# Finite-size exciton insulator in graphene dots & magnetic field effects on topological graphene

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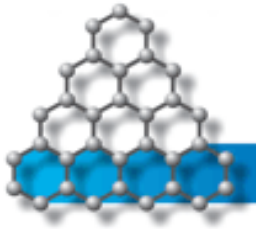


DFG
Schwerpunktprogramm 1459
Graphene

SFB | TR12

# Outline

- Graphene quantum dot:  N particle problem
  - No-pair model: Hartree-Fock calculations
  - Accuracy of no-pair model:  Exact diagonalization of full QED Hamiltonian for N=2,3
  - Wigner molecule formation
  - finite-size excitonic instability

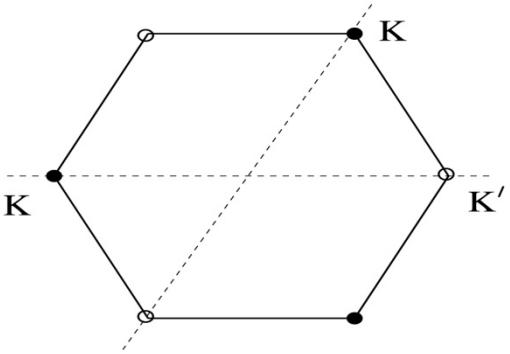
*Paananen, Egger & Siedentop, PRB 83, 085409 (2011)*
*Paananen & Egger, PRB 84, 155456 (2011)*
*Häusler & Egger, preprint (2013)*

- Landau levels & helical edge states in topological monolayer graphene with enhanced spin-orbit interactions

*De Martino, Hütten & Egger, PRB 84, 155420 (2011)*

# Band structure

- Two independent K points in first Brillouin zone: „valley“ d.o.f.
- Band gap vanishes at K points (Dirac points, E=0)
- Lowest-order **k.p** scheme: „relativistic“ Dirac light cone dispersion close to Dirac point
  - Emergent Lorentz invariance
- Here: study effects of
  - Coulomb interaction in „Dirac dot“
  - Spin-orbit coupling




$$E(\vec{q}) = \pm v|\vec{q}|$$

$$\vec{q} = \vec{k} - \vec{K}$$

$$v \approx c/300$$

# Coulomb interaction effects

*Review: Kotov et al., Rev. Mod. Phys. 2012*

- Emergent Lorentz invariance broken by Coulomb interaction
  - Retardation effects (almost) negligible
  - Coulomb field lines are in 3D
- Strength parametrized by (bare) fine structure constant

$$\alpha = \frac{E_C}{E_k} = \frac{e^2}{\varepsilon \hbar v} \approx \frac{2.2}{\varepsilon}$$

  - For density *n*, typical kinetic energy: $E_k = \hbar v \sqrt{n}$
  - Typical Coulomb energy: $E_C = \frac{e^2}{\varepsilon r} \approx \frac{e^2 \sqrt{n}}{\varepsilon}$
  - Condensed-matter strong-coupling variant of $QED_{2+1}$

# Monolayer graphene: (bulk) interaction effects

- α is density-independent: no bulk Wigner crystallization in graphene!
- Fermi liquid theory applies away from Dirac point (doped graphene)
- What happens near Dirac point (undoped graphene)?
  - Density of states vanishes
  - No screening of 1/r Coulomb tail (up to renormalization of dielectric constant)

# Weak-coupling results

*Gonzalez et al., Nucl. Phys. B 1994*

- One-loop RG calculation: logarithmic growth of Fermi velocity at low energies

$$v(k) = v\left(1 + \frac{\alpha}{4}\ln\left(\frac{\Lambda}{k}\right)\right)$$

Cutoff scale (for validity of Dirac cone spectrum)

  - Corresponds to slow logarithmic RG flow $\alpha \to 0$ at low energy scales
  - Weak interactions are marginally irrelevant
  - Experimentally observed (ARPES, cyclotron resonance)

*Elias et al., Nature Physics 2011*

- Same conclusion from two-loop or RPA calculations for $\alpha < 1$

*Son, PRB 2007*

# Dirac liquid vs excitonic insulator

- Perturbative analysis: quasi-particle decay rate has linear scaling with energy
  - consistent with ARPES and STM experiments
  - resembles marginal Fermi liquid: „Dirac liquid“
- For $\alpha > \alpha_c$ : spontaneous mass gap generation theoretically predicted (not observed so far)
  - proliferation of electron-hole pairs
  - excitonic insulator, chiral symmetry breaking
  - Schwinger-Dyson self-consistent gap equation predicts gap in meV regime
  - QMC simulations: $\alpha_c \approx 1.1$

*Drut & Lähde, PRL 2009*

# Mesoscopic geometry: Quantum Dots

- Bulk system: complicated many-body problem
- Here: finite-size setting
  - mathematically well defined & experimentally realizable
- N interacting Dirac quasi-particles on top of filled Dirac sea
  - Magnetic confinement *De Martino, Dell'Anna & Egger, PRL 2007*
  - Quasibound states in electrostatic potentials *Silvestrov & Efetov, PRL 2006*
  - Finite-size „flake": circular dot with „no out-current" (infinite mass) boundary condition [results shown in this talk] *Berry & Mondragon, Proc. R. Soc. London A 1987*
- Single-particle states define noninteracting artificial atom energy levels
  - In contrast to atomic physics: interactions much stronger!

# N particle problem

- „Naive“ interacting N-particle problem for Dirac fermions is ill-defined

*Brown & Ravenhall, Proc. R. Soc. London A 1951*

$$H = v\sum_{n=1}^{N}\left[\vec{\sigma}_n \cdot \vec{p}_n + M(\vec{x}_n)\sigma_{z,n}\right] + \sum_{m<n}\frac{\alpha\hbar v}{\left|\vec{x}_m - \vec{x}_n\right|}$$

- For weak interaction: No-pair model (Furry picture) with fixed N *Sucher, Phys. Rev. 1957, 1958, 1980*
  - Project single-particle spectrum to positive energies
  - Neglect excitation of electron-hole pairs
  - Here protected by finite-size gap between negative and positive energy levels *Egger et al., J. Phys. A 2010*
- Accuracy of no-pair approximation ?

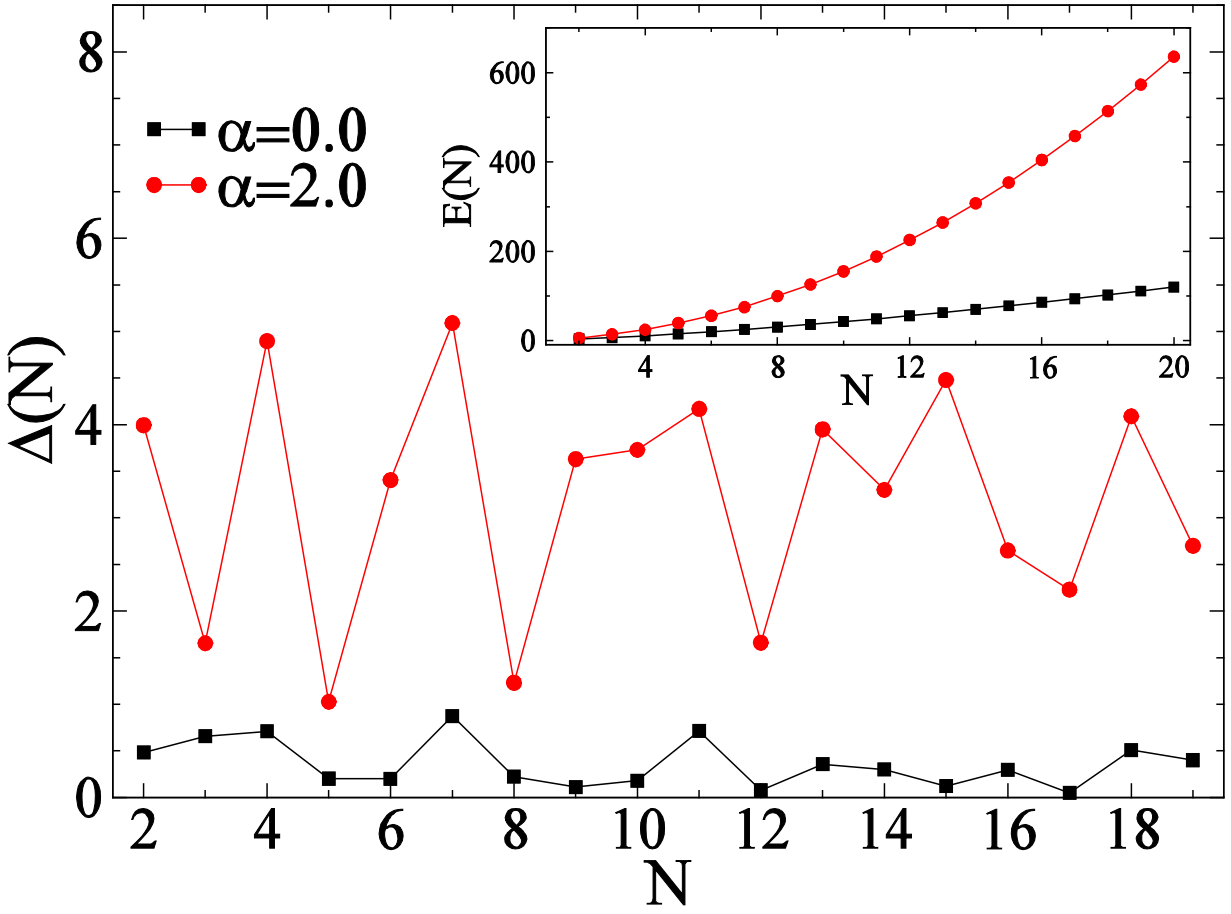
# Hartree-Fock results for no-pair model

*Paananen, Egger & Siedentop, PRB 2011*

- Simplest approach: RHF calculations
  - Unexpectedly accurate even for strong interactions (within no-pair model): Benchmarked vs exact diagonalization for N=2,3
  - Energies agree within <1% for $\alpha=2$
- Results for artifical atom holding up to N=20 electrons:
  - Ground state energy
  - Density (and spin density) expectation value
  - Pair correlation function

# Addition spectrum

addition energy: $\Delta(N) = E(N+1) + E(N-1) - 2E(N)$



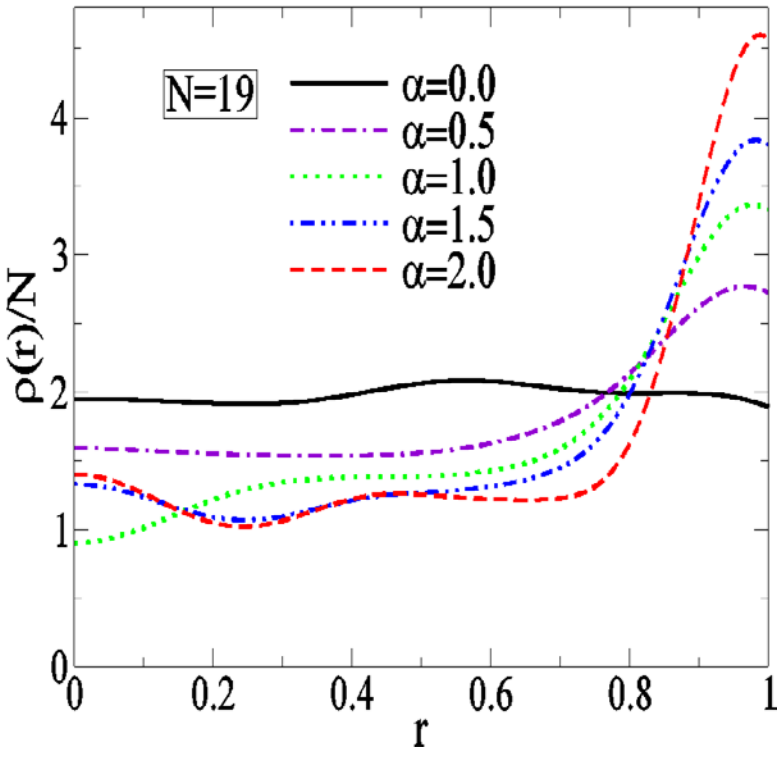

Magic numbers different & more pronounced with interactions !

Measurable by Coulomb blockade spectroscopy…

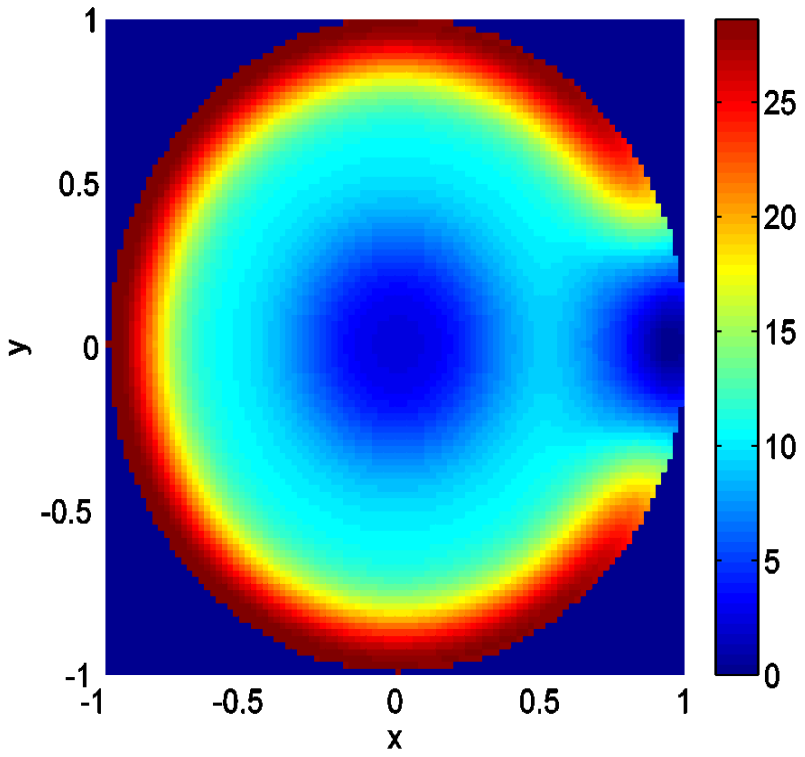
Energy unit: $\hbar v / R$

# Wigner crystallization

radial density profile




pair correlations: spatial shells with sequence 15-3-1



# Wigner crystallization

- Electrostatic energy starts to dominate over kinetic energy for $\alpha > 1$
- Particles maximize their distance & form „crystal“ – here ring-like arrangement
  - Spatial shell filling sequence agrees well with classical result (minimization of electrostatic energy)
- Wigner crystallization favored in confined geometry (no Wigner crystal in bulk graphene!)
- Crossover from Dirac liquid regime to „Wigner molecule“ is similar to standard 2DEG case

*Egger, Häusler, Mak & Grabert, PRL 1999*

# Beyond no-pair model: „QED“ approach

*Paananen & Egger, PRB 2011*

- Expand second-quantized field operator

$$\Psi(\vec{x}) = \sum_a \Phi_a^{(+)}(\vec{x}) c_a + \sum_{\tilde{a}} \Phi_{\tilde{a}}^{(-)}(\vec{x}) d_{\tilde{a}}^+$$

  - $a$ $(\tilde{a})$ labels single-particle states $\Phi_a^{(+)}$ $\left(\Phi_{\tilde{a}}^{(-)}\right)$ with positive (negative) energy
  - Noninteracting reference state = filled Dirac sea

- QED Hamiltonian $H = \sum_a E_a c_a^+ c_a + \sum_{\tilde{a}} \left|E_{\tilde{a}}\right| d_{\tilde{a}}^+ d_{\tilde{a}} + H_I$

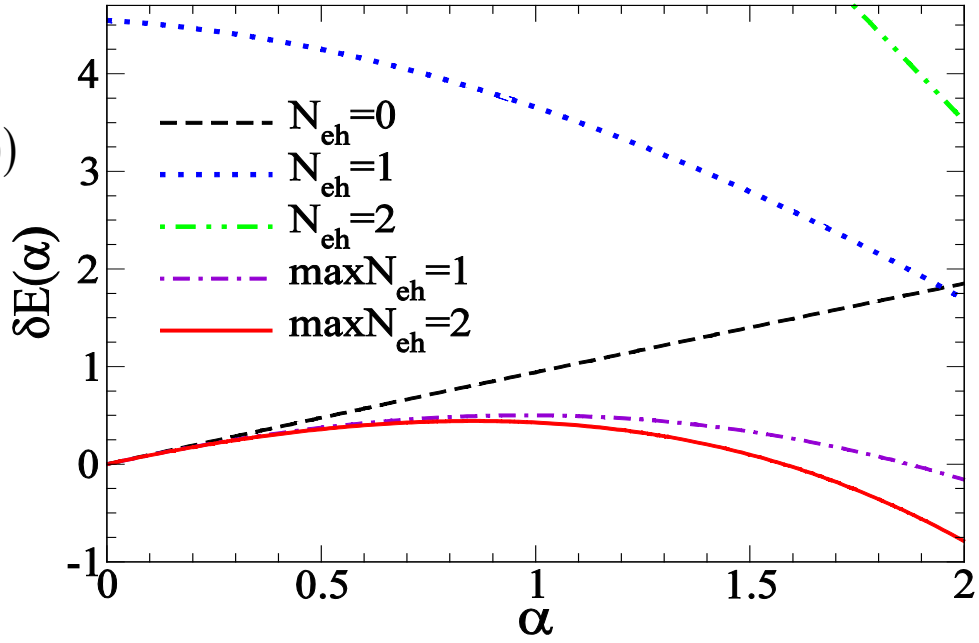
$$H_I = \frac{\hbar v \alpha}{2} \int \frac{d\vec{x} d\vec{x}'}{\left|\vec{x} - \vec{x}'\right|} : \Psi^+(\vec{x}) \Psi^+(\vec{x}') \Psi(\vec{x}') \Psi(\vec{x}) :$$

# Exact diagonalization

- Electron ($N_e$) and hole ($N_h$) numbers are not conserved
- Define particle number as $N=N_e-N_h$
  - N = number of particles on top of filled Dirac sea for $\alpha \rightarrow 0$
  - Conserved by full Hamiltonian
  - Number of electron-hole pairs $N_{eh}$ not conserved!
  - No-pair model follows for $N_{eh}=0$
- Exact diagonalization for N=2,3 with up to $N_{eh}=2$ electron-hole pairs feasible

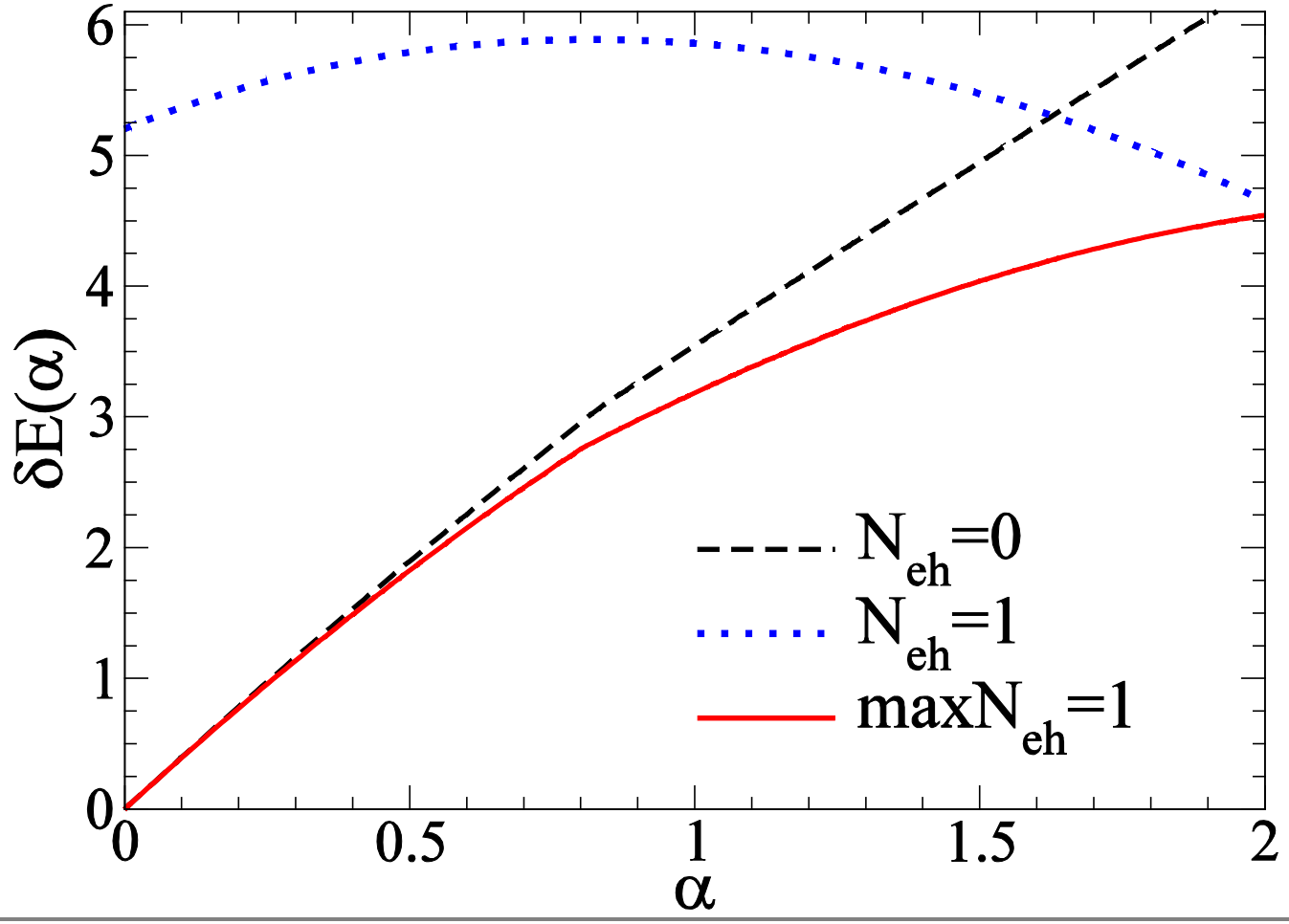
# N=2: exact diagonalization

$$\delta E(\alpha) = E(\alpha) - E(0)$$




- No-pair result for interaction energy accurate only for $\alpha < 0.5$
- Electron-hole pairs proliferate for $\alpha > 1$
- Finite-size crossover to excitonic instability, no-pair model breaks down!

# N=3: exact diagonalization



# Wigner molecule revisited

- HF analysis reporting Wigner molecule formation for $\alpha>1$ relied on no-pair model – but no-pair model breaks down for $\alpha>1$
- ED of full QED model with N=3 shows pronounced density correlations & numerical results for pair correlations similar to no-pair predictions
- Wigner molecule formation only weakly affected by electron-hole proliferation

# Spin-orbit effects: topological graphene

*Castro Neto et al., RMP 2009*

$$H_{SOI} = \pm\Delta\,\tau_z\sigma_z + \frac{\lambda}{2}\left(\pm\,\tau_x\sigma_y - \tau_y\sigma_x\right)$$

spin Pauli matrices

- Δ: intrinsic SOI
- λ : „Rashba“ SOI (curvature, electric field)
- Enhancement of pristine (small) values:
  - *Ab initio* calculations: Indium or Thallium adatom deposition yields up to Δ≈100 K *Weeks et al., PRX 2012*
  - Graphene experiments on Ni surfaces report large values for λ *Varykhalov et al., PRL 2008*
  - Colossal enhancement of spin-orbit couplings observed in weakly hydrogenated graphene

*Balakrishnan et al., Nature Phys. 2013*

# Kane-Mele model: „quantum spin Hall“ (QSH) phase

*Kane & Mele, PRL 2005*

- Topological insulator for $\Delta > \lambda/2$: bulk band gap but gapless excitations at boundary
- Helical edge liquid : right- and left-moving states have opposite spin polarization
  - Spin-independent disorder backscattering strongly suppressed (protected by time reversal symmetry)
- Observed in HgTe wells *König et al., J. Phys.Soc.Jpn. 2008*
- Possibility of QSH phase in graphene!
  - what happens in (perpendicular) magnetic field?

# Graphene band structure with SOI and magnetic field

- Consider piecewise constant magnetic field B
  - Cyclotron orbits: magnetic length $l = \sqrt{\hbar c / 2eB}$
  - Energy scale $\hbar\omega_c = \hbar v / l \sim \sqrt{B}$

    B=1T: ≈ 36 meV ($l$ ≈ 18 nm)
  - Also include spin Zeeman energy

    $$E_Z = g\mu_B B << \hbar\omega_c$$
- Exact spinor eigenstates: parabolic cylinder functions of order p

*De Martino, Hütten & Egger, PRB 2011*

# Homogeneous field: Landau levels

Normalizability: p=n=0,1,2,3,… ⟹ Landau levels solve the quartic equation

$$\left[(E+E_Z)^2 - n(\hbar\omega_c)^2 - \Delta^2\right]\left[(E-E_Z)^2 - (n+1)(\hbar\omega_c)^2 - \Delta^2\right] = \lambda^2\left[(E-\Delta)^2 - E_Z^2\right]$$

- Standard result for $\Delta = \lambda = E_Z = 0$: $E_{\pm,n} = \pm\hbar\omega_c\sqrt{n}$
- Recover $\Delta = E_Z = 0$ results *Rashba, PRB 2009*
- General case: no zero modes in presence of SOI
- Particle hole symmetry generally broken
- Exact solution for n=0 and spin down:

$$E_{n=0,\downarrow} = \Delta - E_Z$$

# QSH phase without time reversal symmetry?

- Quartic equation can be solved analytically, but expressions lenghty & not illuminating
- Study fate of QSH phase in the magnetic field for simpler limit λ=0 : QSH phase for B=0
  - Can QSH phase survive time reversal symmetry breaking (B>0)? *Yang et al., PRL 2011*
- Then spin σ conserved, quartic equation yields

$$E_{\pm,n,\sigma} = \sigma E_Z \pm \sqrt{n(\hbar\omega_c)^2 + \Delta^2}$$

  - no zero energy states: $E_{0,\sigma} = \sigma(E_Z - \Delta)$

# Edge states for $\lambda=0$

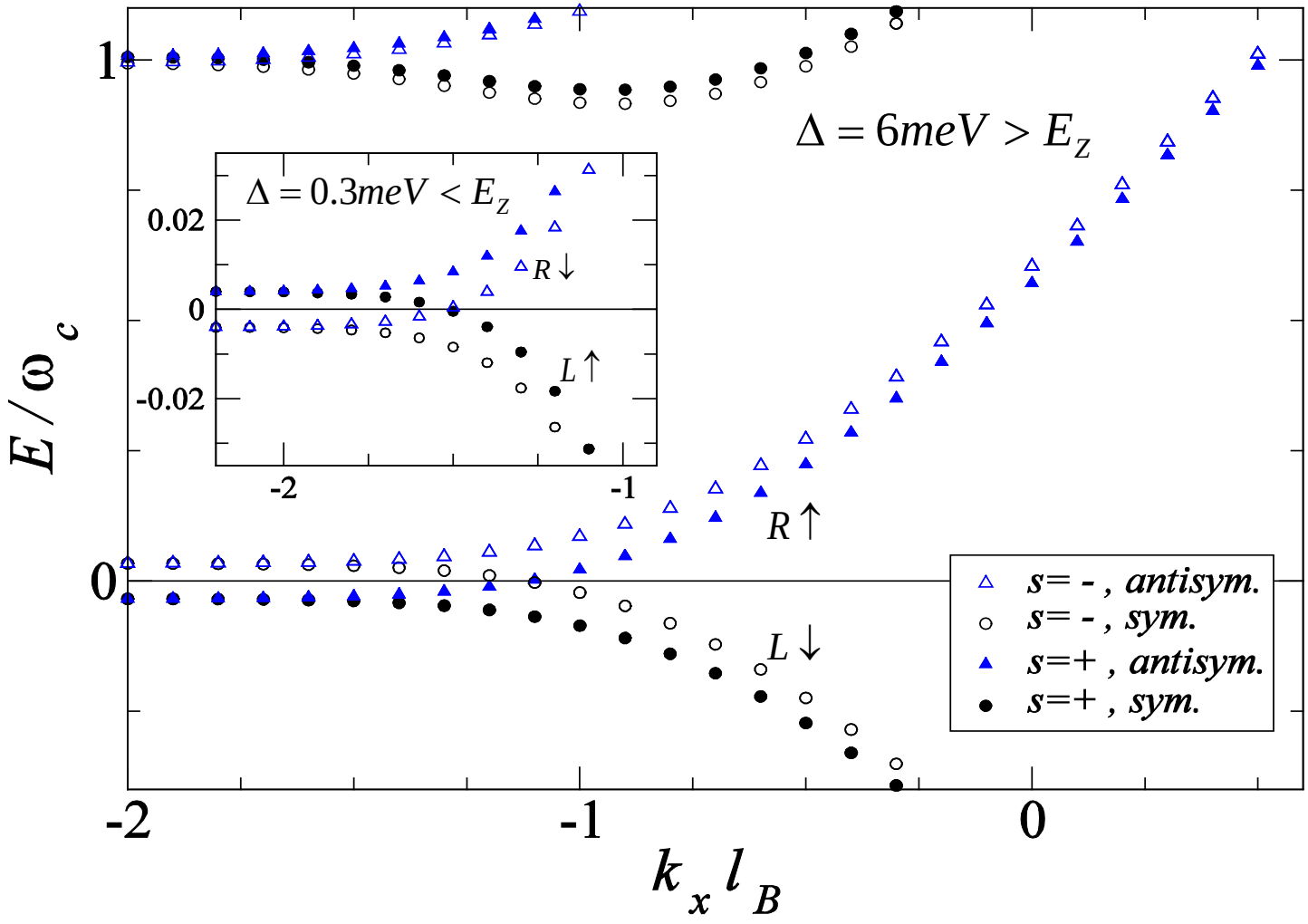
*De Martino, Hütten & Egger, PRB 2011*

- Semi-infinite geometry y<0 with armchair boundary condition at y=0
  - Wavenumber $k_x$ conserved
  - For $k_x < 0$: distance from boundary set by $|k_x|$
- Order p of cylinder function now arbitrary real
  - determined by boundary condition (with symmetric or antisymmetric valley combinations)

$$\left( \sqrt{p(\hbar\omega_c)^2 + \Delta^2} \mp \sigma E_Z \right) D_{p-1}(2k_x l) + \hbar\omega_c D_p(2k_x l) = 0$$

  - Dispersion: $E_{\pm,\sigma}(k_x) = \sigma E_Z \pm \sqrt{p(k_x)\,(\hbar\omega_c)^2 + \Delta^2}$

# Edge states: numerical solution



# Stability of QSH phase

- ✓ Standard chiral Hall edges recovered for Δ=0
- ➢ QSH phase with helical edge liquid near Dirac point for $\Delta > E_Z$
- ➢ Quantum phase transition at $\Delta = E_Z$
- ➢ Spin-filtered Hall edge state for $\Delta < E_Z$

*Abanin, Lee & Levitov, PRL 2006*

- ➢ Both phases similar but with opposite spin current!

# Conclusions

- N particle problem in graphene dots
  - No-pair model quantitatively accurate for $\alpha < 0.5$
  - Electron-hole pairs proliferate for $\alpha > 1$
  - Finite-size excitonic instability & Wigner crystallization
- QSH phase in graphene with enhanced SOI survives for broken time reversal symmetry
  - topological insulator with helical edge states