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

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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)

- 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

- Emergent Lorentz invariance broken by Coulomb interaction
- Retardation effects (almost) negligible
- Coulomb field lines are in 3D
- Strength parametrized by (bare) fine structure constant
  \[
  \alpha = \frac{E_C}{E_k} = \frac{e^2}{\varepsilon \hbar \nu} \approx \frac{2.2}{\varepsilon}
  \]
- For density \( n \), typical kinetic energy: \( E_k = \hbar \nu \sqrt{n} \)
- 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

- $\alpha$ 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

- 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)
  \[ \text{Elias et al., Nature Physics 2011} \]
- Same conclusion from two-loop or RPA calculations for \( \alpha < 1 \)
  \[ \text{Son, PRB 2007} \]
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]  
- 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
  

- For weak interaction: No-pair model (Furry picture) with fixed N
  

  - 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

- 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 artificial atom holding up to N=20 electrons:
  - Ground state energy
  - Density (and spin density) expectation value
  - Pair correlation function

Paananen, Egger & Siedentop, PRB 2011
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

- Expand second-quantized field operator

\[ \Psi(\vec{x}) = \sum_a \Phi^{(+)}(\vec{x})c_a + \sum_{\tilde{a}} \Phi^{(-)}(\vec{x})d_{\tilde{a}}^+ \]

- \( a (\tilde{a}) \) labels single-particle states \( \Phi^{(+)}(\Phi^{(-)}) \) with positive (negative) energy

- Noninteracting reference state = filled Dirac sea

- QED Hamiltonian

\[ H = \sum_a E_a c_a^+ c_a + \sum_{\tilde{a}} E_{\tilde{a}} d_{\tilde{a}}^+ d_{\tilde{a}} + H_I \]

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

Paananen & Egger, PRB 2011
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

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

\( \Delta \): intrinsic SOI

\( \lambda \): „Rashba“ SOI (curvature, electric field)

Enhancement of pristine (small) values:

- \textit{Ab initio} calculations: Indium or Thallium adatom deposition yields up to \( \Delta \approx 100 \) K
  
  \( \text{Weeks et al., PRX 2012} \)

- Graphene experiments on Ni surfaces report large values for \( \lambda \)
  
  \( \text{Varykhalov et al., PRL 2008} \)

- Colossal enhancement of spin-orbit couplings observed in weakly hydrogenated graphene
  
  \( \text{Balakrishnan et al., Nature Phys. 2013} \)
Kane-Mele model: „quantum spin Hall“ (QSH) phase

- **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

Possibility of QSH phase in graphene!
- what happens in (perpendicular) magnetic field?

*Kane & Mele, PRL 2005*

*Konig et al., J. Phys. Soc. Jpn. 2008*
Graphene band structure with SOI and magnetic field

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

  $B=1T: \approx 36 \text{ meV} \quad (l \approx 18 \text{ nm})$

- Also include spin Zeeman energy
  \[ E_Z = g \mu_B B \ll \hbar \omega_c \]

- Exact spinor eigenstates: \textit{parabolic cylinder functions of order} $p$
  
  De Martino, Hütten & Egger, PRB 2011
Homogeneous field: Landau levels

Normalizability: \( p=n=0,1,2,3,\ldots \) → 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 \( \text{Rashba, PRB 2009} \)
- 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 lengthy & not illuminating
- Study fate of QSH phase in the magnetic field for simpler limit $\lambda=0$ : QSH phase for $B=0$
  - Can QSH phase survive time reversal symmetry breaking ($B>0$)?
  - Yang et al., PRL 2011
- Then spin $\sigma$ 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 $\lambda=0$

- 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)

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

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

De Martino, Hütten & Egger, PRB 2011
Edge states: numerical solution

\[ \Delta = 6 \text{meV} > E_z \]

\[ \Delta = 0.3 \text{meV} < E_z \]

\[ B = 15T \]
Stability of QSH phase

- Standard chiral Hall edges recovered for $\Delta=0$
- 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 $\Delta < E_Z$

Both phases similar but with opposite spin current!

*Abanin, Lee & Levitov, PRL 2006*
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