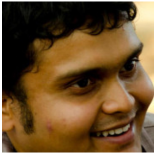
Vacancy-induced low-energy states in undoped graphene

Bhatt-Lee physics in the Kitaev model & crossover behaviour in Chiral Orthogonal universality class. . .

Kedar Damle, Group Seminar OIST May '17
Tata Institute, Bombay



Sambuddha Sanyal

Motivation

- Random impurity potentials localize electron wavefunctions in $d = 1$
  Weak-localization in $d = 2$, mobility edge in $d = 3$ ...
  (Gang of Four 1979)
- What about hopping disorder?
- Right way to ask this question: Are symmetries preserved by disordered Hamiltonian different?

Bipartite random hopping problem

- Random (real) nearest neighbour hopping on bipartite lattices H has bipartite or "chiral" symmetry: Every state at energy ϵ has partner at energy $-\epsilon$ (wavefunction changes sign on one sublattice)
- Bipartite symmetry broken by random potentials or next-nearest neighbour hops

The question

- $\epsilon = 0$ is special in such problems
  Natural question: Does anything interesting happen?

Some answers in $d = 1$

- Density of states diverges very strongly as $\epsilon \to 0$
  $\rho(\epsilon) \sim |\epsilon|^{-1} \frac{1}{\log^3(\Omega/|\epsilon|)}$
  Dyson ('53), Theodorou & Cohen ('76), Eggarter & Riedinger ('78)
  Simplest example of strong-disorder renormalization group fixed point
  Motrunich, KD, Huse ('00,'01)
- Also: Diverging length scale as $\epsilon \to 0$ limit—Loosely identified with localization length (not-quite . . .)

Some answers in $d = 2$

- Gade & Wegner ('91-93): Density of states diverges somewhat less strongly as $\epsilon \to 0$
  $\rho(\epsilon) \sim |\epsilon|^{-1} \exp(-b \log^{1/x}(\Omega/|\epsilon|))$ with $x = 2$
  Think this is arcane?
- Then try this:
  Real answer has $x = 3/2$, due to a strong-disorder effect.
  Motrunich, KD, Huse ('02); Motrunich, Ph.D thesis ('01).
  confirmed field-theoretically by Mudry, Ryu, Furusaki ('03)

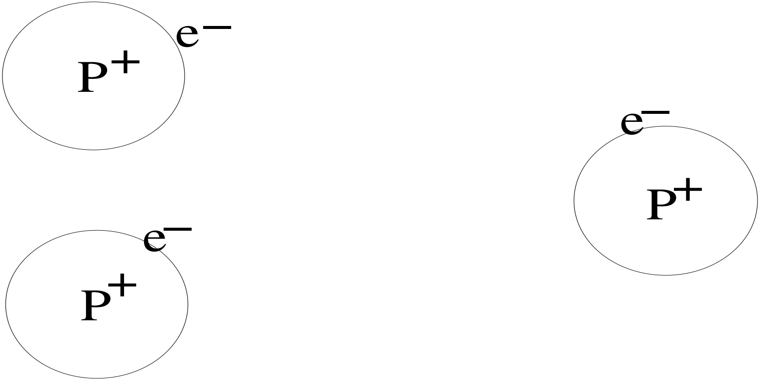
Vacancy-disorder

- Another kind of disorder: Missing sites in tight-binding model
  Natural if substitutional impurities correspond to missing orbital
- Question: Does vacancy-disorder change the asymptotic low-energy behaviour of $\rho(\epsilon)$?
  Notice: No change in symmetries of microscopic H

Our focus today

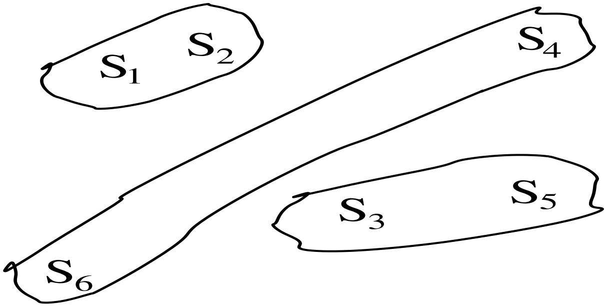
- Vacancies in tight-binding model for graphene
- Vacancies modeled by deleteting sites
  No interactions, no warping, no substrate charges, single-band model . . .
  Simplest possible abstraction of complicated system

Switch topics: Bhatt-Lee physics in Si:P



- Low density of P dopants in Si $\rightarrow$ Half-filled "Hubbard model" on random lattice
  Electrical insulator
- At low energies: Physics of $S = 1/2$ local moments

Low energy spin physics



- $\sum_{i,j} J_{ij}\vec{S}_i \cdot \vec{S}_j$ with broad distribution of J_{ij}
- Singlet pairs with broad distribution of binding energies
- $T\chi(T)$: Pairs with binding energy $< T$
  $\chi(T) \sim \frac{N(T)}{T} \sim \frac{1}{T^\alpha}$ with α set by concentration of P
  (Bhatt & Lee)

Asymptotically exact?

- In $d = 1$, picture asymptotically exact for the random-exchange antiferromagnetic chain
  $\chi(T) = \frac{\Gamma_T^{-2}}{T}$ as $T \to 0$.
  ($\Gamma_T \equiv \log(J/T)$ [J: overall scale of antiferromagnetic exchange].)
  (Dasgupta & Ma, D. S. Fisher)
- For $d > 1$, status unclear (strong-disorder RG inconclusive)
  (Motrunich & Huse)

Bhatt-Lee physics of diluted SU(2) symmetric Majorana spin liquid

- Tractable example of a disordered SU(2) symmetric Majorana spin liquid in $d = 2$
  with $\chi(T) = \frac{\mathcal{C}}{4T} + \frac{N(\Gamma_T)}{4T}$ as $T \to 0$
- $N(\Gamma_T)$ consistent with Bhatt-Lee physics
  $N(\Gamma_T) \sim \Gamma_T^{-y}$ for $T_{\rm cr} \ll T \ll J$
  $N(\Gamma_T) \sim \Gamma_T^{1/3} \exp(-c\Gamma_T^{2/3})$ for $T \ll T_{\rm cr}$

Asymptotically exact realization of Bhatt-Lee physics

- Following Bhatt-Lee—
  $\mathcal{C} \rightarrow$ Density of free-moments
  $N(\Gamma_T) \rightarrow$ Density of singlet-pairs with binding energies smaller than T

Raises (interesting?) question: Alternate Strong-disorder RG approach to go beyond tractable limit?

Connection to chiral orthogonal universality class and Graphene

- $\chi(T) \propto \kappa(T)$ for particle-hole-symmetric canonical free-fermions with vacancy disorder.
  $N(\Gamma) \rightarrow$ integrated DOS for single-particle energies
  $0 < |\epsilon| < J \times 10^{-\Gamma}$ (*i.e.* excluding zero modes)
- Vacancy-induced crossover in DOS in chiral orthogonal universalitty class
  Another example of same crossover: Undoped graphene with vacancy disorder

Setting: Honeycomb model of Yao & Lee

$$\mathcal{H} = J \sum_{\langle \vec{r}\vec{r}' \rangle_\lambda} \tau^\lambda_{\vec{r}} \tau^\lambda_{\vec{r}'} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}'} - \sum_{\vec{r}} \vec{B} \cdot \vec{S}_{\vec{r}} \ . \quad (1)$$

- $\vec{\tau}$: "Orbital degrees of freedom that remain dynamical at low energy
- $\vec{S} = \frac{\vec{\sigma}}{2}$: spin-half moments
- Original motivation: Low-energy effective Hamiltonian for a frustrated $S = 1/2$ model on the decorated honeycomb lattice with multi-spin interactions
  Each $\vec{S}$: Low-energy projection of total spin of three spins.
  $\tau^z = \pm 1$: Two different low energy doublets that make up low energy sector

Majorana representation

- $\sigma^z_{\vec{r}} = -ic^x_{\vec{r}}c^y_{\vec{r}}$
  $\tau^z_{\vec{r}} = -ib^x_{\vec{r}}b^y_{\vec{r}}$
  and cyclic permutations
- $c^\lambda_{\vec{r}}$ and $b^\lambda_{\vec{r}}$ are Majorana (real) fermion operators.

Single-site Hilbert space doubled by this representation

Constraint on fermion states

- $D_{\vec{r}} \equiv -i c_{\vec{r}}^{x} c_{\vec{r}}^{y} c_{\vec{r}}^{z} b_{\vec{r}}^{x} b_{\vec{r}}^{y} b_{\vec{r}}^{z} = +1$ at each site $\vec{r}$
  Curious fact: $D = -1$ sector also provides faithful representation of $\vec{\sigma}$ and $\vec{\tau}$.
  $\rightarrow$
  No "unphysical" states. Instead: Two copies of physical states at each site
- In $D = +1$ sector: $\sigma_{\vec{r}}^{\alpha} \tau_{\vec{r}}^{\beta} = i c_{\vec{r}}^{\alpha} b_{\vec{r}}^{\beta}$
  Similar reduction in $D = -1$ sector

Reduction leads to exact solution

- On bond with orientation λ ($\lambda = x, y, z$) $\langle rr' \rangle \lambda$, get term:
  $u_{\langle rr' \rangle \lambda}(i\vec{c}_r \cdot \vec{c}_{r'})$
  with $u_{\langle rr' \rangle \lambda} = -ib_r^\lambda b_{r'}^\lambda$
- Three copies of Kitaev's non-interacting Majorana model, all coupled to same static Z_2 gauge field

Majorana fermion Hamiltonian

$$\mathcal{H} = \frac{J}{2} \sum_{\alpha=x,y,z} \sum_{\langle \vec{r}\vec{r}' \rangle_\lambda} u_{\langle \vec{r}\vec{r}' \rangle_\lambda} (ic^\alpha_{\vec{r}} c^\alpha_{\vec{r}'} + h.c.) + B \sum_{\vec{r}} ic^x_{\vec{r}} c^y_{\vec{r}} \tag{2}$$

where $\vec{B} = B\hat{z}$.

- Convenient: Canonical fermions $f_{\vec{r}} = (c^x_{\vec{r}} - ic^y_{\vec{r}})/2$
- $S^z_{\vec{r}} = ic^x_{\vec{r}} c^y_{\vec{r}} = f^\dagger_{\vec{r}} f_{\vec{r}} - 1/2$
- Want to compute: $m^z \equiv \sum_r \langle S^z_{\vec{r}} \rangle / 2L^2$ as function of B and obtain $\chi(T) = \frac{dm^z}{dB}$ at $B = 0$

Calculating susceptibility

- Hamiltonian H for f fermions:
  Tight-binding model with static Z_2 gauge-fields u determining signs of each hopping matrix element $t = u|J|$
- $\chi(T)$ related to f fermion compressibility $\kappa(T)$ at particle-hole-symmetric chemical potential $\mu \equiv B = 0$.
- c^z Majorana plays no role in susceptibility calculation
- $\chi(T) = \frac{1}{T} \int d\epsilon \rho_{\text{tot.}}(\epsilon) \frac{e^{\epsilon/T}}{(e^{\epsilon/T}+1)^2}$
  where $\rho_{\text{tot}}(\epsilon)$ is full DOS of H

Projection issues?

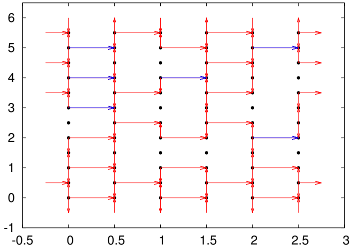
- In usual Kitaev model: Projection gives subleading corrections in thermodynamic limit
  Subtle for impurity susceptibility etc
  (Pedrocchi-Chesi-Loss, Zschocke-Vojta)
  (building on: Willans-Chalker-Moessner, Baskaran-Mandal-Shankar, Yao-Zhang-Kivelson)
- What happens here?
  Again: Only subleading corrections in general.
- For specific boundary conditions: Coefficient of subleading corrections zero

Flux-binding

- Lieb-Loss heuristics:
  Each vacancy binds static π-flux in ground-state sector.
  Gap to other flux sectors
  (Kitaev, Willans-Chalker-Moessner)
- At low temperature, χ dominated by this flux-sector

Flux-attachment

- Send flux-strings off to one open edge



Connection to vacancy-impurities in Graphene

- Without flux-attachment, H is tight-binding model for graphene with compensated vacancies
- Study numerically with and without flux attachment

Dilution

- Remove honeycomb lattice sites at random
- Global “compensation”: Equal number of vacancies on A and B sublattices
  Protocol: Randomly/alternately pick sublattice, then pick random site to remove, ensure global compensation
- Exclusion constraints on vacancies—prevent disconnecting lattice into clusters, prevent dangling bonds.
- Choices eliminate “graph zeroes”

Choice of geometry

- Semi-open $L \times L$ unit cells ($2L^2$ sites in undiluted sample) and armchair edges
- Vacancies excluded from interrupting armchair edge
- L chosen even and *antiperiodic boundary conditions* or odd and periodic boundary conditions
- Choices eliminate boundary-induced graph zeroes.
- Any zero modes will now be “nontrivial”

Computational details

- Form H^2, the square of the tight-binding Hamiltonian H (with hopping amplitude $t = 1$ between nearest-neighbours), and work with the $(1 - n_v)L^2 \times (1 - n_v)L^2$ block $(T_{AB})^\dagger T_{AB}$ where T_{AB} is the matrix of hopping amplitudes from undeleted B sublattice sites to undeleted A sublattice sites
- Fully multiprecision implementation of the ALGOL routines in Wilkinson's handbook to count eigenvalues of $(T_{AB})^\dagger T_{AB}$ below $10^{-2\Lambda}$.
- Results checked at moderate L and moderate Λ against LAPACK routines.

Formulary

- $\rho_{\text{tot}}(\epsilon) = \rho(\epsilon) + w\delta(\epsilon)$
- $N(\Gamma) = 2\int_0^{10^{-\Gamma}} \rho(\epsilon)d\epsilon$
  $(\Gamma = \log_{10}(1/|\epsilon|))$
- Modified Gade-Wegner form:
  $\rho(E) \sim \frac{1}{|\epsilon|} e^{-b|\ln\epsilon|^{1/x}}$
  equivalently:
  $N(\Gamma) = a\Gamma^{1-\frac{1}{x}} e^{-b\Gamma^{\frac{1}{x}}}$
  ($x = 3/2$, two free parameters a and b)
- Dyson form:
  $\rho(\epsilon) \sim \dfrac{1}{|\epsilon|[\log[1/|\epsilon|]]^{1+y}}$
  equivalently:
  $N(\Gamma) = c\Gamma^{-y}$ (two free parameters c and y)

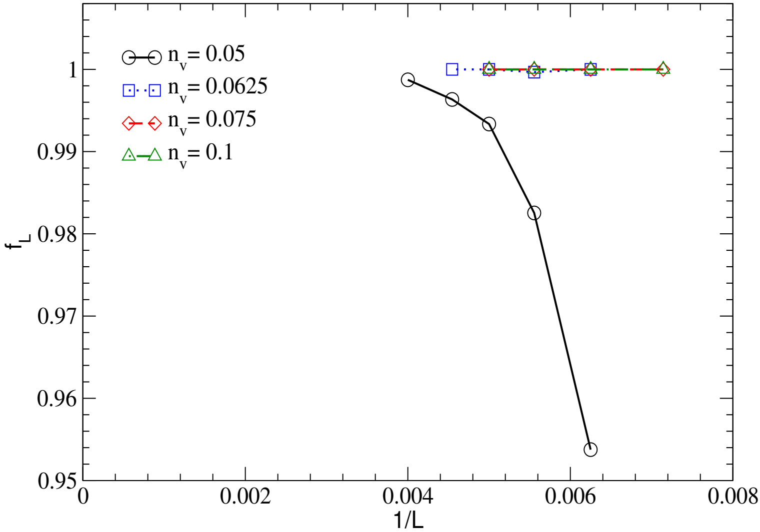
Computational details—II

- For each sample, computations first done in a coarse-grid of $\Lambda = \Gamma_i$, then $N_{\text{tot}}(\Gamma)$ “filled in” iteratively when needed. Final grid spacing $\Delta(\Gamma) = 0.5$.
- Lowest-nonzero gap $10^{-\Gamma_g}$ in a given sample obtained with accuracy of $\Delta(\Gamma_g) = 0.5$.
- w_L (number of zero modes per unit volume) given by $N_{\text{tot}}(\Gamma, L)$ after “last” downward step.
- “Last”: Grid extends to Γ_{max} as high as 100—stability checked by varying precision
- Study $N_L(\Gamma) = N_{\text{tot}}(\Gamma, L) - w_L$ and w_L for ~ 3000 samples

Alternate (less painful) protocol

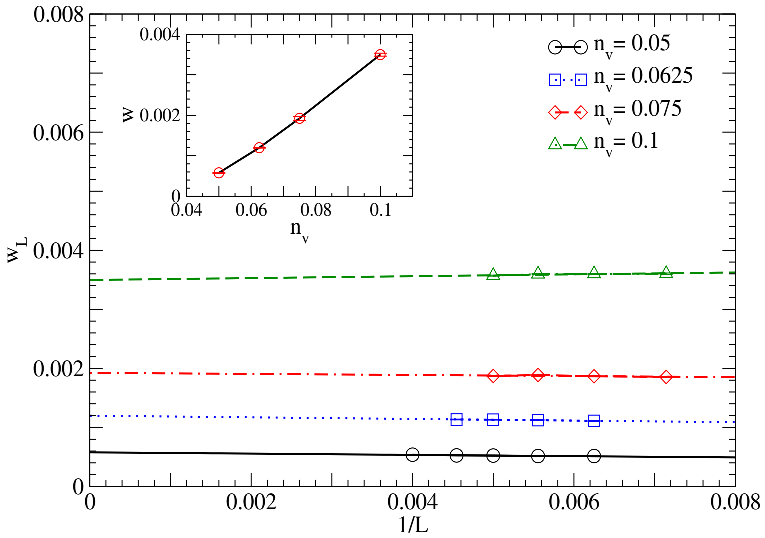
- Keep track of differences $N_{\text{tot}}(\Gamma_{i+1}) - N_{\text{tot}}(\Gamma_i)$
- Obtain $|\epsilon|\rho(\epsilon)$ directly
- Poorer statistical properties, but finesses zero mode question

Zero modes



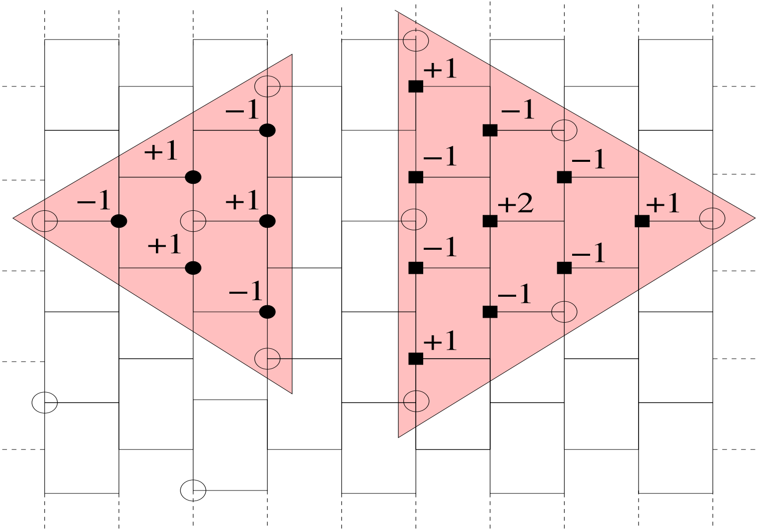
$n_v = 0.05$
$n_v = 0.0625$
$n_v = 0.075$
$n_v = 0.1$
f_L
1
0.99
0.98
0.97
0.96
0.95
0
0.002
0.004
0.006
0.008
1/L

Zero modes



0.008
0.006
0.004
0.002
0
w_L
0
0.002
0.004
0.006
0.008
1/L
n_v = 0.05
n_v = 0.0625
n_v = 0.075
n_v = 0.1
0.004
0.002
0
w
0.04
0.06
0.08
0.1
n_v

Rigorous lower-bound on zero modes



4-triangle and $\mathcal{R}_6$ motifs

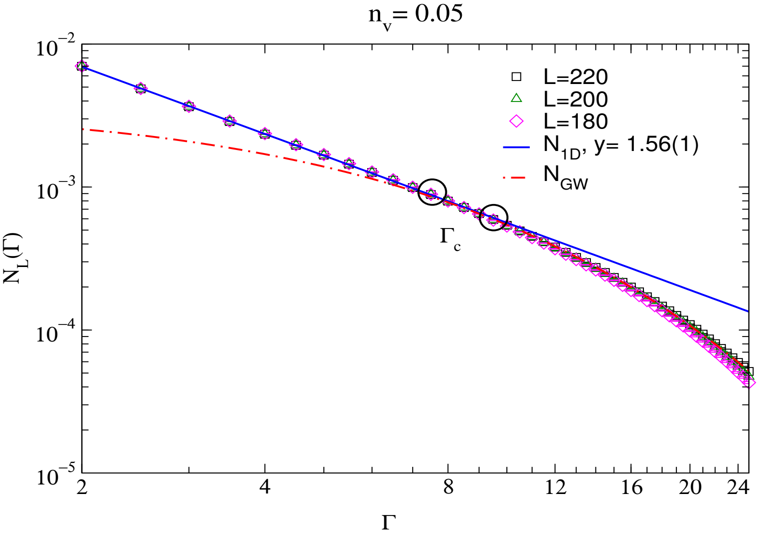
$$w_L^{(i)} \geq \left[\max(N_{\Delta_{4A}}^{(i)}, N_{\Delta_{4B}}^{(i)}) \right] / L^2$$

Implies $w \geq n_{\Delta_4}$ (concentration of 4-triangles)

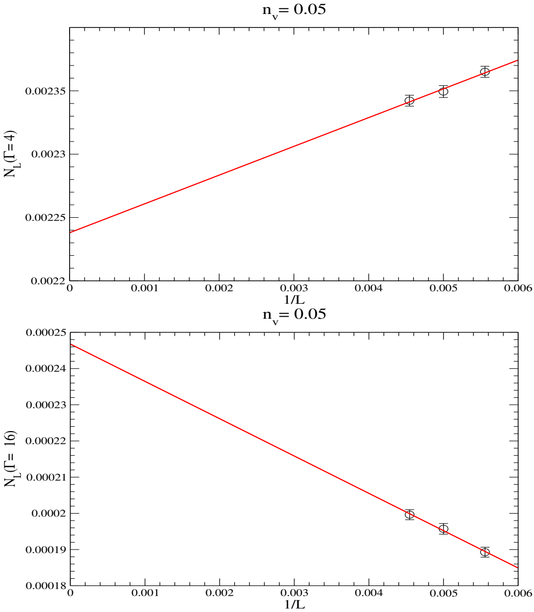
Robust to hopping disorder

- $\mathcal{R}_6$ mode robust to bond disorder (but not 4-triangles).
- More general $\mathcal{R}$-type zero modes possible, also robust to bond disorder
- Dominate over 4-triangles except for asymptotically small n_v (out of reach)

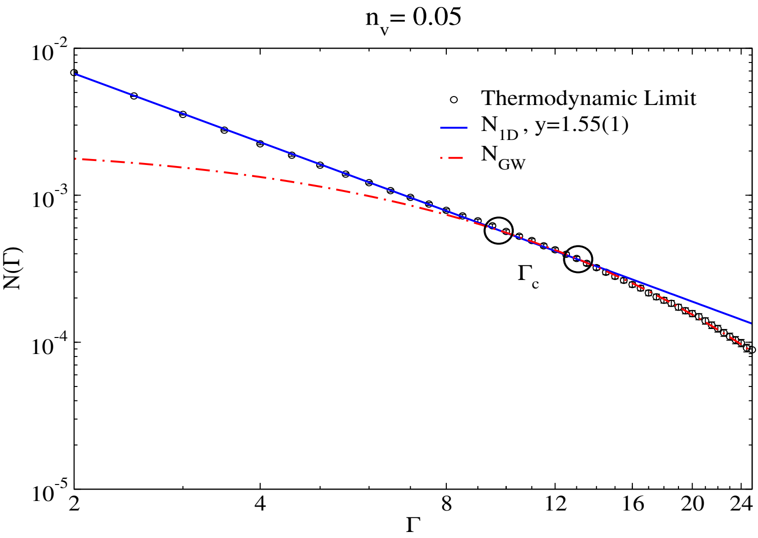
$N(\Gamma)$ for $n_v = 0.05$



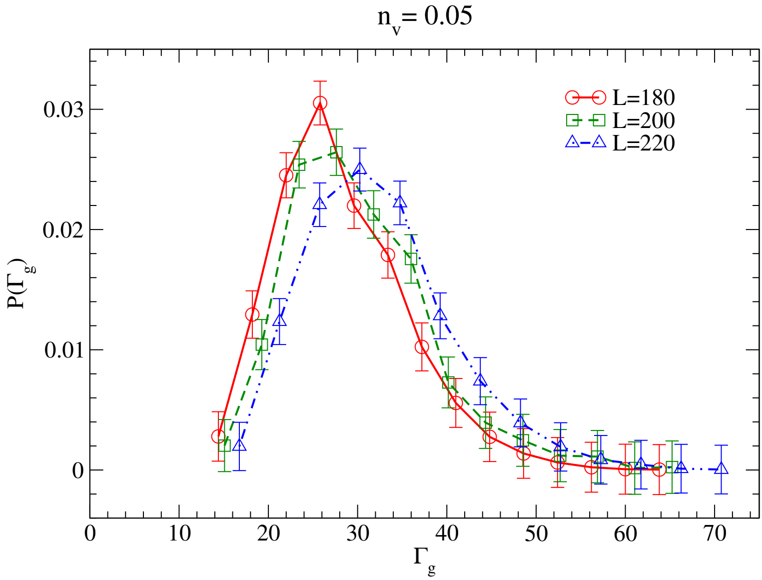
Taking the thermodynamic limit



Thermodynamic limit: $n_v = 0.05$

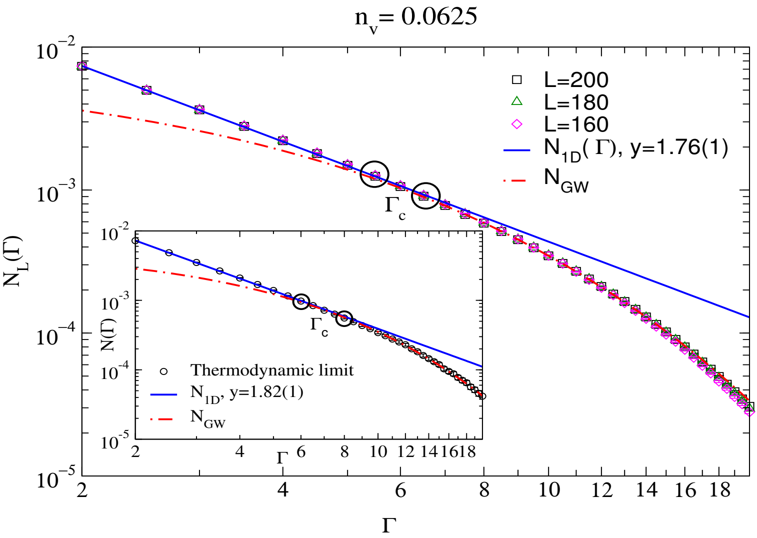


Γ^*_{gap}

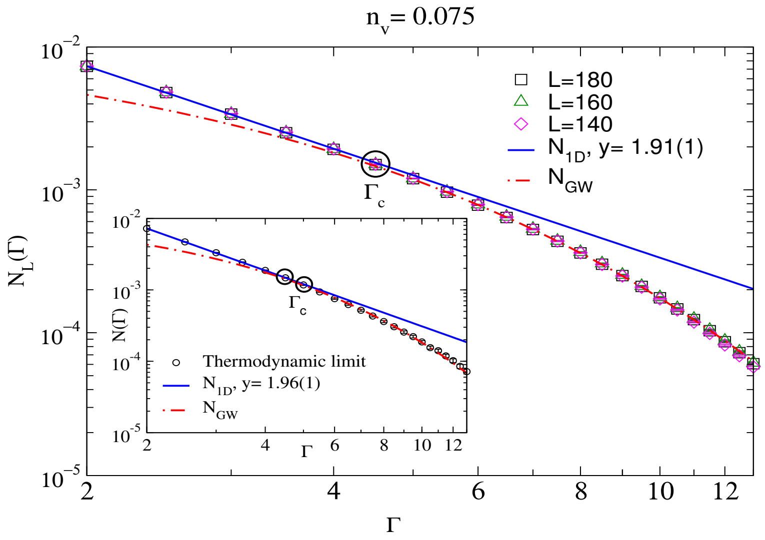


$n_v = 0.05$
L=180
L=200
L=220
$P(\Gamma_g)$
Γ_g
0.03
0.02
0.01
0
0
10
20
30
40
50
60
70

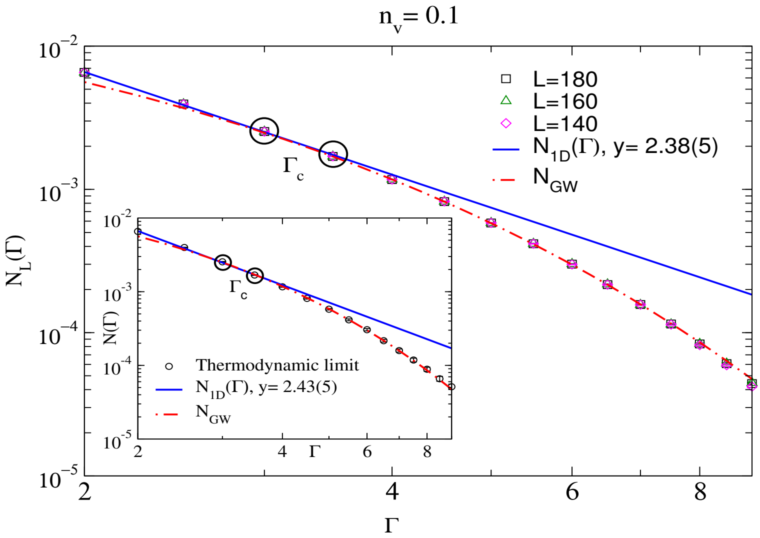
$N(\Gamma)$ for $n_v = 0.0625$



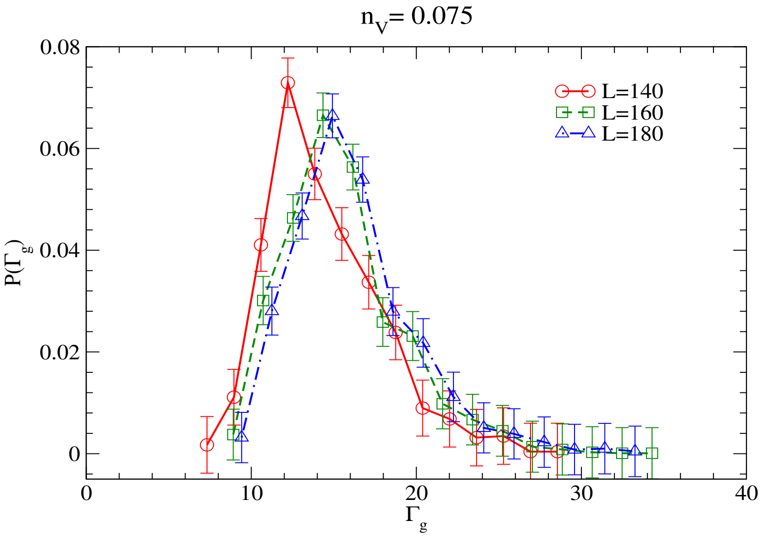
$N(\Gamma)$ for $n_v = 0.075$



$N(\Gamma)$ for $n_v = 0.1$

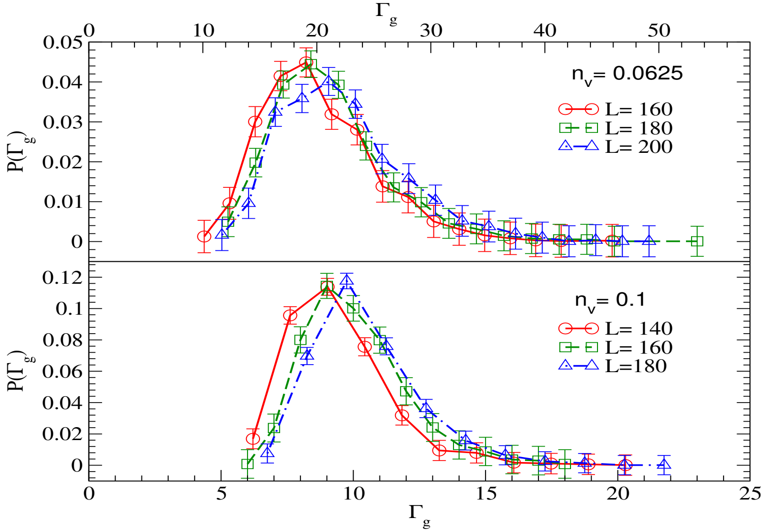


Γ^*_{gap}



n_V= 0.075
L=140
L=160
L=180
$P(\Gamma_g)$
Γ_g
0
0.02
0.04
0.06
0.08
0
10
20
30
40

Γ^*_{gap}

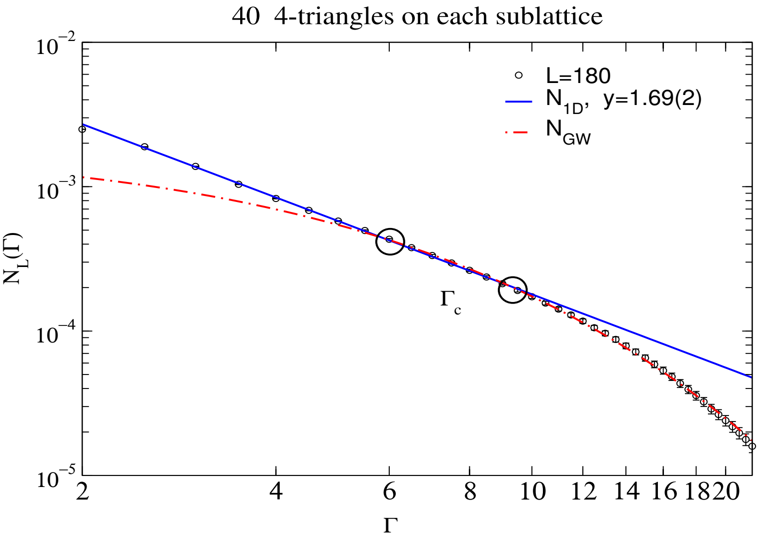


Γg
0
10
20
30
40
50
0.05
0.04
0.03
0.02
0.01
0
P(Γg)
nv= 0.0625
L= 160
L= 180
L= 200
0.12
0.1
0.08
0.06
0.04
0.02
0
P(Γg)
nv= 0.1
L= 140
L= 160
L=180
0
5
10
15
20
25
Γg

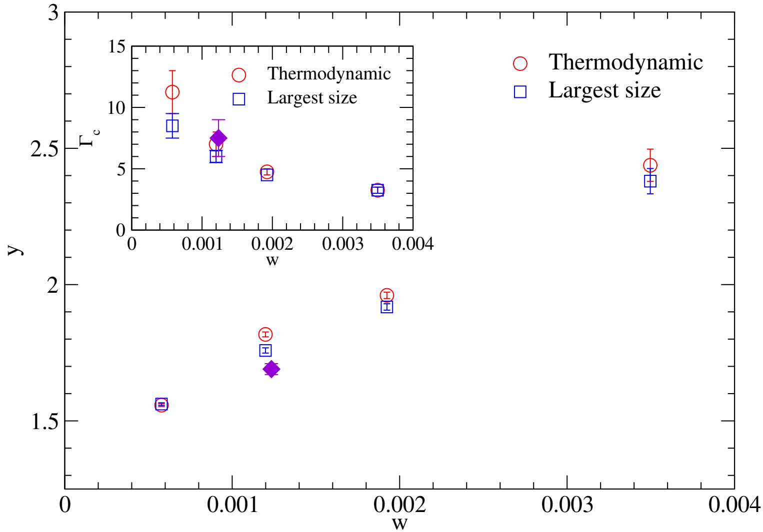
Physics:

- w depends on n_v *and* correlations between positions of vacancies
- Is crossover Γ_c and intermediate asymptotic exponent y “quasi-universal”?
- Operational definition of “Quasi-Universality”:
  Vary n_v, vary correlations.
  If resulting w is same, crossover Γ_c and y same...

Toy-model: Dilution by 4-triangles ($n_v = 0.0049$)

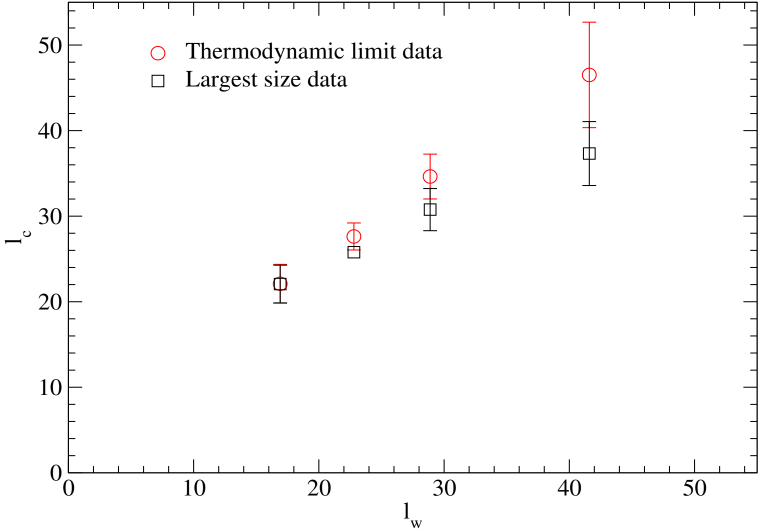


Check crossover systematics



Filled symbol: 4-triangle diluted sample

Another aspect of crossover systematics

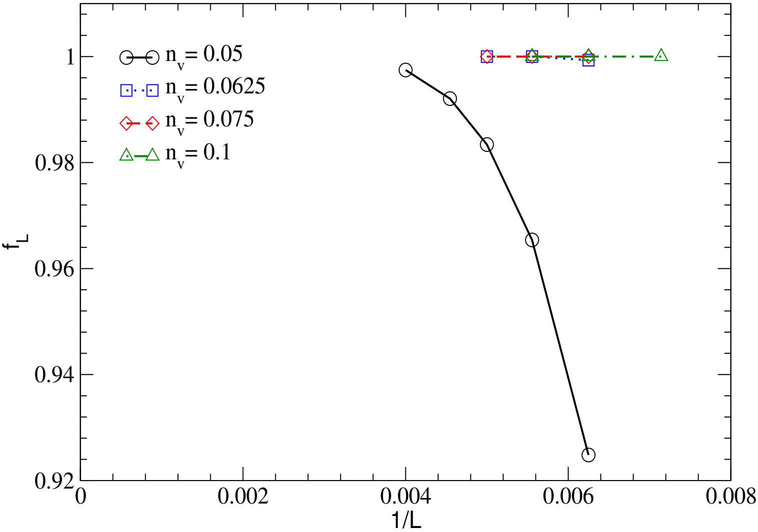


$l_c \equiv 1/\sqrt{N(\Gamma_c)}$

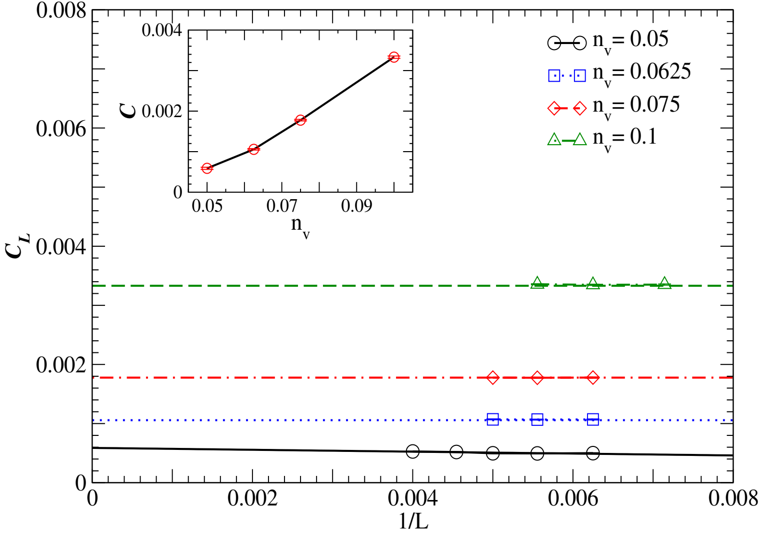
$l_w \equiv 1/\sqrt{w}$

Caution: Not claiming $l_c = l_w$, only $l_c \sim l_w$.

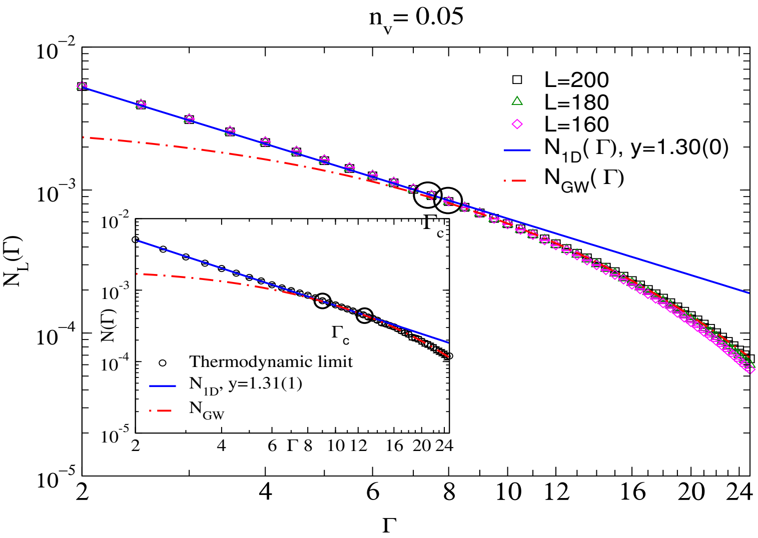
Kitaev: Zero modes



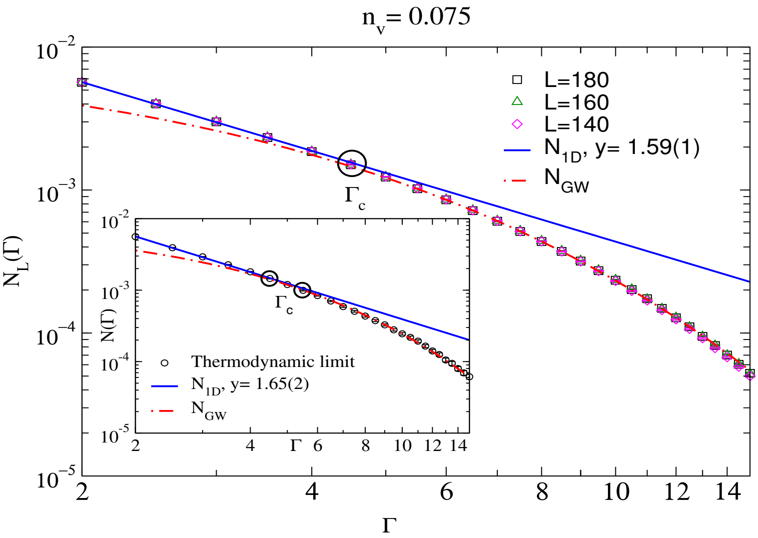
Kitaev: Zero modes



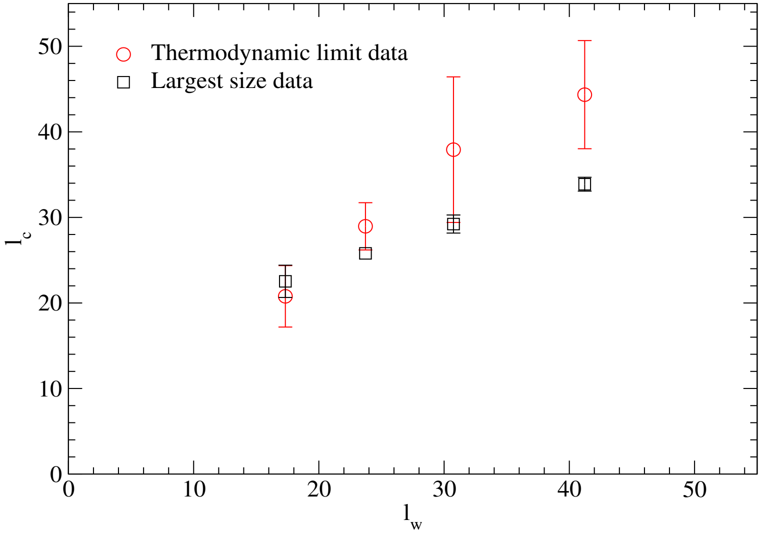
Kitaev: $N(\Gamma)$



Kitaev: $N(\Gamma)$



Kitaev: Crossover systematics



Comments on other work

Evers group: $0 < y < 1$
(Hafner *et. al.* 2014)
Mirlin group prediction: $y = 0.5$
(Ostrovsky *et. al.* 2014)
Willans-Chalker-Moessner (in gapped phase of Kitaev): $y = 0.7$

Acknowledgements

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