Ground state properties of graphene in Hartree-Fock theory

Mathieu LEWIN

Mathieu.Lewin@math.cnrs.fr

(CNRS & Université de Cergy-Pontoise)

joint work with C. Hainzl (Tuebingen, Germany) & C. Sparber (Chicago, USA)

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Graphene

- Spectrum of non interacting graphene:

Locally, same as 2D massless Dirac operator

\[ v_F \sigma \cdot (-i \nabla) = v_F \sigma \cdot \rho = -iv_F (\sigma_1 \partial_{x_1} + \sigma_2 \partial_{x_2}) := v_F D^0 \]

on \( L^2(\mathbb{R}^2, \mathbb{C}^2) \), with \( \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \), \( \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \), \( v_F \) = effective velocity

The effect of long range interactions

- **Short range interactions**: no effect on shape of excitation spectrum [GM-10]

- **Long range (Coulomb) interactions**: renormalization group (perturbative) methods give effective operator \( v_{\text{eff}}(p) \sigma \cdot p \) with

| Continuous graphene, instantaneous interactions | \( v_{\text{eff}}(p) \sim |p| \rightarrow 0 \log(\Lambda/|p|) \) | [GGV-94,Mish-07] |
| Continuous graphene, retarded interactions | \( v_{\text{eff}}(p) - v_* \sim |p| \rightarrow 0 |p|^\eta \) | [GMP-10] |
| with \( v_* < c \) |  |
| Hubbard model, retarded interactions | \( v_{\text{eff}}(p) - c \sim |p| \rightarrow 0 |p|^\eta \) | [GMP-12] |

- It was also proposed that a gap should open (Peierls instability) through lattice deformations [FL-11,GMP-12]

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Dirac cones reshaped by interaction effects in suspended graphene

D. C. Elias\textsuperscript{1}, R. V. Gorbachev\textsuperscript{1}, A. S. Mayorov\textsuperscript{1}, S. V. Morozov\textsuperscript{2}, A. A. Zhukov\textsuperscript{3}, P. Blake\textsuperscript{3}, L. A. Ponomarenko\textsuperscript{1}, I. V. Grigorieva\textsuperscript{1}, K. S. Novoselov\textsuperscript{1}, F. Guinea\textsuperscript{4*} and A. K. Geim\textsuperscript{1,3}
Effective Hamiltonian

**Most popular model:** Dirac gas with instantaneous Coulomb interactions

\[ H^V = -i v_F \int_{\mathbb{R}^2} \Psi^*(x) \sigma \cdot (\nabla \Psi)(x) \, dx + \int_{\mathbb{R}^2} V(x) \rho(x) \, dx \]

\[ + \frac{1}{2} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} \frac{\rho(x) \rho(y)}{|x - y|} \, dx \, dy \]

- \[ \Psi^*(x) \sigma (y) \tau + \Psi(y) \tau \Psi^*(x) \sigma = 2 \delta(x - y) \delta_{\sigma \tau} \]

- \[ \rho(x) = \frac{1}{2} \sum_{\sigma = 1}^{2} [\Psi^*(x) \sigma, \Psi(x) \sigma] \]

- \[ e^2 / \kappa = \hbar = 1 \text{ where } \kappa = \text{dielectric constant of substrate} \]

**Outline:**

- (HF) ground state when \( V \equiv 0 \)
- (HF) perturbed ground state when \( V \neq 0 \) need to add an ultraviolet cut-off!

Hartree-Fock approximation

- Any state in fermionic Fock space has a density matrix

\[ \gamma(x, y)_{\sigma, \tau} = \langle \Psi(x)_{\sigma}^* \Psi(y)_{\tau} \rangle \]

which is such that \( 0 \leq \gamma \leq 1 \) on \( L^2(\mathbb{R}^2, \mathbb{C}^2) \) (Pauli principle)

- Conversely, to any \( 0 \leq \gamma \leq 1 \), there exists a corresponding preferred state in Fock space, called Hartree-Fock or quasi-free. Its (formal) energy is

\[ \mathcal{E}_{\text{HF}}^V(\gamma) = v_F \text{tr} \, D^0(\gamma - 1/2) + \int_{\mathbb{R}^2} \rho_{\gamma - 1/2}(x) \, V(x) \, dx \]

\[ + \frac{1}{2} \int_{\mathbb{R}^2 \times \mathbb{R}^2} \frac{\rho_{\gamma - 1/2}(x) \, \rho_{\gamma - 1/2}(y) - |(\gamma - 1/2)(x, y)|^2}{|x - y|} \, dx \, dy \]

- The energy diverges like the volume, even with a UV cut-off
- The (formal) minimizer for \( v_F = +\infty \) is the free Dirac/Fermi sea:

\[ \gamma^0 = 1(D^0 \leq 0) \]


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The energy of translation-invariant states for $V \equiv 0$

Let $\mathcal{H}_\Lambda := \{ f \in L^2(\mathbb{R}^2, \mathbb{C}^2) : \text{supp}(\widehat{f}) \subset B(0, \Lambda) \}$ [\Lambda \simeq 0.1 \ \AA^{-1} \text{ in graphene}]

- A translation-invariant HF state on $\mathcal{H}_\Lambda$ has $\gamma = \gamma(p)$ and its density is constant:

$$
\rho_{\gamma_{-1/2}} = \frac{1}{(2\pi)^2} \int_{B(0,\Lambda)} \text{tr}_{\mathbb{C}^2} \left( \gamma(p) - \frac{1}{2} \right) \, dp
$$

**Example:** $\gamma = \gamma^0 = 1(D^0 \leq 0)$, then

$$
\gamma^0(p) - \frac{1}{2} = -\frac{\sigma \cdot p}{2|p|} \implies \rho_{\gamma^0_{-1/2}} \equiv 0
$$

- Using that $|x|^{-1} = |k|^{-1}$, one finds that the energy per unit volume of any translation-invariant HF state $\gamma = \gamma(p)$ with $\rho_{\gamma_{-1/2}} \equiv 0$ is

$$
\mathcal{T}(\gamma) = \frac{1}{(2\pi)^2} \left( v_F \int_{B(0,\Lambda)} \text{tr}_{\mathbb{C}^2} \left( \sigma \cdot p \gamma_{\text{ren}}(p) \right) \, dp - \frac{1}{2} \int_{\mathbb{R}^2} \frac{\gamma_{\text{ren}}(x)^2}{|x|} \, dx \right)
$$

with $\gamma_{\text{ren}} = \gamma - 1/2$
Mean-field operator of interacting Dirac sea

**Proposition (The mean-field operator [HLS12])**

For any $\Lambda, v_F > 0$, define the operator $D^0 = v_F D^0 - \gamma^0_{\text{ren}}(x - y) |x - y|^{-1}$ on $\mathcal{F}_\Lambda$. Then we have

$$D^0 = v_{\text{eff}}(p) \sigma \cdot p \quad \text{with} \quad v_{\text{eff}}(p) = v_F + g \left( \frac{\Lambda}{|p|} \right),$$

$$g(R) = \frac{1}{2\pi} \int_0^\pi \int_0^R \frac{\cos \theta}{\sqrt{r^2 - 2r \cos \theta + 1}} rdr d\theta.$$

The function $g$ is increasing on $[1, \infty)$ and it is such that $g(1) \approx 0.1324$ and $g(r) \sim_{r \to \infty} \log(r)/4$. Since $g > 0$, we have

$$\gamma^0 = 1(D^0 \leq 0).$$

**Idea of proof.** In Fourier space, the second term is

$$- \frac{1}{2\pi} \int_{|k| \leq \Lambda} \frac{\gamma^0_{\text{ren}}(k)}{|p - k|} dk = \sigma \cdot \left( \frac{1}{4\pi} \int_{|k| \leq \Lambda} \frac{k}{|k| |p - k|} dk \middle|_{p g(|p|)} \right).$$

The Dirac sea is the absolute minimizer

\[ h(\nu_F) := \sup_{\text{supp} \hat{\varphi} \subset B_1} \frac{\langle \varphi, |x|^{-1} \varphi \rangle}{\langle \varphi, |p|(\nu_F + g(|p|^{-1}))\varphi \rangle} \]
\[ \leq \frac{1}{\nu_F + g(1)} \sup_{\varphi} \frac{\langle \varphi, |x|^{-1} \varphi \rangle}{\langle \varphi, |p|\varphi \rangle} = \frac{\Gamma(1/4)^2}{2(\nu_F + g(1))\Gamma(3/4)^2} \]

Corollary (The Dirac sea is the absolute minimizer [HLS-12])

If \( \nu_F > h^{-1}(2) \), e.g. \( \nu_F > 2.0560 \), then \( \gamma^0 \) is the unique global minimizer of \( \mathcal{I} \).

Rmk. In massive 3D case [LS-00, HLS-07], \( \gamma^0 \) depends on coupling constant

Proof. Compute with \( F(p) = \gamma(p) - \gamma^0(p) \)

\[ \mathcal{I}(\gamma) - \mathcal{I}(\gamma^0) = \frac{1}{(2\pi)^2} \left( \int_{B(0,\Lambda)} \text{tr}_{C^2} \left( D^0(p) F(p) \right) dp - \frac{1}{2} \int_{\mathbb{R}^2} \frac{|\tilde{F}(x)|^2}{|x|} dx \right) \]

Then \( \text{tr}_{C^2} \left( D^0(p) F(p) \right) \geq \text{tr}_{C^2} \left( |D^0(p)| F(p)^2 \right) \geq h(\nu_F)^{-1} \int_{\mathbb{R}^2} |\tilde{F}(x)|^2 |x|^{-1} dx \)

Now we assume $V \neq 0$

**Theorem (Locally perturbed ground state [HLS-12])**

Assume $\Lambda > 0$ and $v_F > 2.0560$. For any external field $V = \nu \ast |x|^{-1}$ with $\int_{\mathbb{R}^2} |\hat{\nu}(k)|^2 |k|^{-1} \, dk < \infty$, there exists a ground state, that is, a state $\gamma$ which minimizes the relative energy

$$
\gamma \mapsto "E^{V}_{HF}(\gamma) - E^{0}_{HF}(\gamma^0)"
$$

It solves the self-consistent equation

$$
\gamma = 1 \left( v_F \sigma \cdot (-i \nabla) + V + \rho_{\gamma-1/2} * \frac{1}{|x|} - \frac{(\gamma - 1/2)(x, y)}{|x - y|} \leq 0 \right).
$$

on $\mathcal{H}_{\Lambda}$ and it is such that

$$
\text{tr} \left| \mathcal{D}^0 \right| (\gamma - \gamma^0)^2 < \infty, \quad \rho_{\gamma-1/2} \in L^\infty(\mathbb{R}^2), \quad \int_{\mathbb{R}^2} \frac{|\hat{\rho}_{\gamma-1/2}(k)|^2}{|k|} \, dk < \infty.
$$

The unique minimizer is $\gamma^0$ if $V \equiv 0$.

Rmk. We do not know if $\gamma - \gamma^0$ is compact! The state $\gamma$ could live in a non-equivalent Fock representation.
From the self-consistent equation we can formally compute the linear response.

We write

$$\gamma - \gamma^0 = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\eta \left( \frac{1}{D^0 + \cdots + i\eta} - \frac{1}{D^0 + i\eta} \right)$$

$$\implies \hat{\rho}_{\gamma-\gamma^0}(k) = \hat{\rho}_{\gamma-1/2}(k) = -\frac{B(k)}{1 + B(k)} \hat{\nu}(k) + \cdots$$

for some $B(k) \sim \frac{\pi}{4 \log (\frac{\Lambda}{|k|})}$. One gets the universal behavior:

$$\hat{\rho}_{\gamma-1/2}(k) \big|_{|k| \to 0} \sim -\frac{\pi}{4 \log (\frac{\Lambda}{|k|})} \hat{\nu}(k)$$

No long-range screening, but very long range oscillations. Charge in a ball $B_R$:

$$\int_{|x| \leq R} \rho_{\gamma-1/2}(x) \, dx \bigg|_{R \to \infty} \sim -\frac{\pi}{4 \log R} \int_{\mathbb{R}^2} \nu$$
Sketch of proof of Theorem 2

Following [HLS-05], we show that the relative energy is \( \text{wlsc} \), where

\[
\mathcal{E}^V_{\text{HF}}(\gamma) - \mathcal{E}^0_{\text{HF}}(\gamma^0) = \text{tr} D^0 Q - \frac{1}{2} \int \int_{\mathbb{R}^2 \times \mathbb{R}^2} \frac{|Q(x, y)|^2}{|x - y|^2} - D(\nu, \rho_Q) + \frac{1}{2} D(\rho_Q, \rho_Q)
\]

and \( Q = \gamma - \gamma^0 \).

Since

\[
\text{tr} D^0 Q = \text{tr} |D^0| (Q^{++} - Q^{--}) \geq \text{tr} |D^0| Q^2,
\]

where \( Q^{--} := \gamma^0 Q \gamma^0 \) and so on, the natural topology for \( Q \) is \( |D^0|^{1/2} Q^{\pm \pm} |D^0|^{1/2} \in \mathcal{G}_1 \) and \( |D^0| Q \in \mathcal{G}_2 \). This controls \( D(\rho_Q, \rho_Q) \).

We write

\[
\text{tr} |D^0| (Q^{++} - Q^{--}) = \text{tr} \left( |D^0| - (v_F + g(1)) |p| \right) (Q^{++} - Q^{--})
\]

\[\geq 0\]

\( \text{wlsc} \)

\[+(v_F + g(1)) \text{ tr} |p| (Q^{++} - Q^{--})\]

Sketch of proof of Theorem 2

Lemma (Weak lower semi-continuity)

\[\text{If } Q_n \rightharpoonup Q \text{ in the sense that } |\mathcal{D}^0| Q_n \rightharpoonup |\mathcal{D}^0| Q \text{ weakly in } \mathfrak{S}_2 \text{ and } \begin{align*}
|\mathcal{D}^0|^{1/2} Q_n^{\pm \pm} |\mathcal{D}^0|^{1/2} & \rightharpoonup |\mathcal{D}^0|^{1/2} Q^{\pm \pm} |\mathcal{D}^0|^{1/2} \text{ weakly-}* \text{ in } \mathfrak{S}_1, \end{align*} \text{ then for } \nu_F > 2.0560 \]

\[\liminf_{n \to \infty} \left( \text{tr} |p| (Q_n^{++} - Q_n^{--}) - \frac{1}{2(v_F + g(1))} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} |Q_n(x, y)|^2 \frac{1}{|x - y|} \, dx \, dy \right) \geq \text{tr} |p| (Q^{++} - Q^{--}) - \frac{1}{2(v_F + g(1))} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} \frac{|Q(x, y)|^2}{|x - y|} \, dx \, dy, \]

Proof goes by localizing \( Q_n \) in and outside of a fixed ball, and then using the strong CV inside and Hardy’s inequality outside. Main difficulty: no mass!

Lemma (Localization [LL-10,HLS-12])

\[\text{Let } 0 \leq \gamma \leq 1 \text{ with } \text{tr} |p| \gamma < \infty. \text{ Then for a smooth partition of unity } \chi^2 + \eta^2 = 1, \]

\[\text{tr} |p| \gamma \geq \text{tr} |p| \chi \gamma \chi + \text{tr} |p| \eta \gamma \eta \]

\[-c (\text{tr} |p| \gamma)^{1/2} \left( ||\nabla \chi||^2_{L^2} + ||\nabla \eta||^2_{L^2} \right)^{1/2} \left( ||\nabla \chi||^2_{L^4} + ||\nabla \eta||^2_{L^4} \right)^{1/2}.\]

Conclusion & Perspectives

► Conclusion:
  - Identified the ground state of graphene in a non-perturbative regime
  - Found the expected logarithmic divergence of the effective Fermi velocity
  - Shown the existence of bound states in a local external electric field
  - Linear response suggests that there are very long range oscillations, but no screening

► Perspectives:
  - Better understanding of the best constant $h(v_F)$ in Hardy-like inequality
  - Conductivity
Thematic trimester from April 15 to July 12, 2013, organized by Maria J. Esteban & Mathieu Lewin

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