

Summary-I

LW, Corboz and Troyer, 1407.0029

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

CTQMC

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

$$\nu = 0.80(3)$$

$$\eta = 0.302(7)$$

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

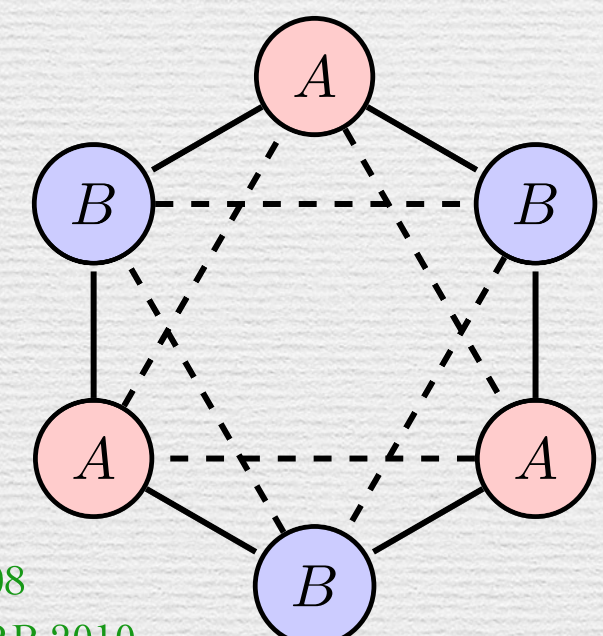
To resolve the discrepancies we need to

- ☐ Make sure to compare with the right theory
- ☐ Bigger systems and more careful data analysis

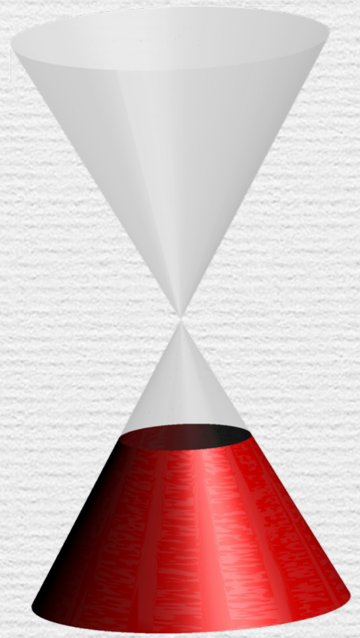
Where do we go from here ?

Half-filled, nearest-neighbor repulsion

Next-nearest-neighbor repulsion



Doped attractive system



Raghu et al, PRL,2008
Weeks and Franz, PRB,2010
García-Martínez et al, PRB,2013
Daghofer and Hohenadler, PRB,2014

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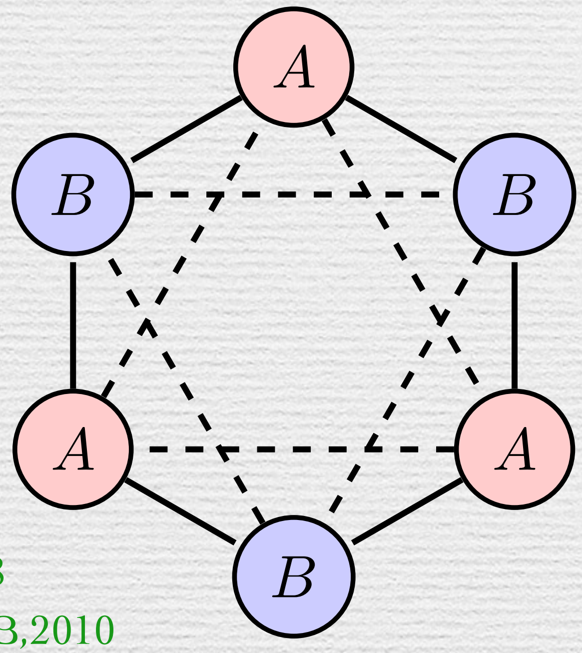

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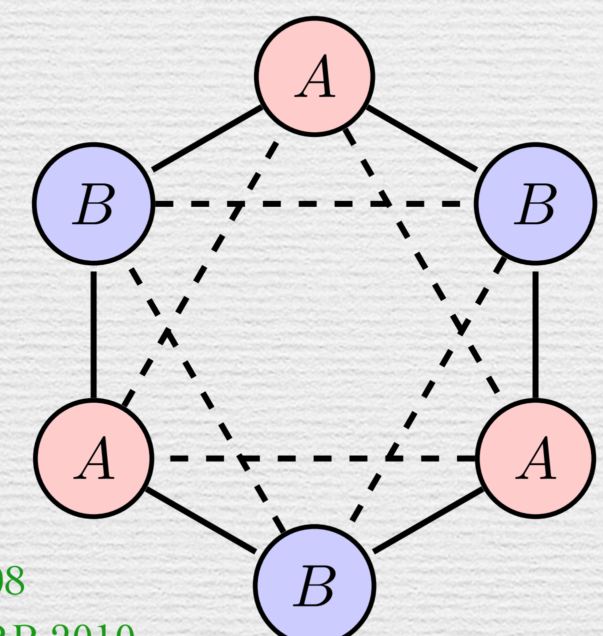

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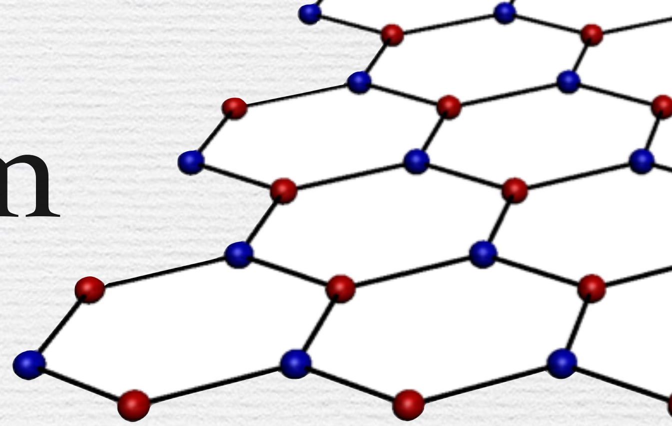
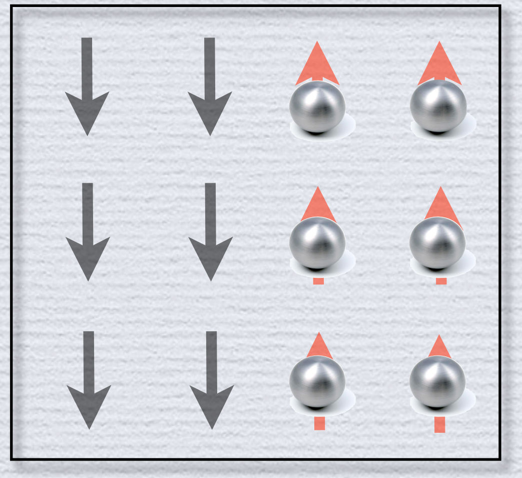


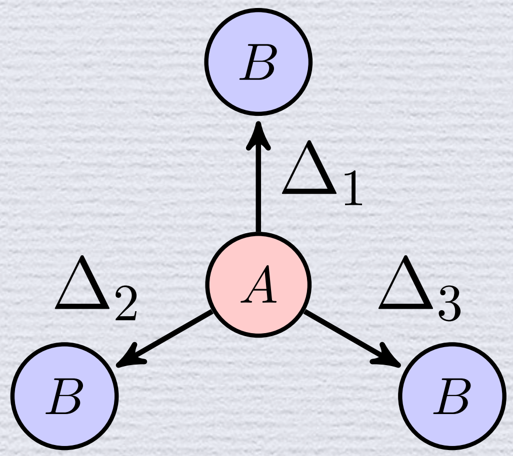
$V < 0$

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

Strong coupling
"Phase separation"



Weak-coupling
Superconductivity

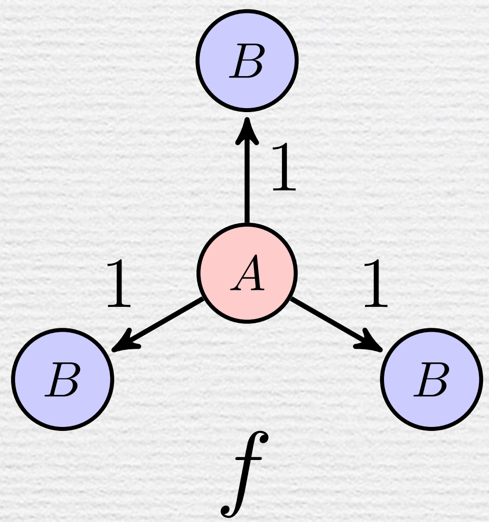


$$\Delta_\delta = \langle \hat{c}_{\mathbf{i}\in A}\hat{c}_{\mathbf{i}+\delta}\rangle$$

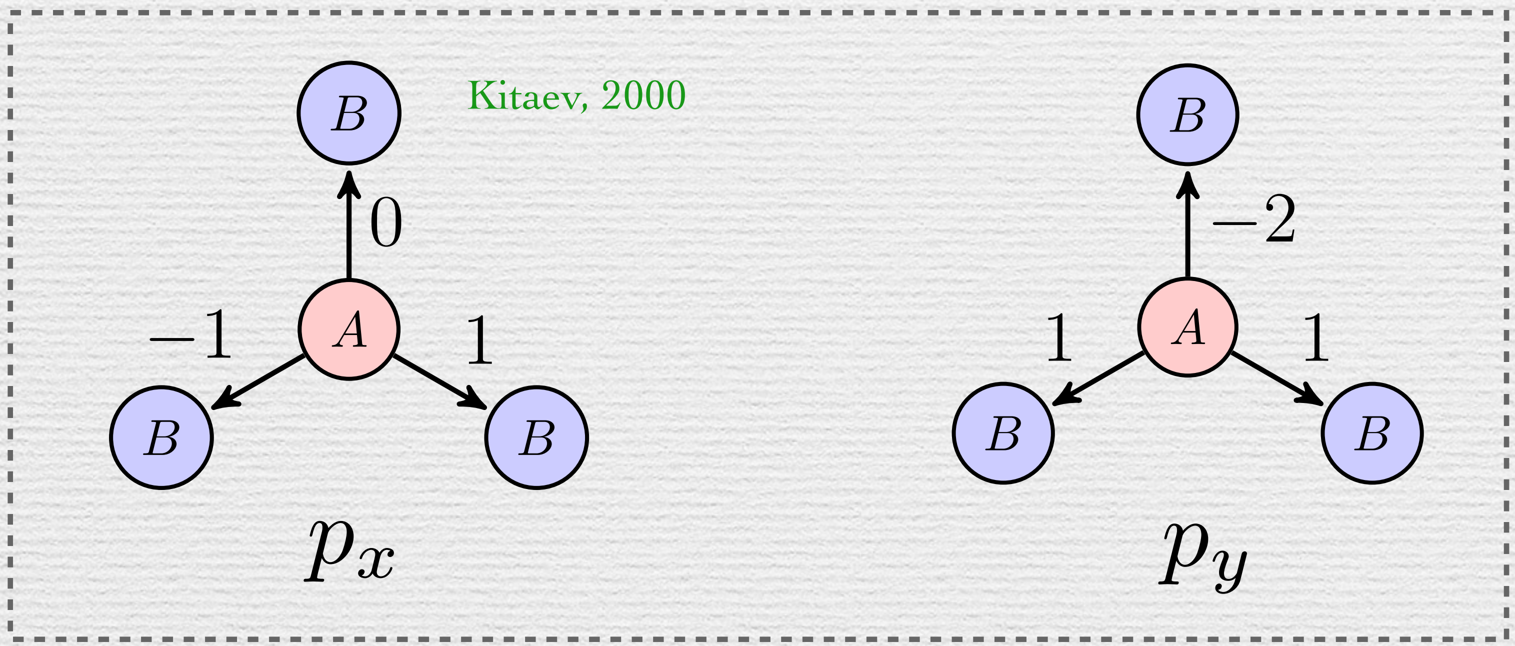
Pairing Symmetries

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



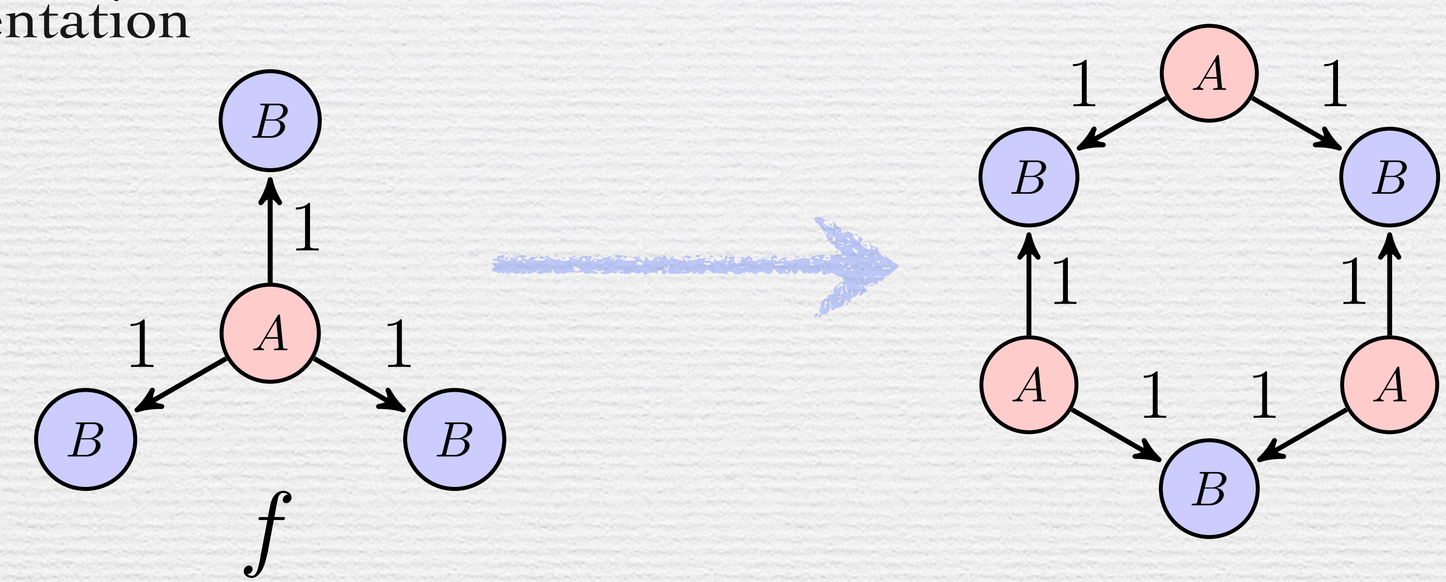
- 2-dim E_1 representation



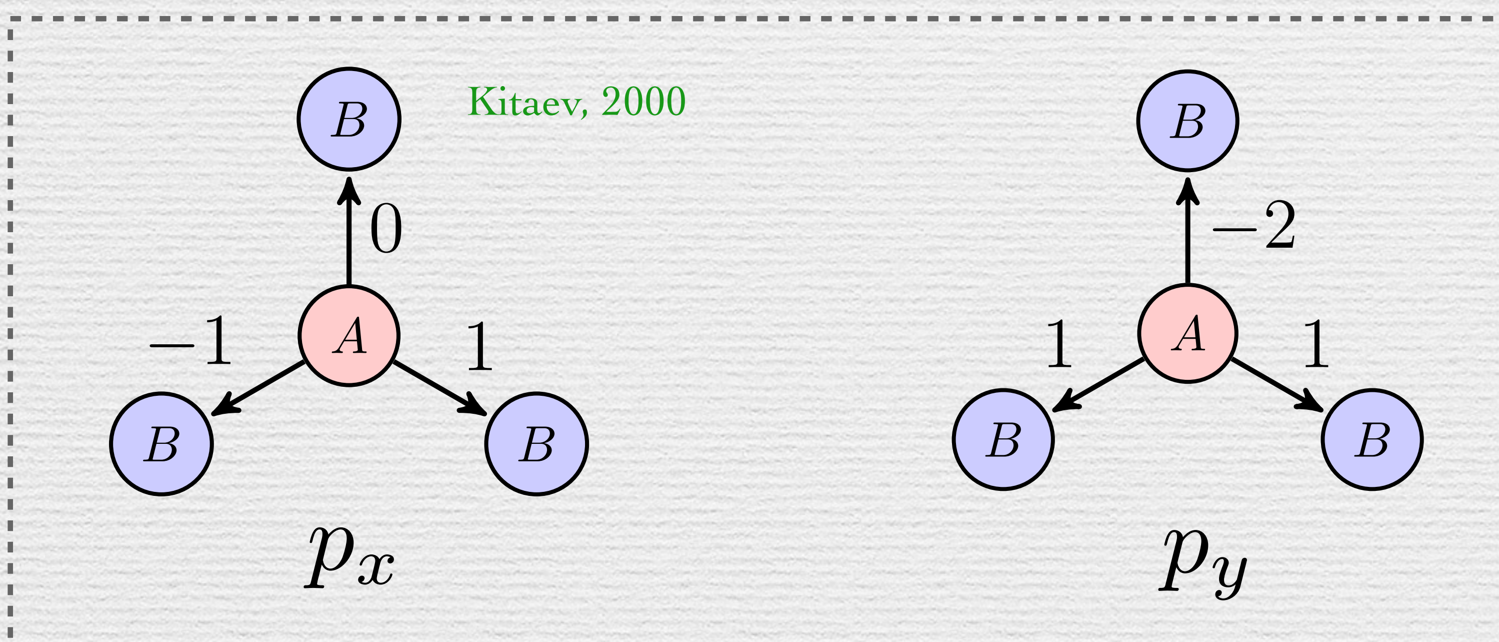
Pairing Symmetries

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



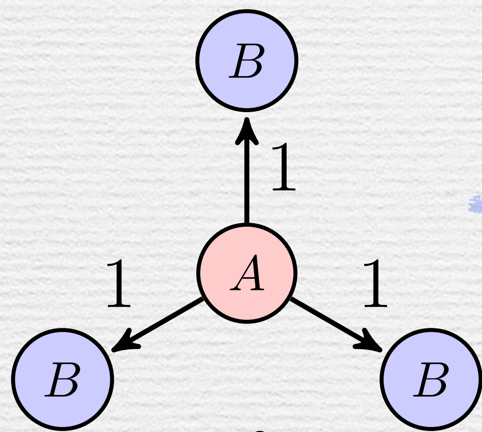
- 2-dim E_1 representation



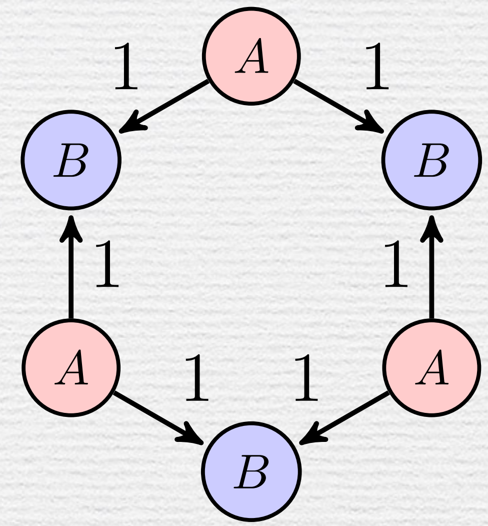
Pairing Symmetries

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

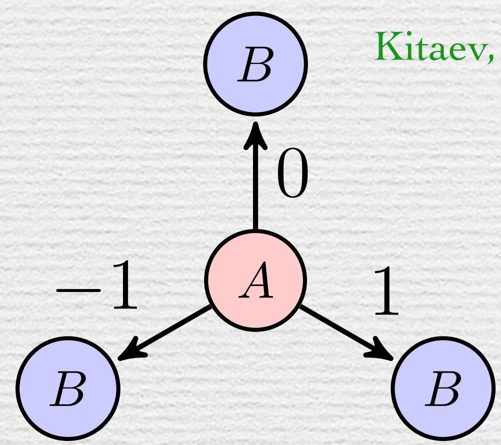
- 1-dim B_1 representation



f

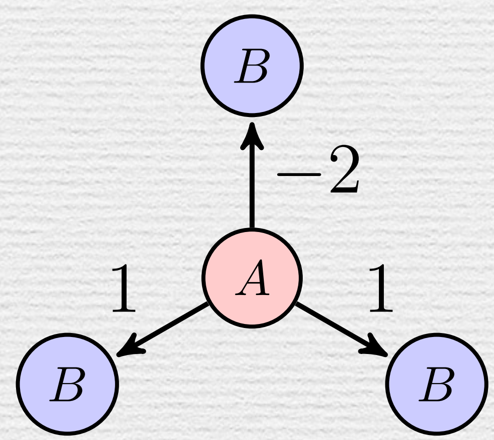


- 2-dim E_1 representation

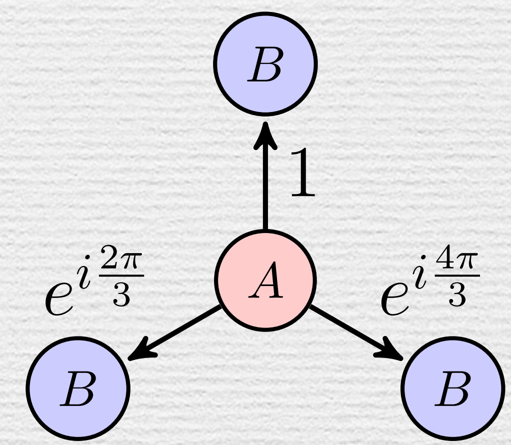


p_x

Kitaev, 2000



p_y



$p_x + ip_y$

Read and Green, PRB, 2000

Pairing Susceptibilities

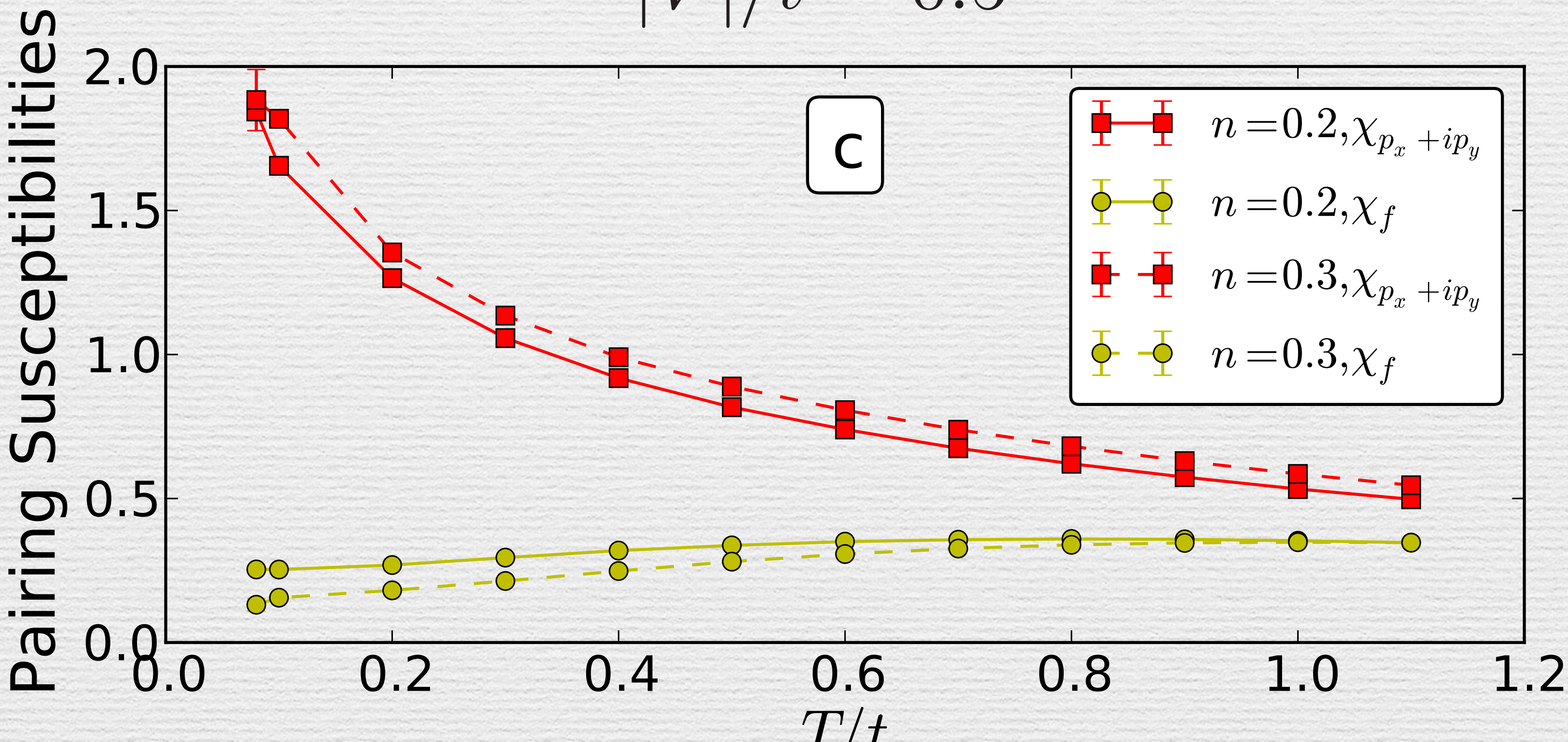
$$\chi_\Gamma = \int_0^\beta d\tau \langle \hat{\Delta}_\Gamma(\tau)\hat{\Delta}_\Gamma^\dagger \rangle$$

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

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

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

$|V|/t = 0.5$



BdG Calculation

$$H_{\mathrm{BdG}} =$$

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

BdG Calculation

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

$$H_{\mathrm{BdG}} =$$

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

BdG Calculation

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

$$H_{\mathrm{BdG}} = \frac{1}{2}\sum_{\mathbf{k}} \begin{pmatrix} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \\ \hat{c}^\dagger_{-\mathbf{k}A} \\ \hat{c}^\dagger_{-\mathbf{k}B} \end{pmatrix}^\dagger \begin{pmatrix} -\mu & z_{\mathbf{k}} & 0 & \Delta_{\mathbf{k}} \\ z^*_{\mathbf{k}} & -\mu & -\Delta_{-\mathbf{k}} & 0 \\ 0 & -\Delta^*_{-\mathbf{k}} & \mu & -z^*_{-\mathbf{k}} \\ \Delta^*_{\mathbf{k}} & 0 & -z_{-\mathbf{k}} & \mu \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \\ \hat{c}^\dagger_{-\mathbf{k}A} \\ \hat{c}^\dagger_{-\mathbf{k}B} \end{pmatrix}$$

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

BdG Calculation

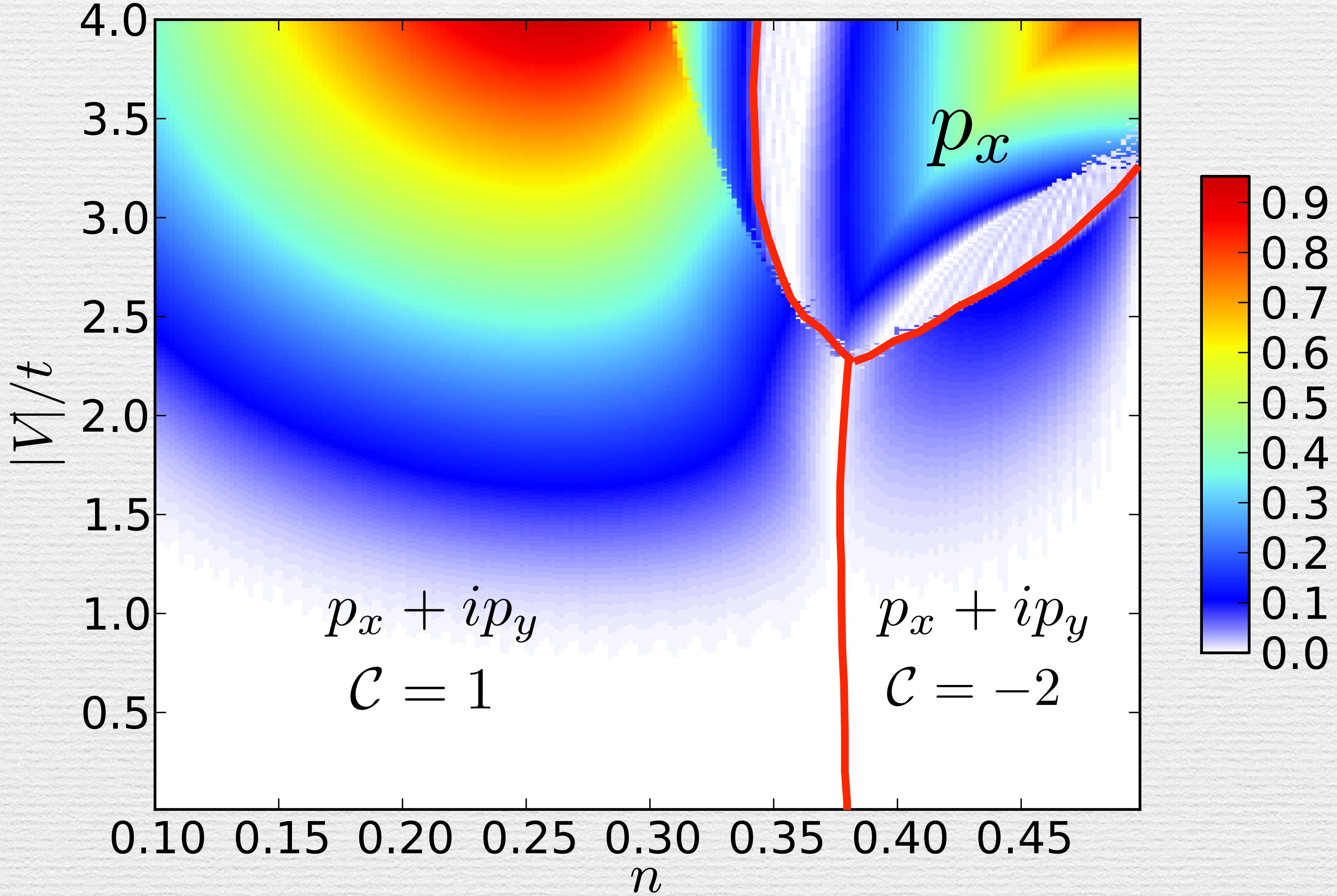
$$-t(1 + e^{-i\mathbf{k}\mathbf{a}_2} + e^{i\mathbf{k}(\mathbf{a}_1 - \mathbf{a}_2)})$$

$$H_{\text{BdG}} = \frac{1}{2}\sum_{\mathbf{k}} \begin{pmatrix} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \\ \hat{c}^{\dagger}_{-\mathbf{k}A} \\ \hat{c}^{\dagger}_{-\mathbf{k}B} \end{pmatrix}^{\dagger} \begin{pmatrix} -\mu & z_{\mathbf{k}} & 0 & \Delta_{\mathbf{k}} \\ z^*_{\mathbf{k}} & -\mu & -\Delta_{-\mathbf{k}} & 0 \\ 0 & -\Delta^*_{-\mathbf{k}} & \mu & -z^*_{-\mathbf{k}} \\ \Delta^*_{\mathbf{k}} & 0 & -z_{-\mathbf{k}} & \mu \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \\ \hat{c}^{\dagger}_{-\mathbf{k}A} \\ \hat{c}^{\dagger}_{-\mathbf{k}B} \end{pmatrix}$$

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

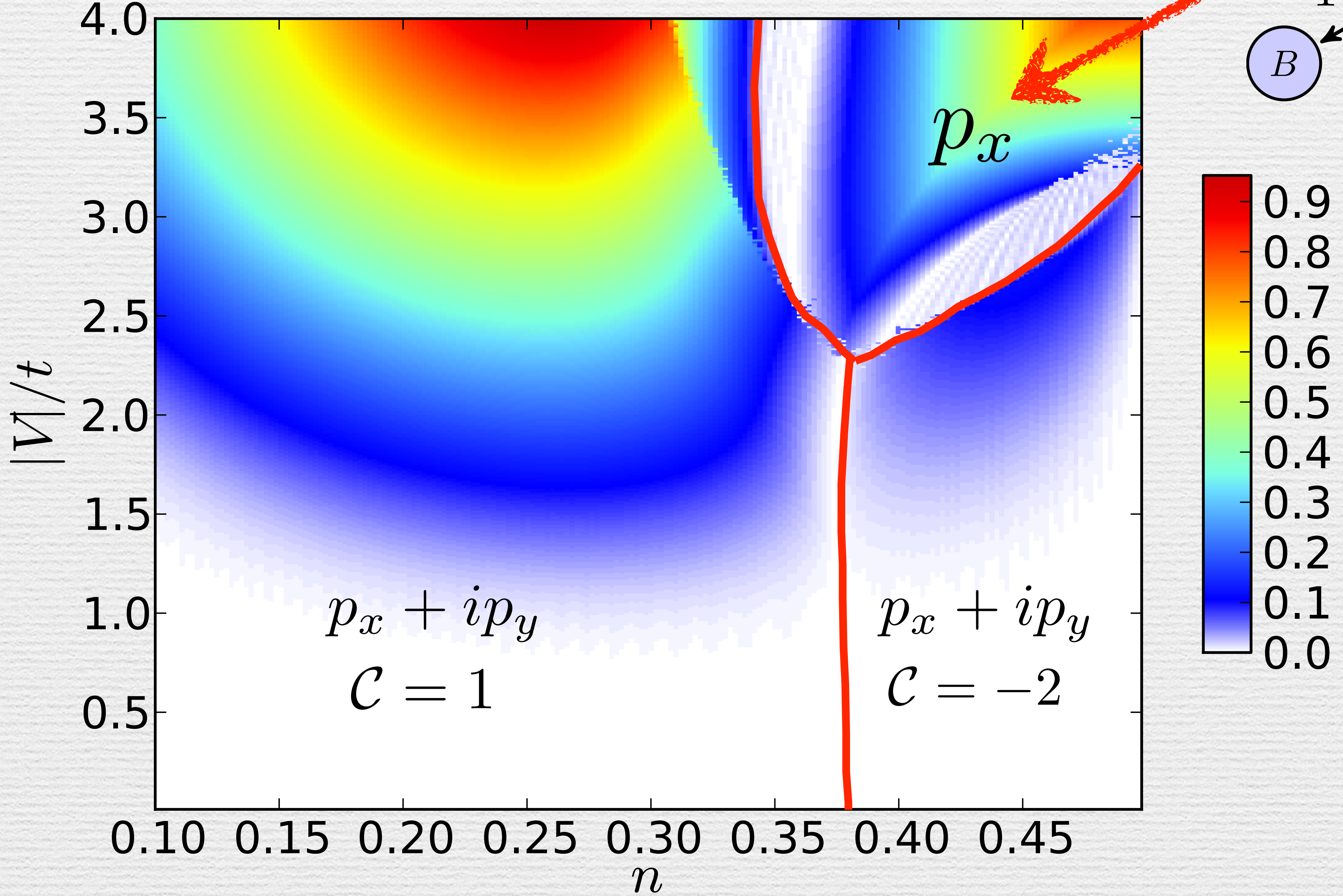
Start with random guesses, iterate until convergence

BdG phase diagram

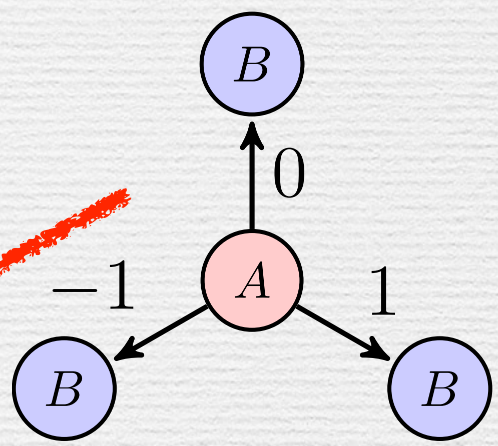


*color indicates size of superconducting gap

BdG phase diagram



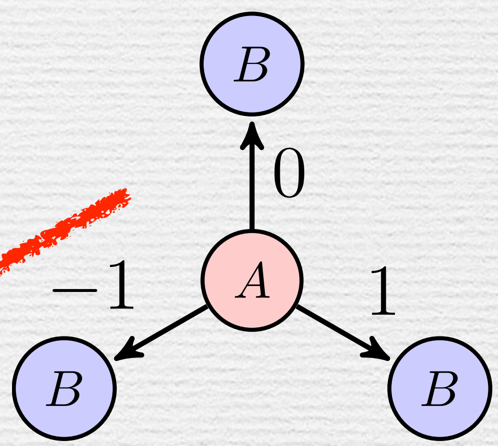
Kitaev, 2000

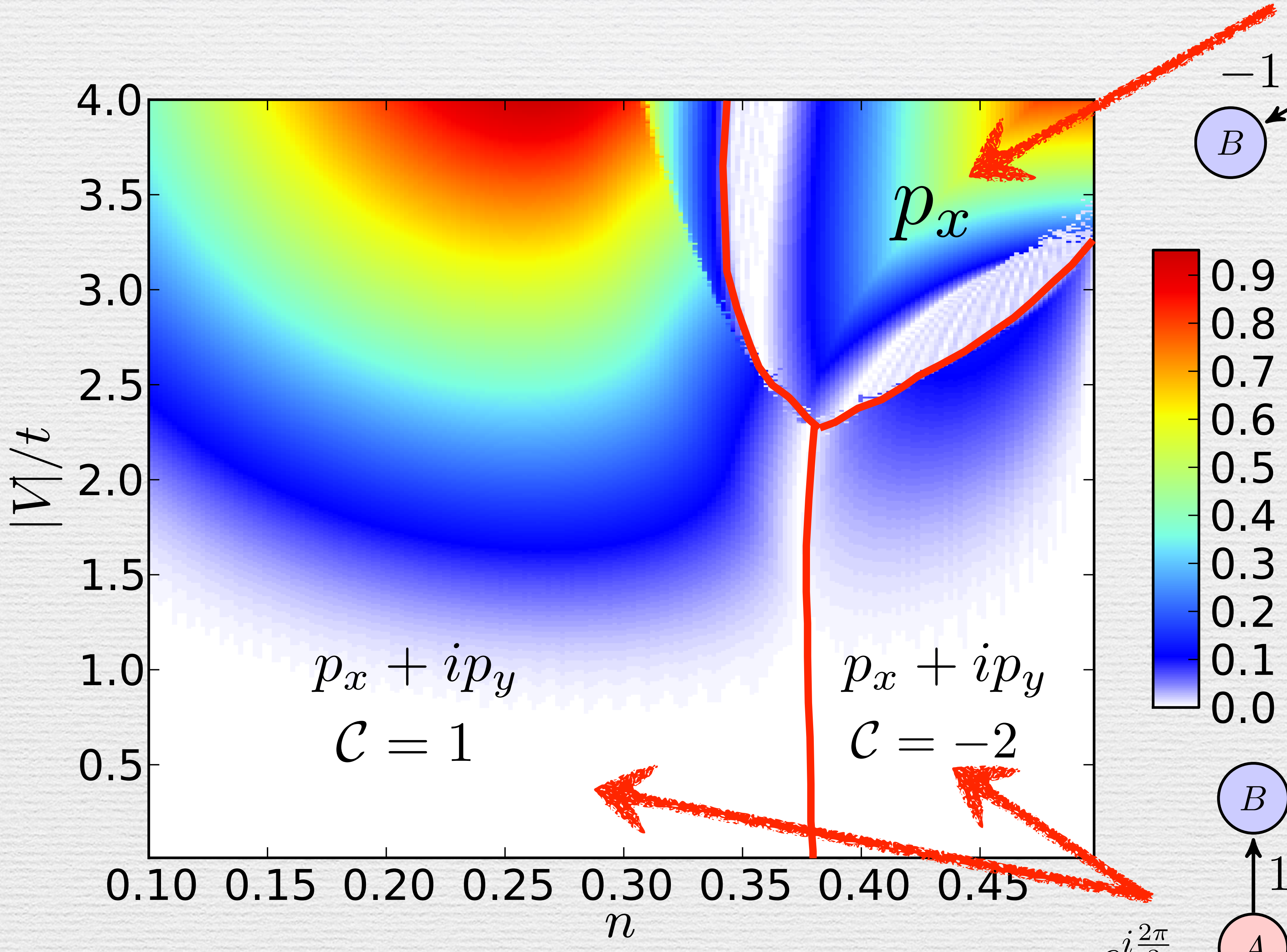


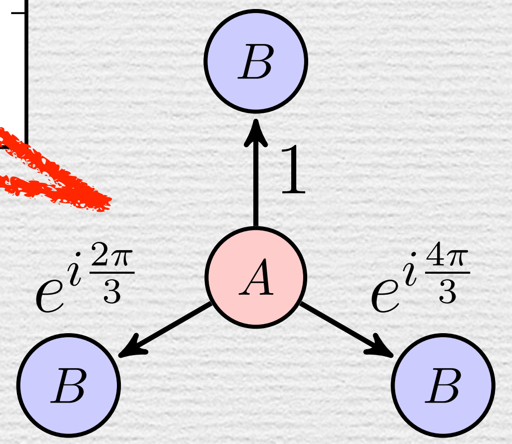
*color indicates size of superconducting gap

BdG phase diagram

Kitaev, 2000



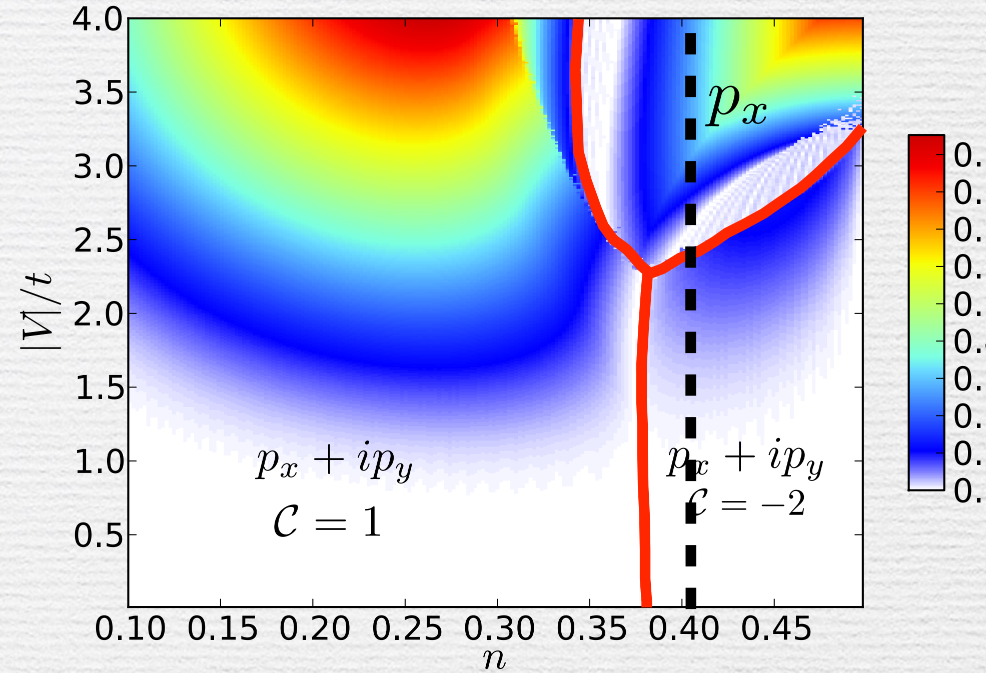




Read and Green, PRB, 2000

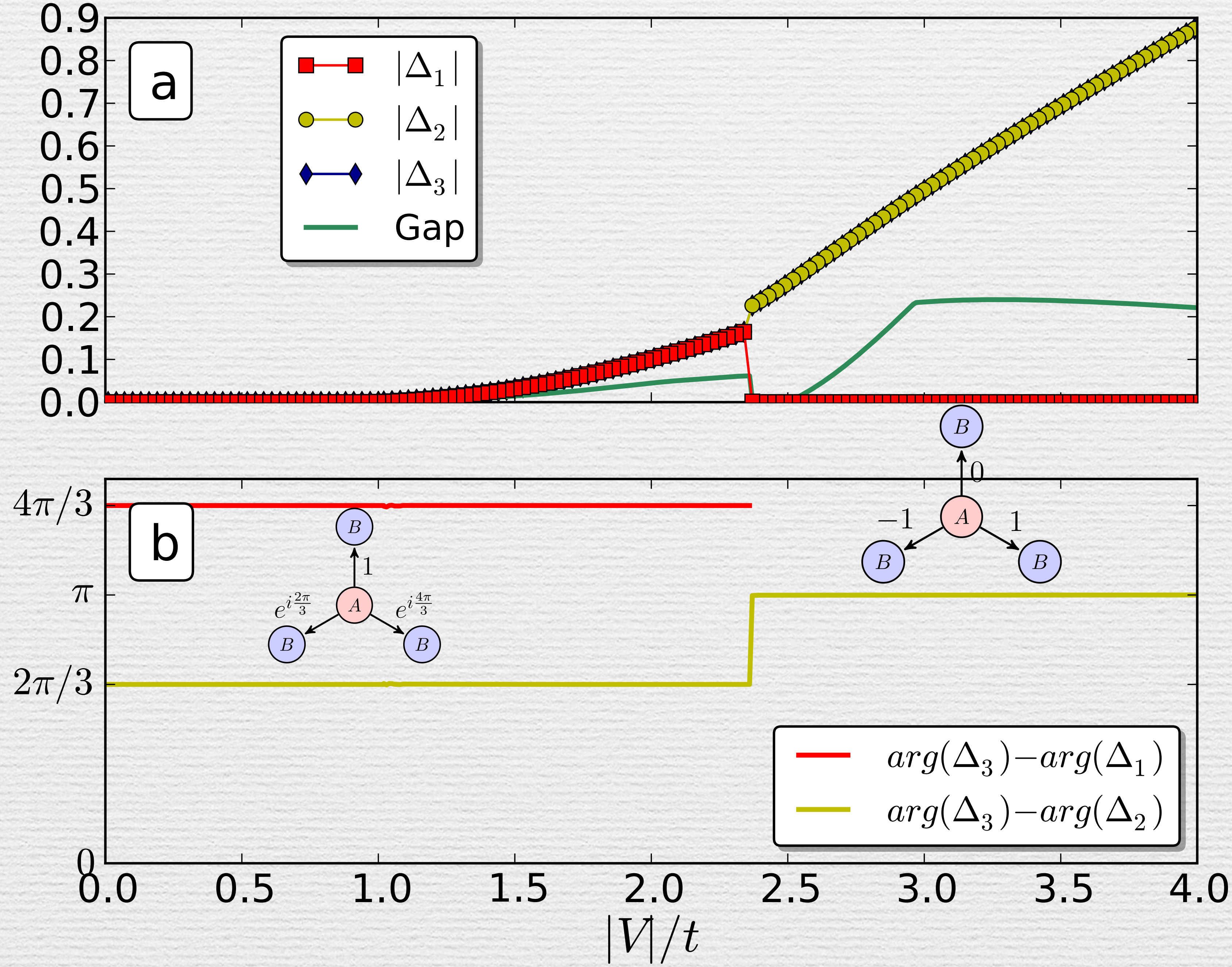
*color indicates size of superconducting gap

Scan V



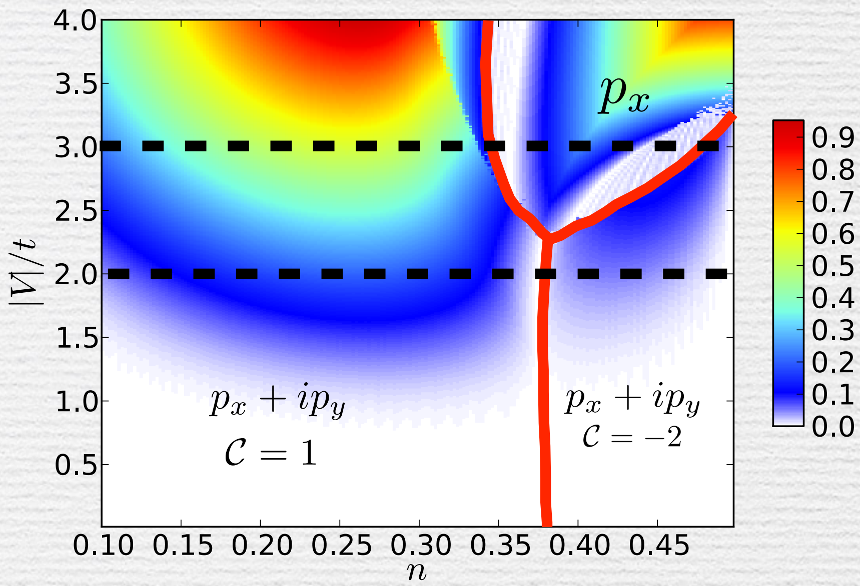
p_x
$p_x + ip_y$
$\mathcal{C} = 1$
$p_x + ip_y$
$\mathcal{C} = -2$
$|V|/t$
n

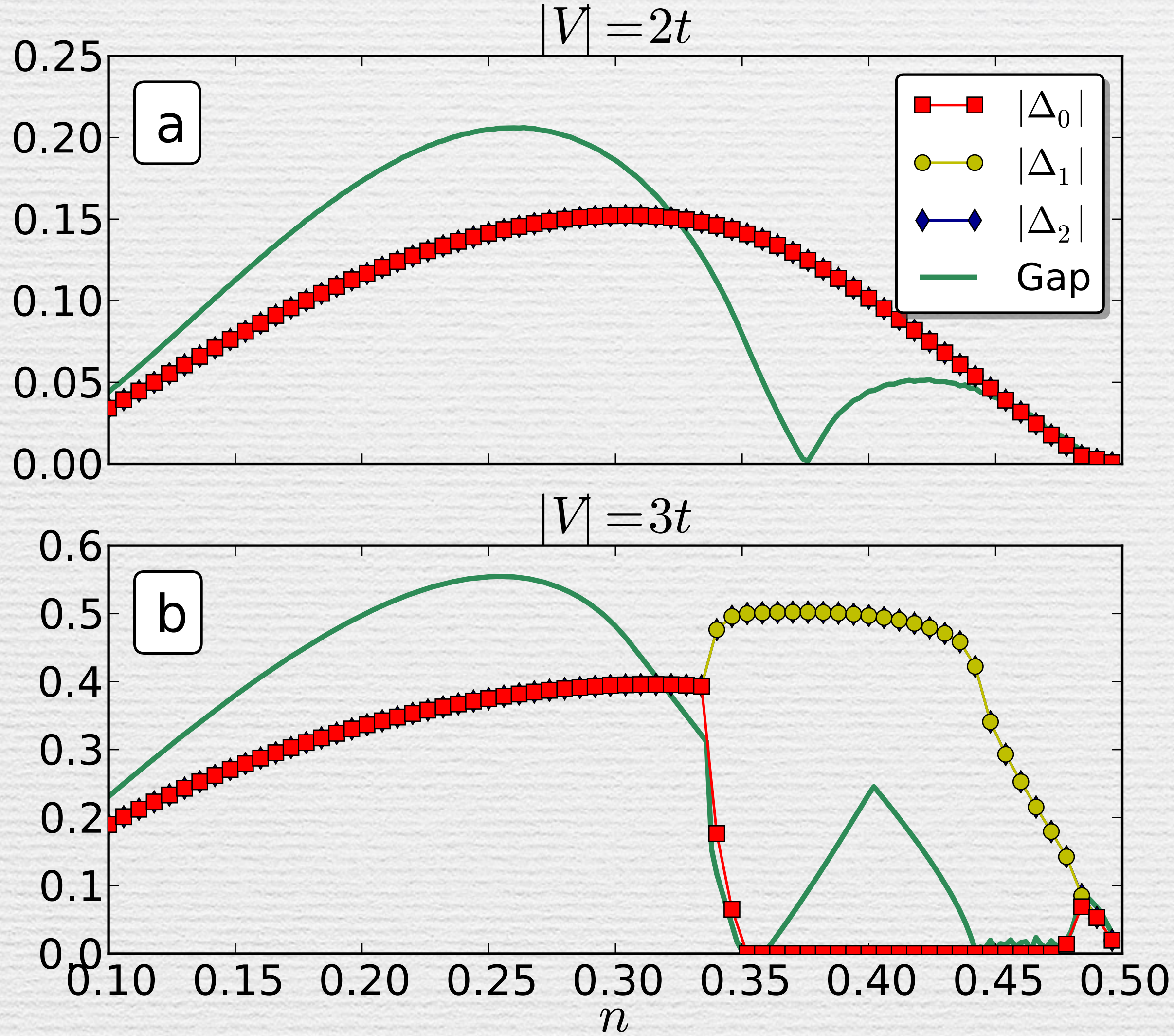
$n = 0.4$



a
$|\Delta_1|$
$|\Delta_2|$
$|\Delta_3|$
Gap
b
$4\pi/3$
π
$2\pi/3$
$arg(\Delta_3) - arg(\Delta_1)$
$arg(\Delta_3) - arg(\Delta_2)$
$|V|/t$

Scan density





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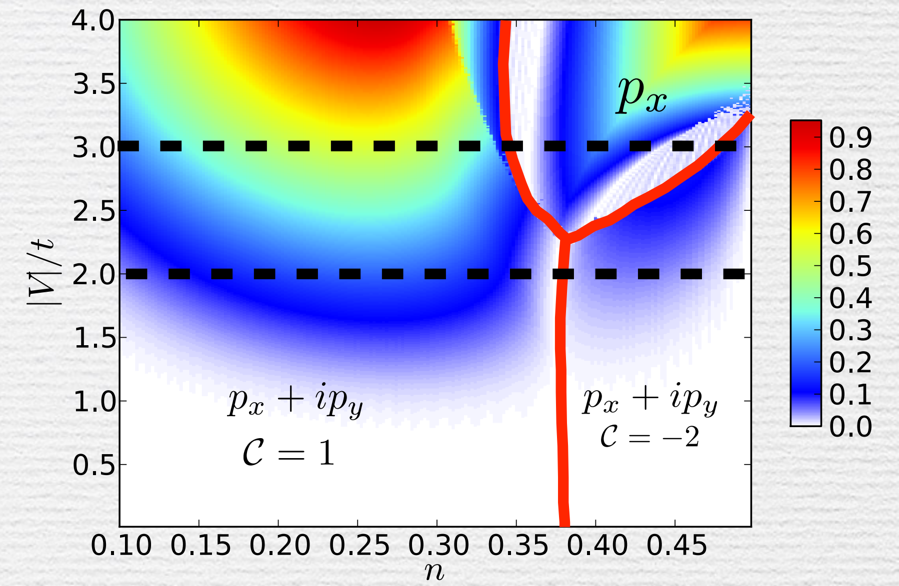

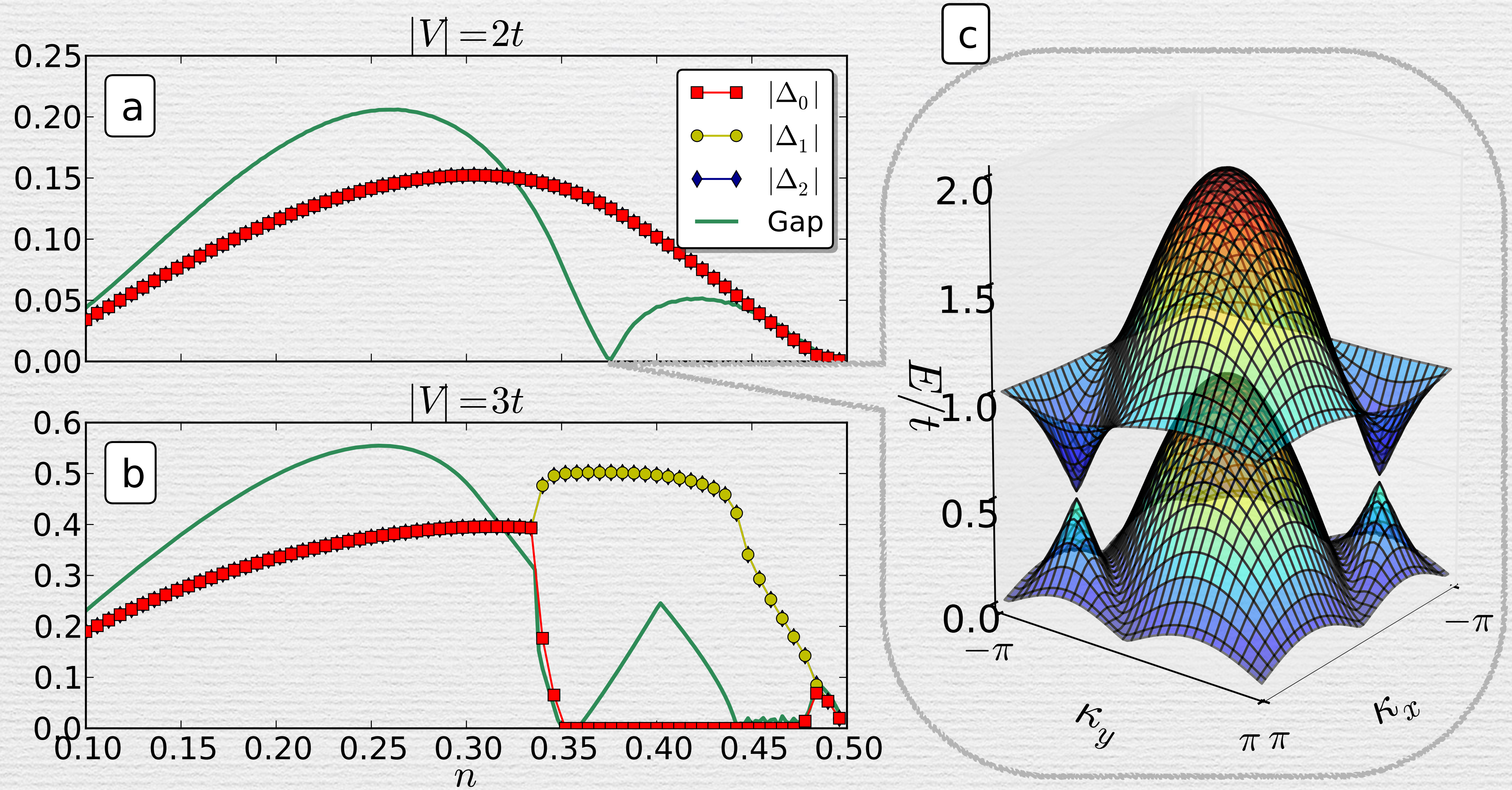

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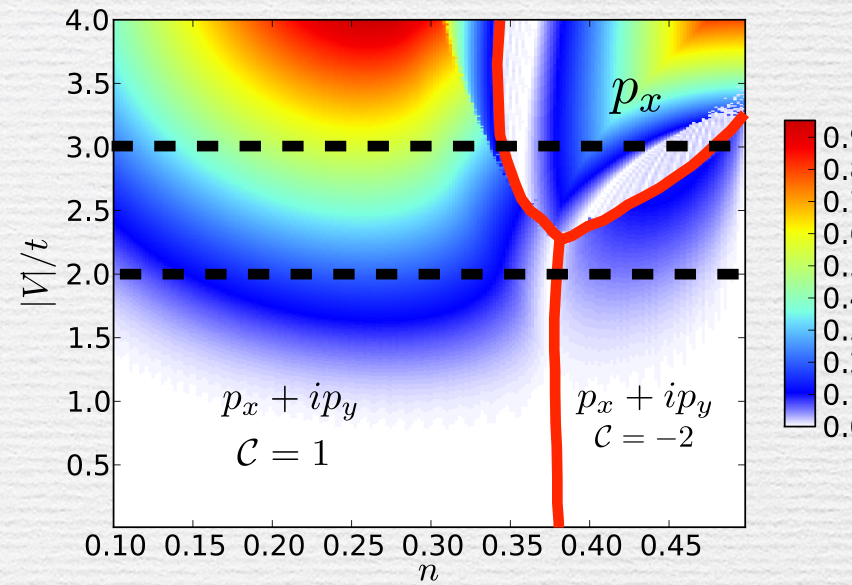
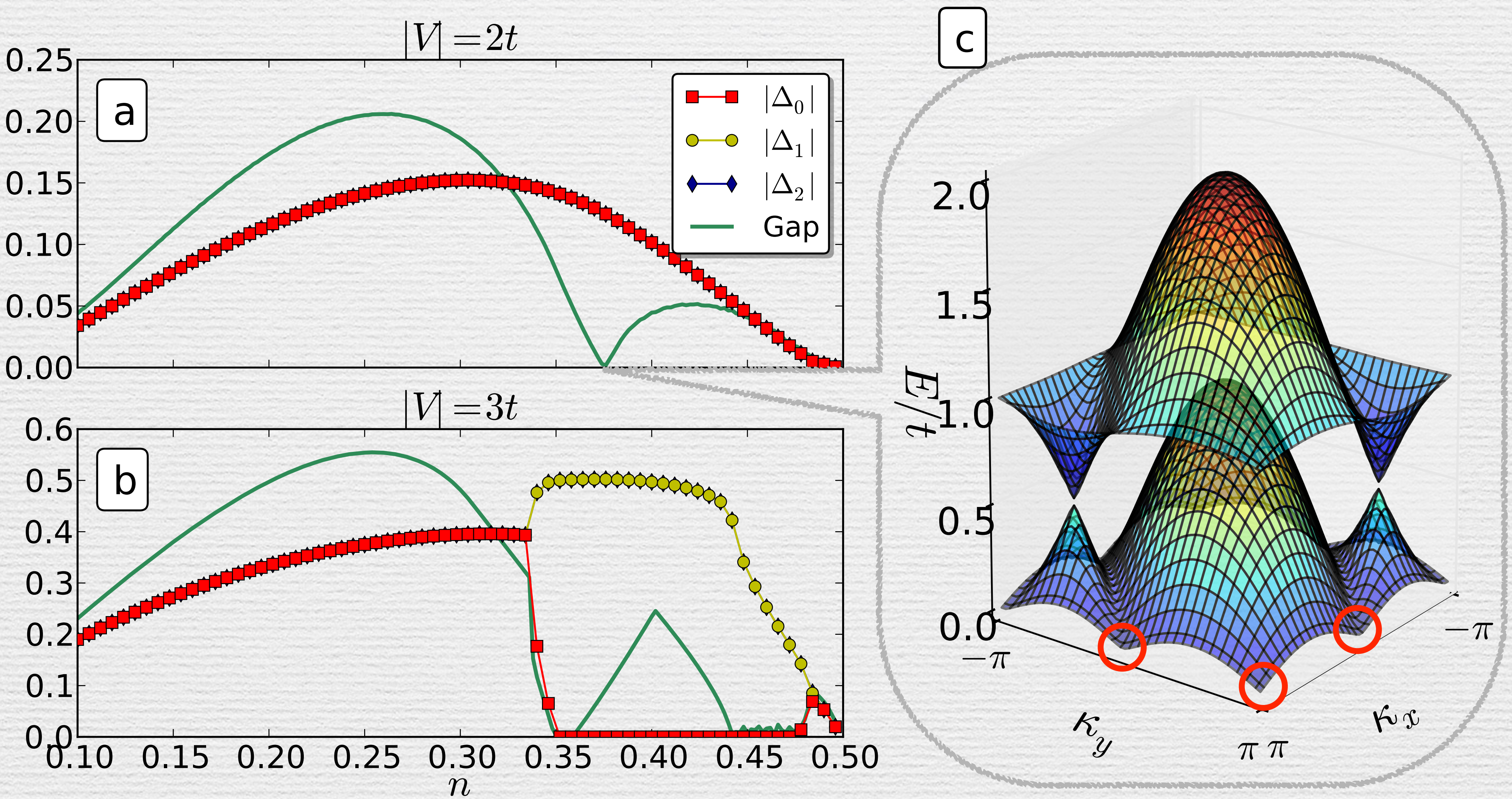
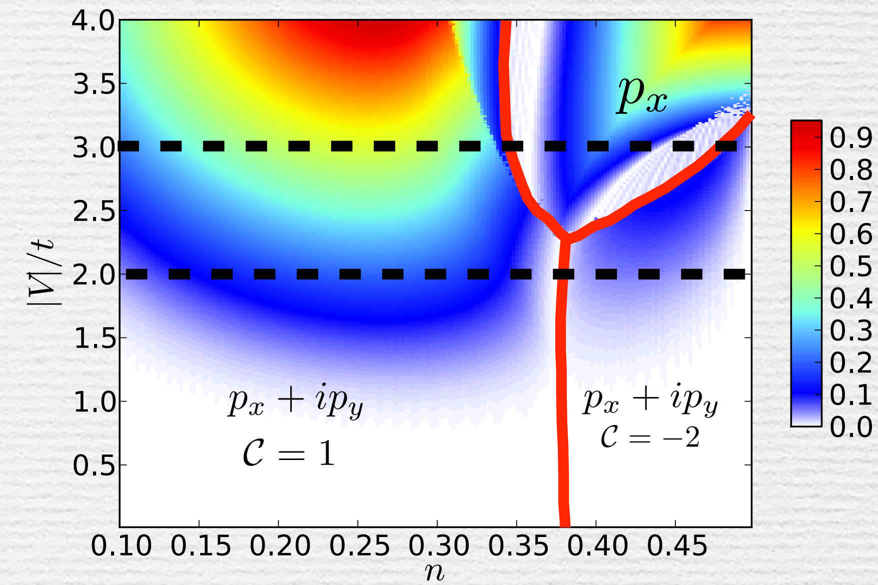
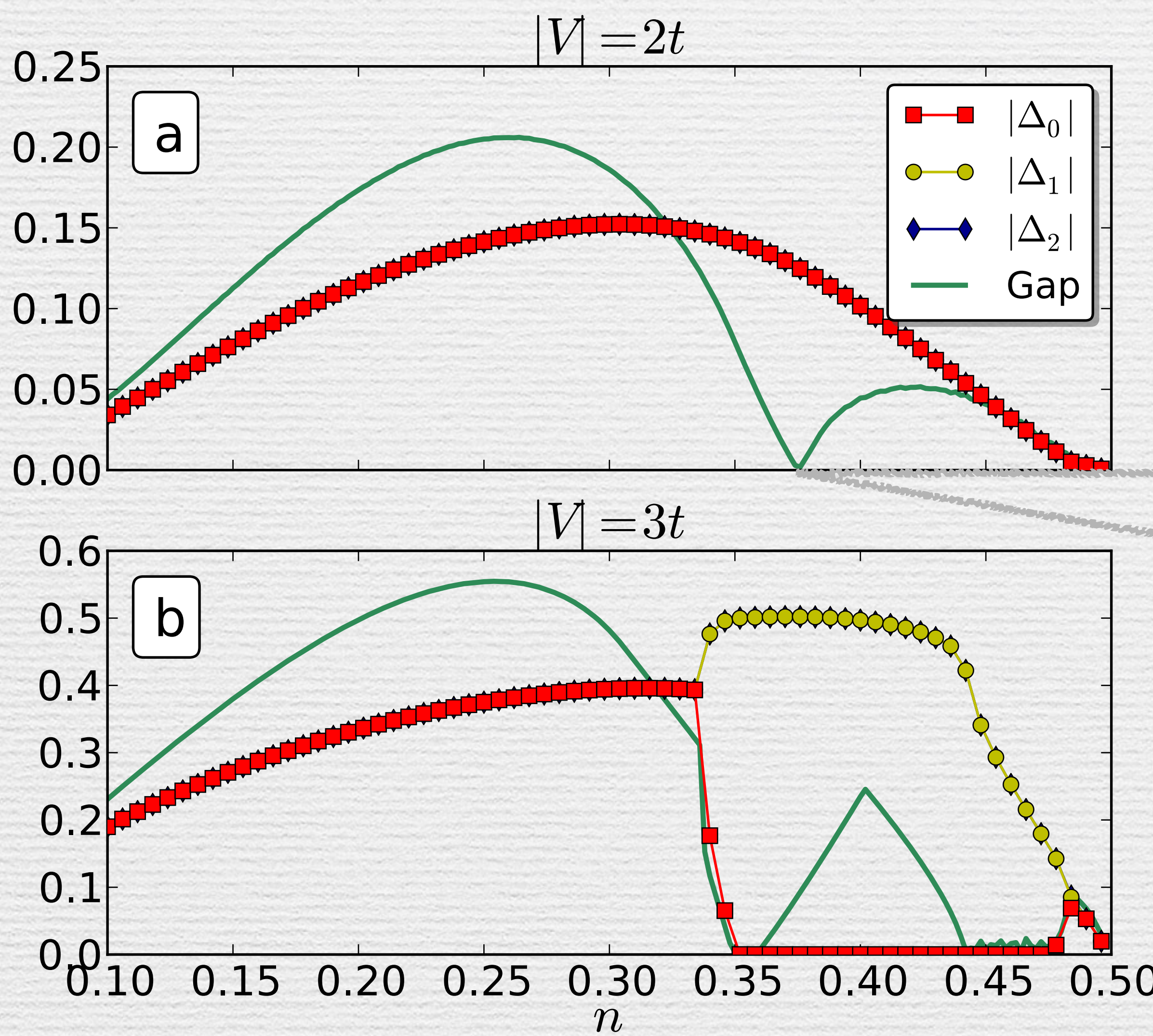
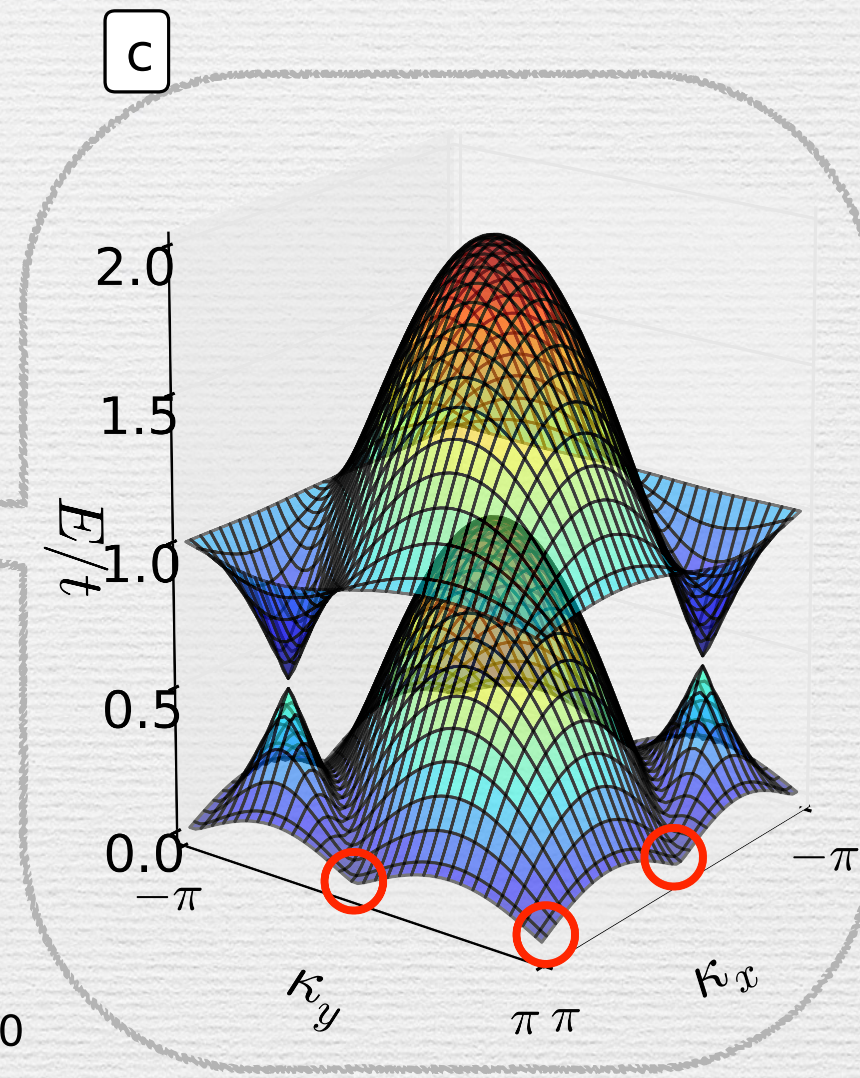


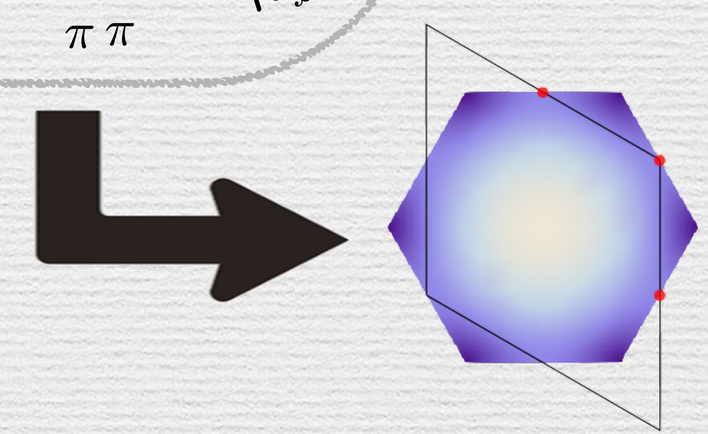


Scan density









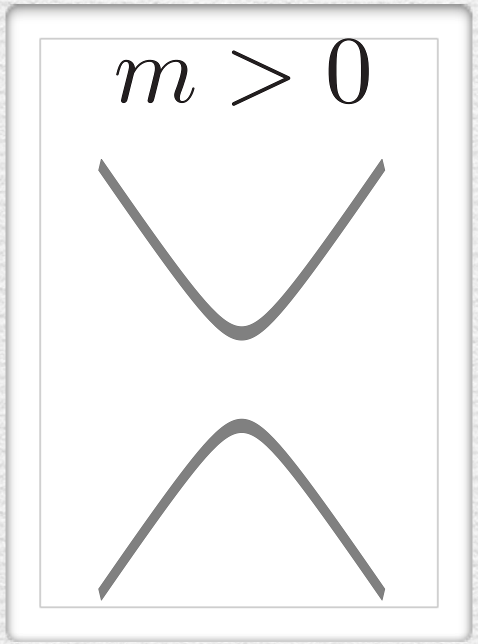
Topological Phase Transition and Dirac Fermions

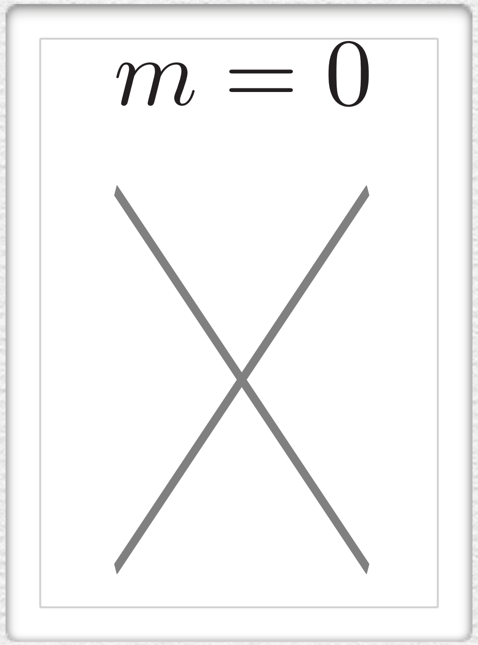
Chern number of a Dirac fermion

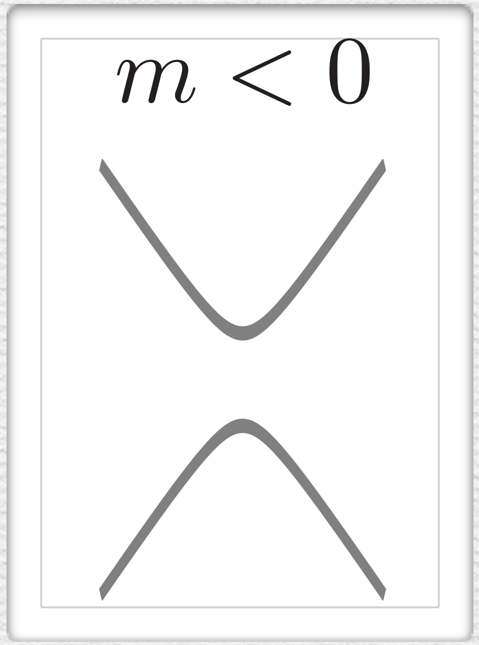
$$\mathcal{C} = \frac{\mathrm{sgn}(m)}{2}$$

Oshikawa, PRB,1994

Ludwig et al, PRB,1994

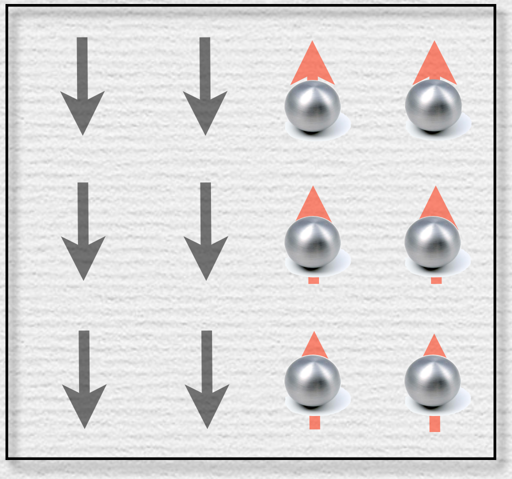


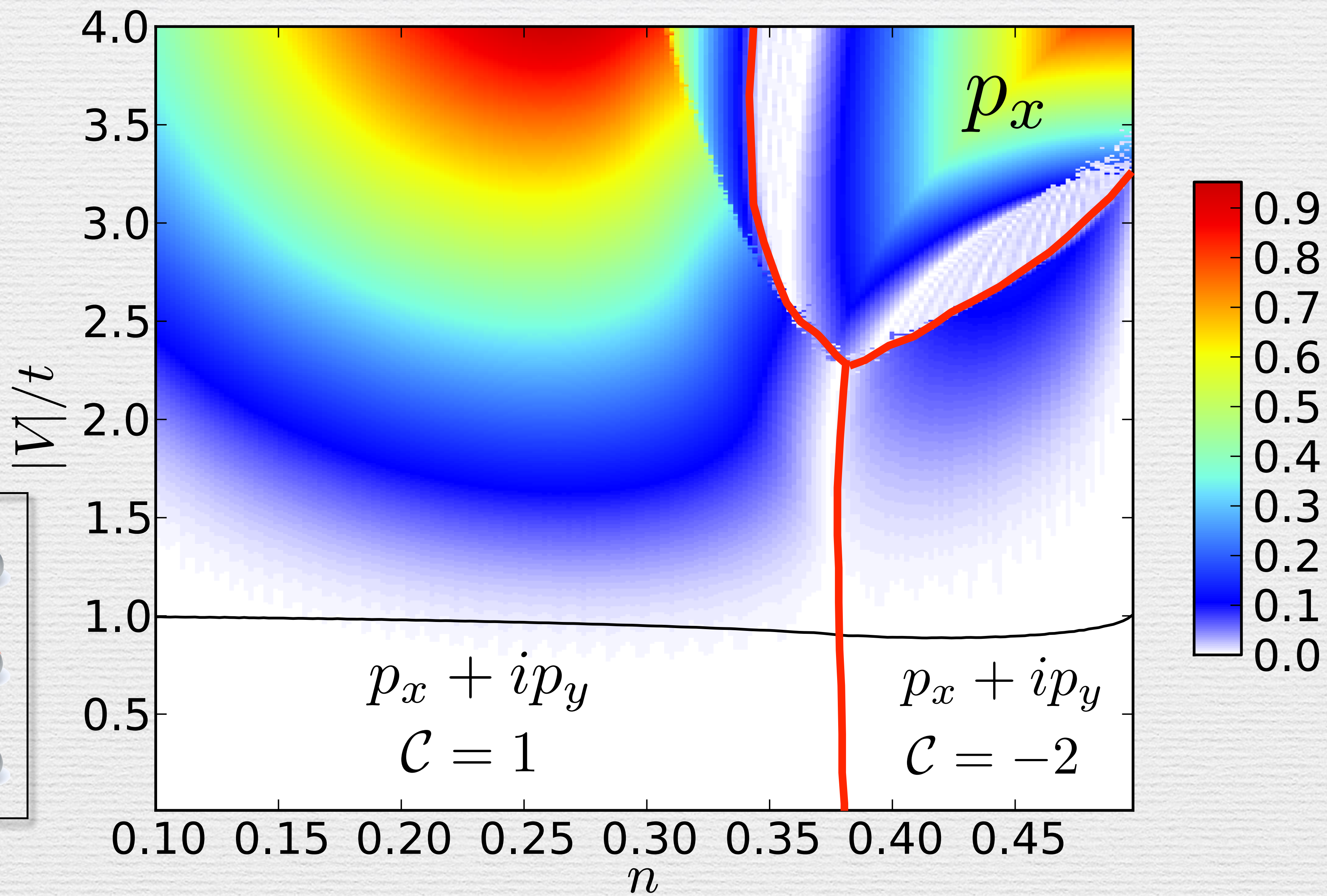




$$\Delta\mathcal{C} = \#\text{ of Dirac points}$$

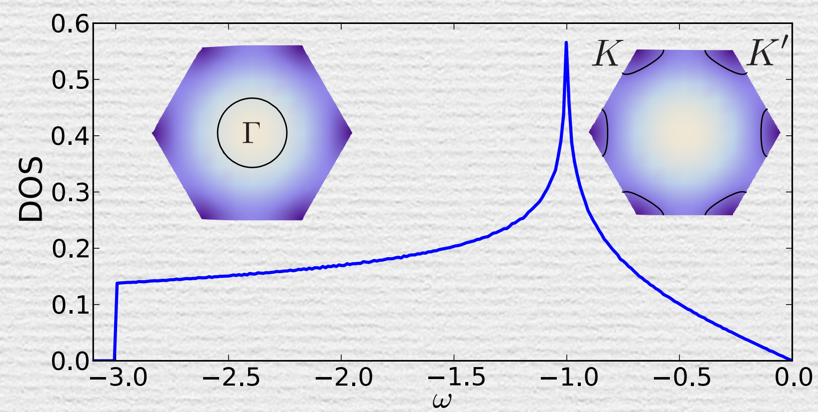
Phase diagram, again





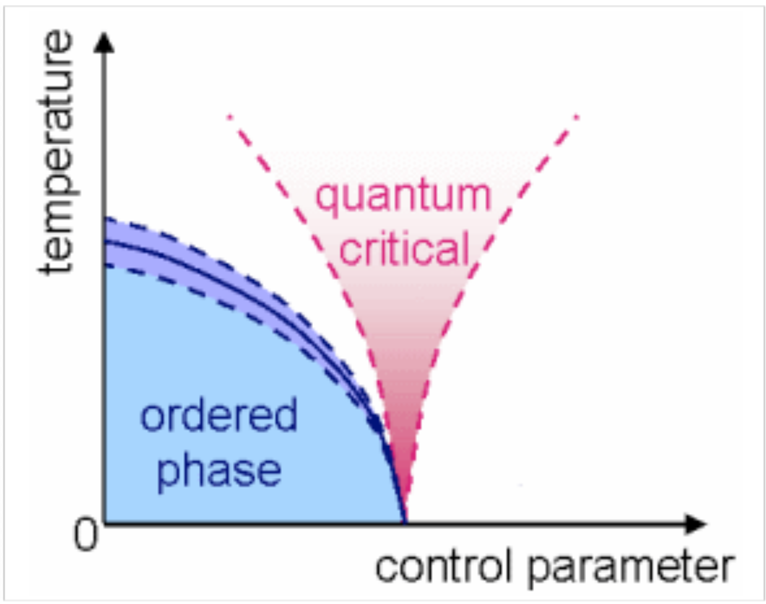
A general "theorem", Cheng, Sun, Galitski and Das Sarma, PRB, 2010

Grassmann Tensor RG, Gu, PRB, 2013



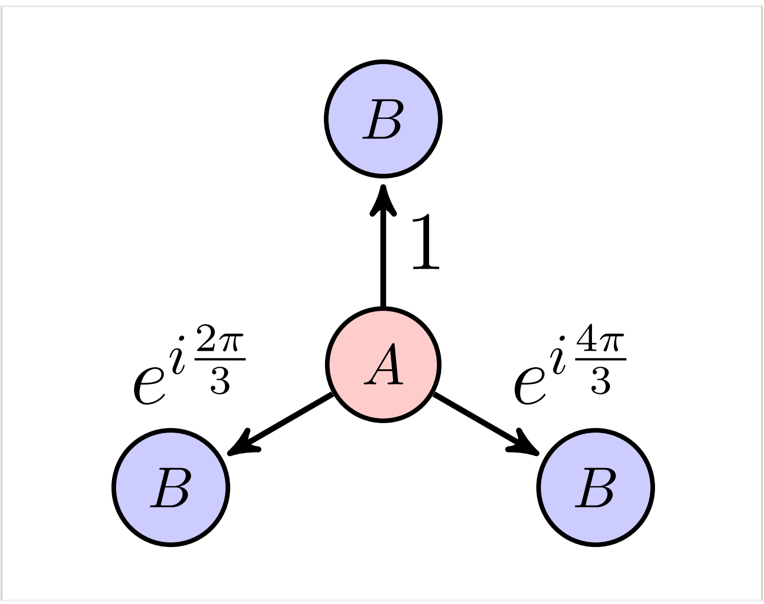
Summary-II

Fermionic
Quantum Critical Point



1407.0029

Topological *Superconductors*



to appear

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

Thank you!