Vacancy-induced crossover in chiral orthogonal universality class

Consequences for a SU(2) symmetric Majorana spin liquid

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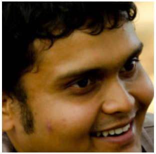
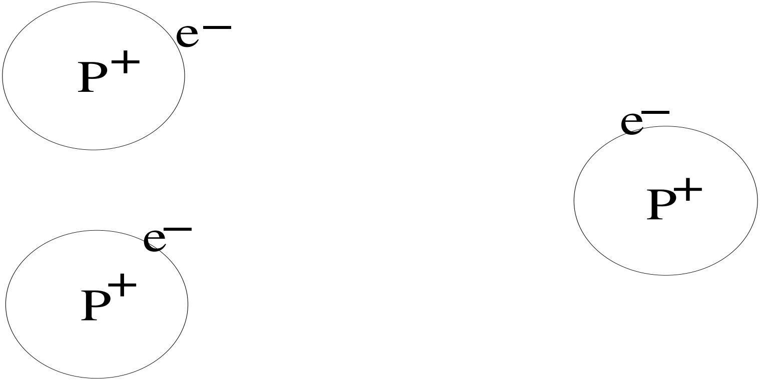
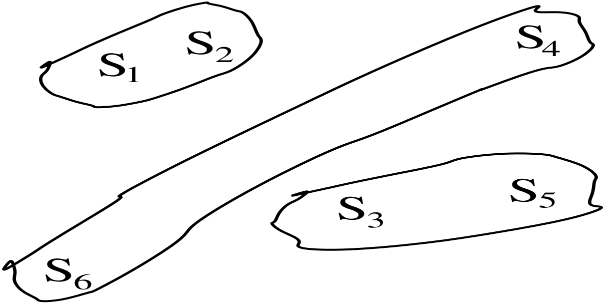


Background: Bhatt-Lee physics in Si:P



- 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)

In this talk: 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 $T \to 0$
- $N(\Gamma_T)$ displays advertised crossover:
  $N(\Gamma_T) \sim \Gamma_T^{-y}$ 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

- $\chi(T) \propto \kappa(T)$ 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

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

- $\vec{\tau}$: “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

- $D_{\vec{r}} \equiv -ic^x_{\vec{r}}c^y_{\vec{r}}c^z_{\vec{r}}b^x_{\vec{r}}b^y_{\vec{r}}b^z_{\vec{r}} = +1$ 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: $\sigma^\alpha_{\vec{r}}\tau^\beta_{\vec{r}} = ic^\alpha_{\vec{r}}b^\beta_{\vec{r}}$
  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
- $\chi(T) = \frac{1}{T} \int d\epsilon \rho_{\mathrm{tot.}}(\epsilon) \frac{e^{\epsilon/T}}{(e^{\epsilon/T}+1)^2}$
  where $\rho_{\mathrm{tot}}(\epsilon)$ 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

Dilution

- Remove honeycomb lattice sites at random (modeling non-magnetic impurities.)
- Global “compensation”: Equal number of vacancies on A and B sublattices
- Short-distance correlations on impurity ensemble—prevent disconnecting small clusters

Flux-binding

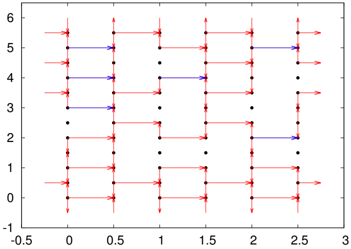
- Lieb-Loss heuristics:
  Each vacancy binds static π-flux in ground-state sector.
  Gap to other flux sectors
  (Kitaev, Willans-Chalker-Moessner)
- At low temperature, χ dominated by this flux-sector

Choice of geometry

- Semi-open $L \times L$ unit cells ($2L^2$ sites in undiluted sample) and armchair edges (to avoid boundary-induced low-energy modes)
- L chosen even, so loop wrapping around periodic direction has length zero mod 4.
- To preserve precise connection to dimer enumeration, *antiperiodic boundary conditions*

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

Computational details

- Form H^2, the square of the tight-binding Hamiltonian H (with hopping amplitude $t = J = 1$ between nearest-neighbours), and work with the $(1-p)L^2 \times (1-p)L^2$ block $(M_{AB})^T M_{AB}$ where M_{AB} is the matrix of connectivity between A and B sublattice sites in the depleted lattice
- Fully multiprecision implementation of the ALGOL routines in Wilkinson's handbook to count eigenvalues of $(M_{AB})^T M_{AB}$ below $10^{-2\Gamma}$.
- Results checked at moderate L and moderate Γ against LAPACK routines.

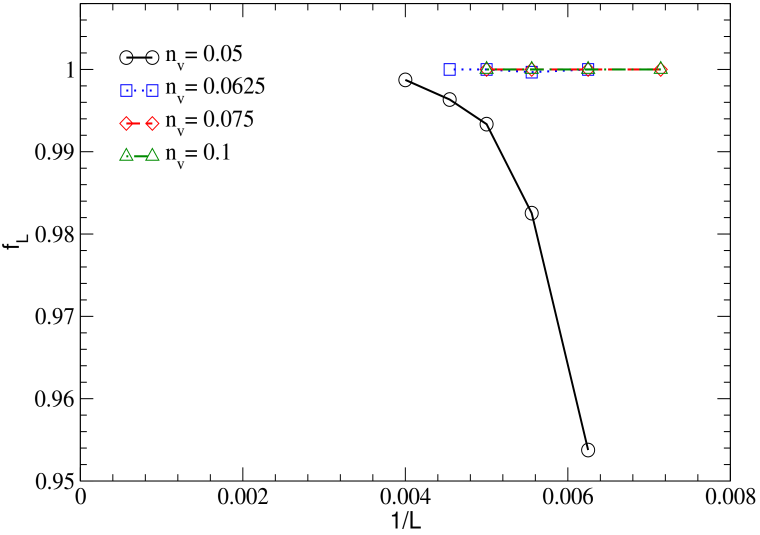
Computational details—II

- For each sample, computations first done in a coarse-grid of Γ, then $N_{\text{tot}}(\Gamma)$ "filled in" iteratively when needed. Final grid spacing $\Delta(\Gamma) = 0.5$.
- So lowest-nonzero gap $10^{-\Gamma_g}$ in a given sample obtained with accuracy of $\Delta(\Gamma_g) = 0.5$.
- w_0, the number of zero modes per unit volume in a given sample empirically equated to value of $N_{\text{tot}}(\Gamma)$ after last downward step in this quantity.
- Our grid extends to Γ_{max} as high as 100 in some cases—stability in these cases checked by varying precision
- Study $N(\Gamma) = N_{\text{tot}}(\Gamma) - w_0$ and w_0 for ~ 4000 samples

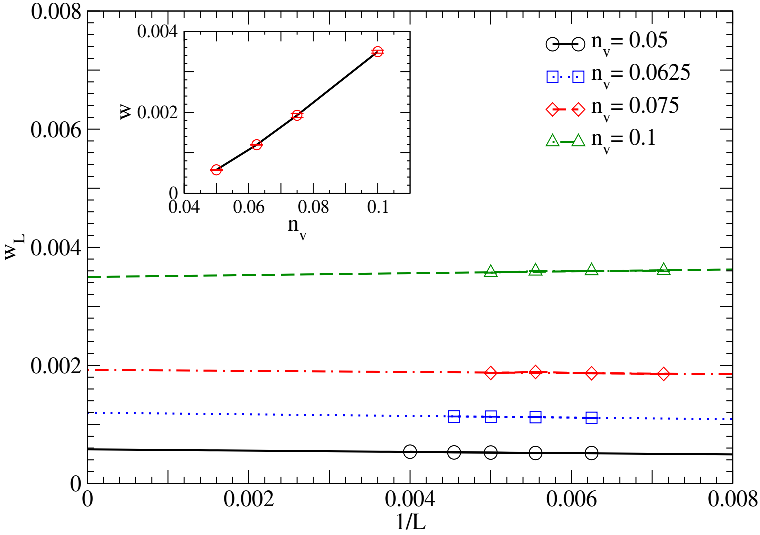
Formulary

- $\rho_{\text{tot}}(\epsilon) = \rho(\epsilon) + w_0\delta(\epsilon)$
- $N(\Gamma) = 2\int_0^{10^{-\Gamma}} \rho(\epsilon)d\epsilon$
- Universal asymptotics of chiral-orthogonal universality class
  $\rho(E) \sim \frac{1}{\epsilon} e^{-b|\ln\epsilon|^{1/x}}$
  equivalently:
  $N(\Gamma) = a\Gamma^{1-\frac{1}{x}} e^{-b\Gamma^{\frac{1}{x}}}$
  ($x = 3/2$, two free parameters a and b)
  (Gade-Wegner, Motrunich-KD-Huse, Mudry-Ryu-Furusaki)
- Analogous $d = 1$ result (Dyson):
  $\rho(\epsilon) \sim \dfrac{1}{\epsilon[\log[1/\epsilon]]^{1+y}}$
  equivalently:
  $N(\Gamma) = q\Gamma^{-y}$ (two free parameters q and y)

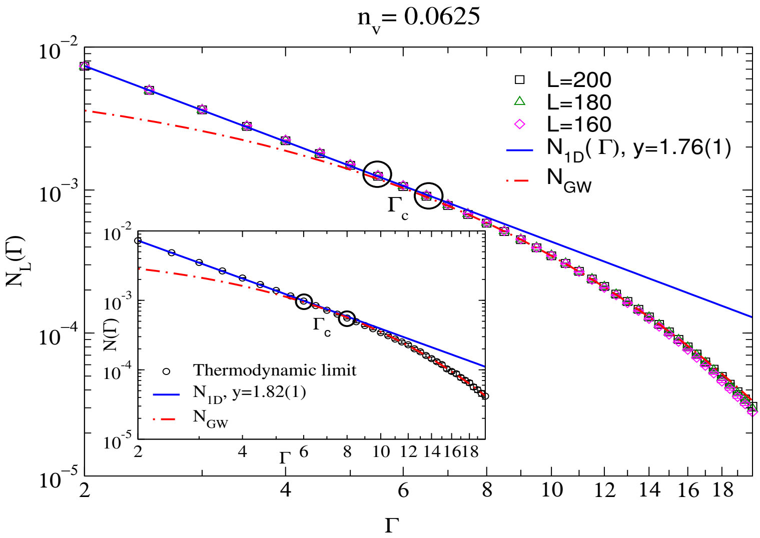
Graphene: Zero modes



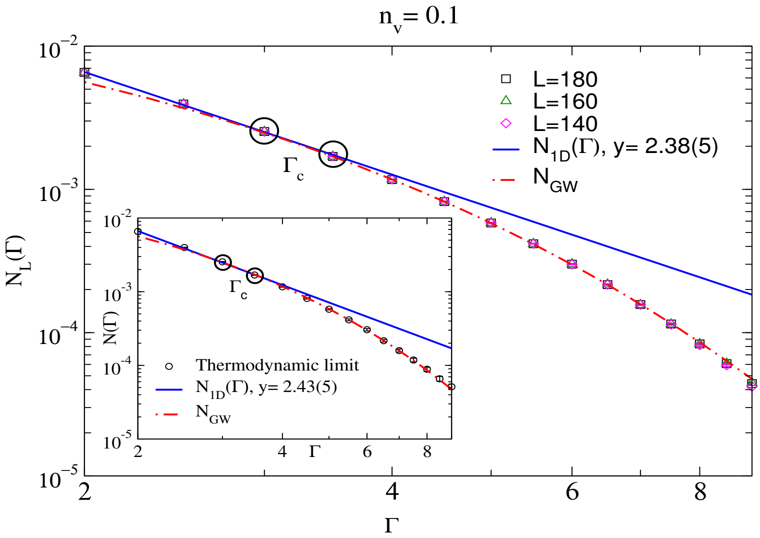
Graphene: Zero modes



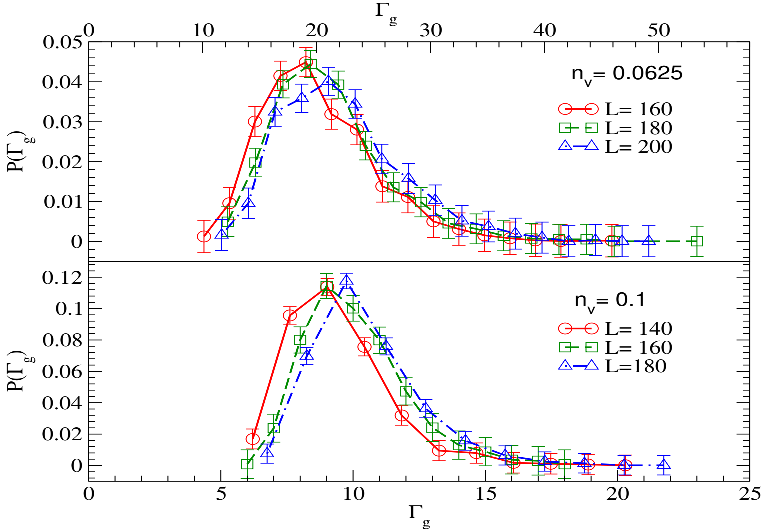
Graphene: $N(\Gamma)$



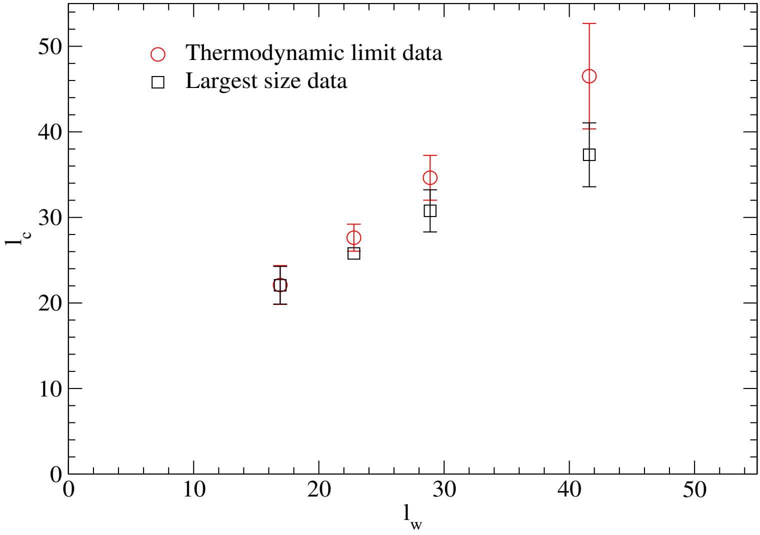
Graphene: $N(\Gamma)$



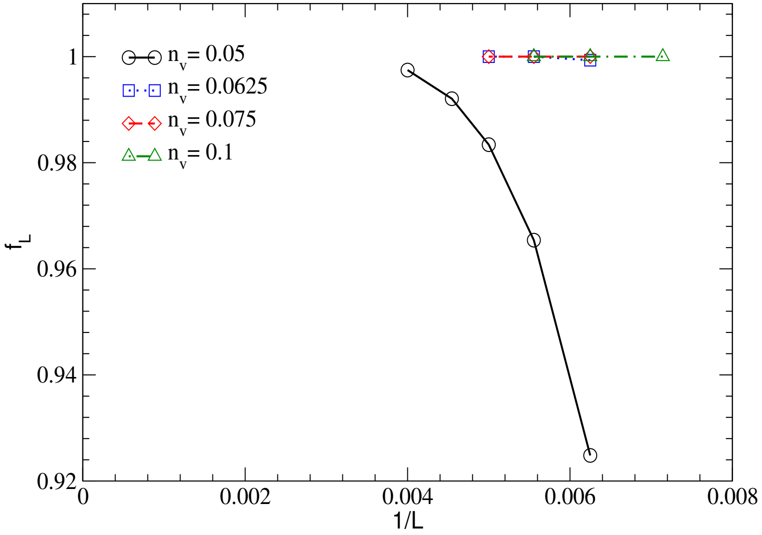
Graphene: Γ^*_{gap}



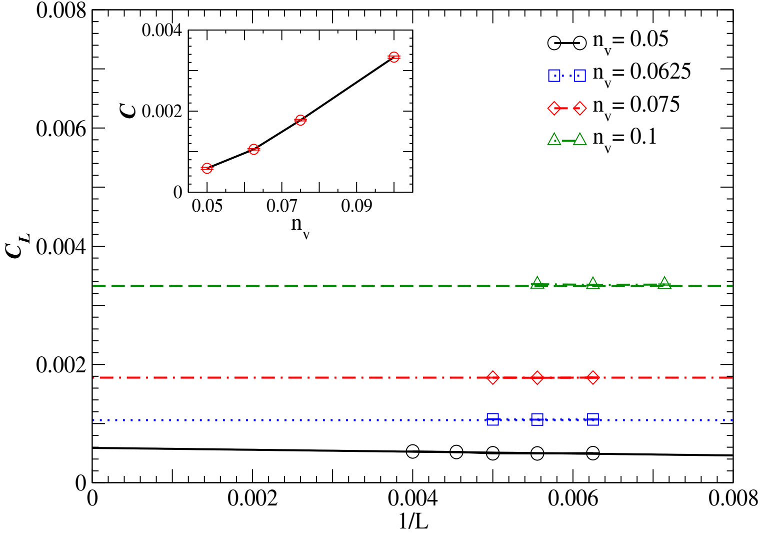
Graphene: Crossover systematics



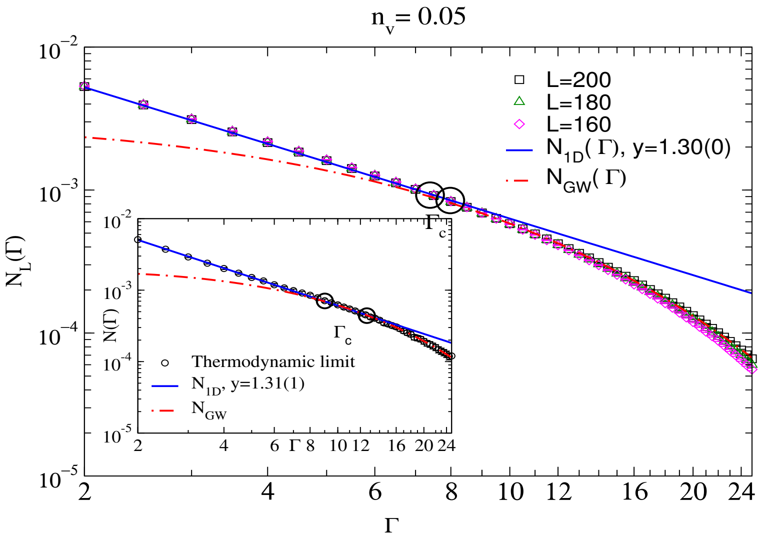
Kitaev: Zero modes



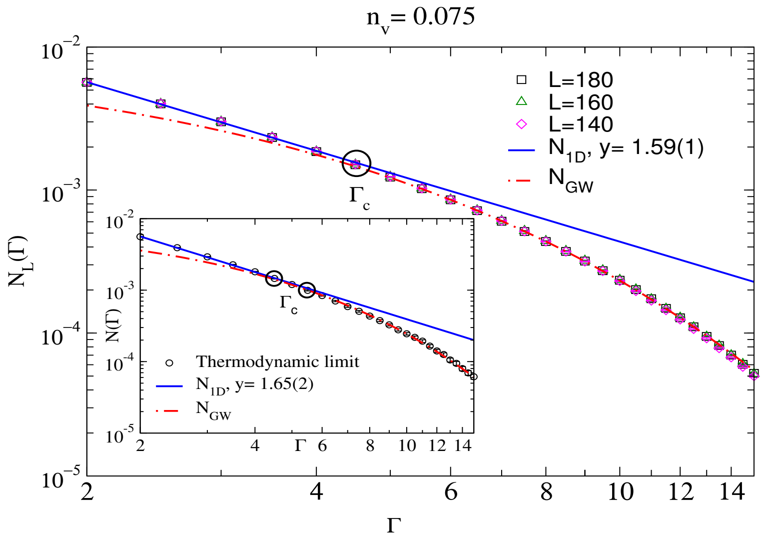
Kitaev: Zero modes



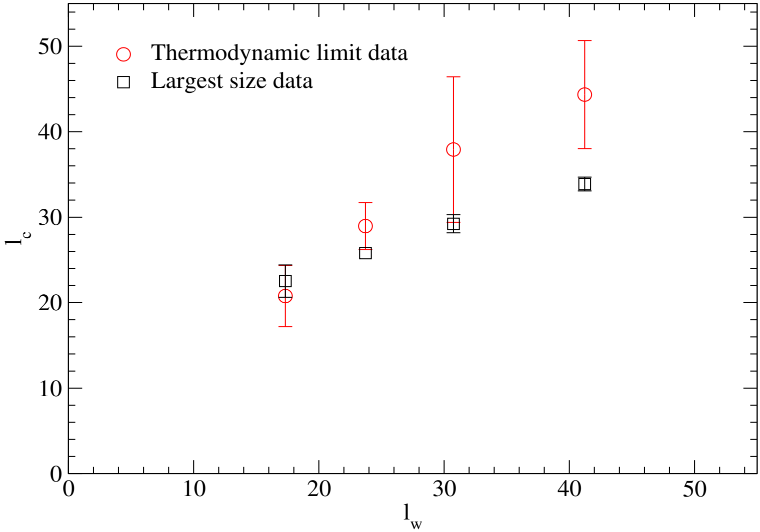
Kitaev: $N(\Gamma)$



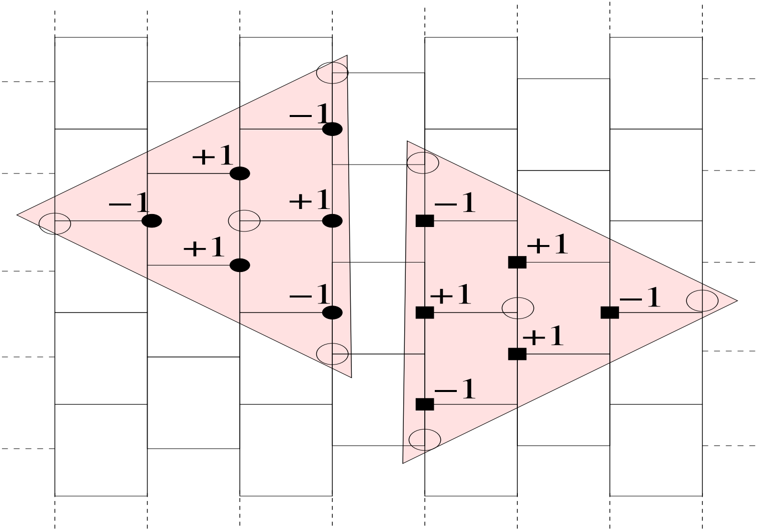
Kitaev: $N(\Gamma)$



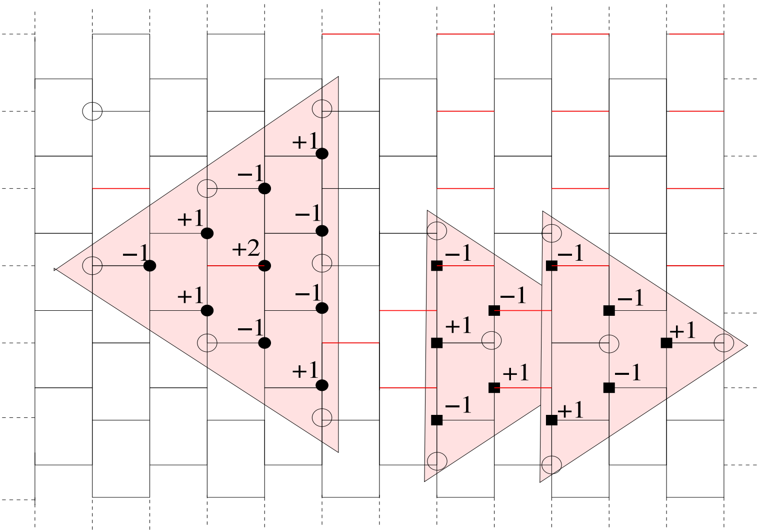
Kitaev: Crossover systematics



Graphene: Lower-bound on zero modes



Kitaev: Lower-bound on zero modes



Comments on other work

Evers group (graphene data): $0 < y < 1$
(Hafner *et. al.* 2014)
Mirlin group prediction (for graphene): $y = 0.5$
(Ostrovsky *et. al.* 2014)
Willans-Chalker-Moessner (in gapped phase of Kitaev): $y = 0.7$
Dynamical range too small to see crossover??

Acknowledgements

- Collaborators:
  Graphene: Sambuddha Sanyal (ICTS-TIFR) and Olexei Motrunich (Caltech)
  SU(2) symmetric Kitaev spin liquid: Sambuddha Sanyal (ICTS-TIFR), John Chalker (Oxford), R. Moessner (MPIPKS)
- Computational resources at TIFR

Data analysis

- Fits of $N(\Gamma)$ attempted to three two-parameter forms: "Gade", "Dyson" and "Griffiths" (see formulary on next page to fix notation)
- For "Gade", exponent in DOS fixed at our value of $2/3$, and subleading terms dropped in converting DOS prediction to prediction for $N(\Gamma)$
- Fits made to largest-size data, using data with $\Gamma < \Gamma^*_{\text{gap}}$, where Γ^*_{gap} is defined as the most probable value of the lowest non-zero gap Γ_g (from peaks in histograms of this quantity)
- Thermodynamic limit of $N(\Gamma)$ obtained at each $\Gamma < \Gamma_{\text{gap}}$ by straight line fits in $1/L$ for three largest sizes.
- N_{thermo} obtained in this way also fit to the same three alternate forms, to see if conclusions change: We accept fit parameters will change, but ask: does the type of best-fit curve change?