Quantum Monte Carlo study of the renormalization of the Fermi velocity in graphene

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INTRODUCTION
The Effect

Dirac cones reshaped by interaction effects in suspended graphene

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[Nature 7, 701 (2011)]

Graphene: Dirac fermions in 2+1D with strong ($\alpha>1$) Coulomb interaction.

Logarithmic divergence of the Fermi velocity near the Dirac points.

Theoretical predictions:
J. Gonzalez, F. Guinea, M. Vozmediano,
Motivation: Experiment vs theory (1)

Graphene: large $\alpha$ theory. Some approximations are needed

a) one-loop RPA:

b) one-loop bare Coulomb

$$\frac{v^*_F}{v_F} = 1 + \frac{\alpha}{4} \ln \frac{\Lambda}{k}$$

c) two loop + GR:

d) one-loop screened Coulomb

“intrinsic graphene”: there is fitting parameter $\varepsilon_G$

e) various variants of screened Coulomb+RPA


Squares: experiment [Èlias et al, Nature 7, 701 (2011)]
Motivation: Experiment vs theory (2)


- For suspended graphene:
  - Experimental data of Ref. 4
  - $v_F^*$ at $E_F$ (bare self-screening)
  - $v_F^*$ at $E_F$ (self-consistent self-screening)
  - $v_F^*(n)$ for $E_F=0$ (with $\omega/\epsilon_{\text{RPA}}$)

- For hBN-encapsulated graphene:
  - Experimental data of Ref. 8
  - $v_F^*$ at $E_F$ in $K\Gamma$-direction
  - $v_F^*$ at $E_F$ in KM-direction
  - $v_F^*(n)$ for $E_F=0$ in KM-direction

Low precision for suspended graphene

Still can not be incorporated in present approximations
Motivation: short-range interaction (1)

Role of short-range interactions in low-energy effective field theory


\[ L = L_0 - ia_0 \sum_\sigma \bar{\Psi}_\sigma \gamma_0 \Psi_\sigma + a_0 \frac{|\nabla|}{2e^2} a_0 + \sum_{x=d,c,f,a} L_x \]

\[ L_x = g_x (\sum_\sigma w_{x,\sigma} \bar{\Psi}_\sigma M_x \Psi_\sigma)^2 + \tilde{g}_x \sum_{\mu=3,5} (\sum_{\sigma \pm 1} w_{x,\sigma} \bar{\Psi}_\sigma M_x \gamma_1 \gamma_\mu \Psi_\sigma)^2 \]

Functions of on-site and the nearest-neighbour interactions


\[ \langle \bar{\Psi} \Psi \rangle \neq 0 \]

\[ \mathcal{L}_4 = \frac{G}{2} (\bar{\Psi}_a \Psi_a)^2 \]

\[ \tilde{g} = G \Lambda / \pi \]

\[ \langle \bar{\Psi} \Psi \rangle = 0 \]
Motivation: short-range interaction (2)

One-loop lattice perturbation theory (LPT)

Fitting with logarithm: coefficient before log is untouched, while cutoff changes noticeably
Motivation: proximity to the phase transitions


Extended Hubbard model on hexagonal lattice [P. Buividovich, D. Smith, M. Ulybyshev, L. von Smekal arXiv:1807.07025, PRB 98, 235129 (2018); See the talk by D. Smith]
Previous attempts to make lattice calculations


BSS-QMC was used (see the plenary talk with the comparison of the algorithms): $N_s^3 N_t$ scaling instead of $(N_s N_t)^{5/4} \ldots 4/3$ scaling of HMC. Maximal lattice size was 15x15. Authors could not get close enough to the Dirac point, but studied the behavior of the Fermi Velocity in the vicinity of the AFM phase transition at large $k$. 

![Graph showing the results for different short-range simulations.](Image)

![Graph showing the results for different long-range simulations.](Image)

![Graph showing the results for different onsite Hubbard model calculations.](Image)
METHODS
Lattice setup for calculations

Standard HMC on GPUs (some algorithmic improvements)
102x102 hexagonal lattice, \( N_t = 160, \beta = 43 \) (in the units of hopping)

1) Graphene on substrate (reduced long-range tail)
2) Graphene on substrate (reduced long-range tail) + modification of short-range Coulomb couplings \( (V_{01} \text{ and } V_{02}) \) (easier to manipulate in experiment?)
3) Suspended graphene

Algorithms:
M. Ulybyshev, P. Buividovich, M. Katsnelson, M. Polikarpov
arXiv:1304.0660,
PRL 111, 056801 (2013);
D. Smith, L. von Smekal,
arXiv: 1403.3620,
PRB 89, 145429 (2014)
Observables

Euclidean correlator in momentum space:

\[
C'(\tau) = \sum_{x,y} \text{Tr} \left( \hat{a}_x^\dagger \bar{\psi}(x) e^{-\tau \hat{H}} \hat{a}_y \psi(y) e^{-(\beta-\tau) \hat{H}} \right)
\]

\[
\text{(x)} \quad \text{representing the single-particle wavefunctions for the free electrons in the vicinity of Dirac points.}
\]

The extraction of the dispersion relation from these correlators can be done in several ways:

1) simple exponential fit with the function \( \cosh \left( \frac{E}{2\tau} \right) \);
2) More sophisticated approaches using analytical continuation from imaginary to real time which include the maximum entropy method (MEM) and the Backus-Gilbert method [A8]. We are going to use all of these algorithms in order to check if the results are in agreement with each other.

A comparison of the profiles for \( v_F \) renormalization for different short-range potentials, constructed similar to Fig. 3b will allow us to

K-K and K-K' lines in order to check warping effects
Analytical continuation (1)


MEM is better than BG in reconstruction of sharp features, but prone to generation of fake peaks at smaller energies.
Analytical continuation (2)

1) Stochastic MEM [K. S. D. Beach, arXiv:cond-mat/0403055]. Central idea: mapping between analytical continuation and thermal average over some system of interacting classical fields. Exact fitting – ground state, MEM – mean-field solution, thus reduction of "fake" fluctuations due to full thermal averaging.

\begin{align*}
mapping \phi : \mathbb{R} \rightarrow [0, 1] \quad \phi(\omega) &= \frac{1}{N} \int_{-\infty}^{\omega} d\nu \, D(\nu) \\
n(x) &= \frac{A(\phi^{-1}(x))}{D(\phi^{-1}(x))} \\
H[n(x)] &= \int_0^\beta \frac{d\tau}{\sigma(\tau)^2} \left| \int_0^1 dx \, \hat{K}(\tau, x)n(x) - \bar{G}(\tau) \right|^2 \\
\langle n(x) \rangle &= \frac{1}{Z} \int \mathcal{D}n \, n(x) e^{-\alpha H[n]} \\
\langle A(\omega) \rangle &= \langle n(\phi(\omega)) \rangle D(\omega)
\end{align*}

2) Simple fit with "discretized exponents" \((1.0-\delta E)^t\) in order to get average over several peaks.
RESULTS
Check against LPT

- For $U_0 = 0.05, \gamma = 2.1447^3$
  - $\Lambda = 2.130 \pm 0.092$
  - $C = 0.0072275 \pm 0.0000941$

- For $U_0 = 0.10, \gamma = 2.1447^3$
  - $\Lambda = 2.087 \pm 0.127$
  - $C = 0.0146203 \pm 0.0003226$

- For $U_0 = 0.15, \gamma = 2.1447^3$
  - $\Lambda = 2.447 \pm 0.154$
  - $C = 0.0196604 \pm 0.0004023$

- For $U_0 = 0.20, \gamma = 2.1447^3$
  - $\Lambda = 1.802 \pm 0.066$
  - $C = 0.0297867 \pm 0.0003840$

+ Fix the cutoff in RPA approximation
Examples of Euclidean correlators (1)

\[ T = 2.315 \times 10^{-2}, \quad U_0 = 3.4, \quad \text{MOD}, \quad \gamma = 1.55452, \quad L = 102, \quad N_t = 160 \]
Examples of Euclidean correlators (2)

$T=2.315e-02$, $U_0=3.4$, $\gamma=2.14473$, $L=102$, $N_t=160$
Graphene on substrate: reduced long-range tail + increased short-range Coulomb (1)
Graphene on substrate: reduced long-range tail + increased short-range Coulomb (1)

T=2.315e-02, U₀=3.4, MOD, γ=1.55452, L=102, Nₜ=160

Spectral function at the Dirac point: proximity to AFM phase transition (similar to Hubbard-Coulomb model on square lattice)?
Graphene on substrate: reduced long-range tail + increased short-range Coulomb (1)

QMC $U_0 = 3.44$, MOD $\gamma = 1.55452$

$\Lambda = 2.496 \pm 0.517$

$C = 0.2030897 \pm 0.0110941$

KK line

KK' line

KK fit $C \ast \ln(\Lambda/k)$
Graphene on substrate: reduced long-range tail (1)
Graphene on substrate: reduced long-range tail (2)

Comparison of the spectral functions at the Dirac point
Graphene on substrate: effect of short-range Coulomb interactions

$$\left( \frac{V_f \text{renorm} - V_f \text{free}}{V_f_0} \right)$$

Exponential fit

$$QMC \ U_0=3.44, \ \gamma=1.55452$$

KK line

KK’ line

KK fit $$C_1*\ln(\Lambda_1/k)$$

$$QMC \ U_0=3.44, \ \text{MOD}, \ \gamma=1.55452$$

KK line

KK’ line

KK fit $$C_2*\ln(\Lambda_2/k)$$

Exponential fit

(k-K) [Å⁻¹]
Graphene on substrate: comparison with RPA and LPT

\[ \frac{(V_f_{\text{renorm}} - V_f_{\text{free}})}{V_f_0} \]

- \( QMC U_0 = 3.44, \gamma = 1.55452 \)
- \( \Lambda = 2.445 \pm 0.277 \)
- \( C = 0.1836326 \pm 0.0057527 \)

**KK line**

\[ KK \text{ line} \]

**KK' line**

\[ KK' \text{ line} \]

**KK fit**

\[ C \ast \ln(\Lambda/k) \]

**RPA**

**LPT**

**Exponential fit**

\[ \exp(-k-k') \]
Quite strong scattering on some collective excitations (enhanced by the long-range Coulomb)
Decreasing role of on-site interaction: We go away from AFM transition.
Suspended graphene (3): only lower branch

Experimental data:

- QMC $U_0 = 3.44$, $\gamma = 2.14473$
- KK line
- KK' line

The bare interaction for $\alpha = 0$, $\omega = 0$, $v_F = 0$, $\Lambda = 75\,\text{Å}$, $\tilde{e} = 1$, $\tilde{\epsilon} = 5$, $\tilde{h} = 10$, $\tilde{a} = 10$, $\tilde{q} = 10$, $\tilde{t} = 10$, $\tilde{\alpha} = 1$, $\tilde{\epsilon} = 0$, $\tilde{\alpha} = 0.2$, $\tilde{\alpha} = 0.5$, $\tilde{\alpha} = 1.0$, $\tilde{\alpha} = 2.0$, $\tilde{\alpha} = 4.0$, $\tilde{\alpha} = 9.0$, $\tilde{\alpha} = 0.1$, $\tilde{\epsilon} = 0.05$ for suspended graphene with $\tilde{t} = 0.05$ for suspended graphene with $\Lambda = 10$ eV and $\tilde{h} = 6$ eV, respectively, $\tilde{u} = 3.44$, $\tilde{t} = 2.14473$ as mentioned in the introduction. This compares well with the usual argument of fixing $\epsilon_0$ and $\alpha_0$ by conserving the total number of states in the Brillouin zone when compared to the tight-binding model.

$\omega = 0$ and $\epsilon_0 = 0$ are obtained, but agrees well with the usual argument of fixing $\epsilon_0$ and $\alpha_0$. The precise value of $\alpha = 0$.

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Summary

1) RPA approximation is indeed an improvement in comparison with one-loop corrections to Fermi velocity, but RPA still deviates quite substantially from the Monte Carlo data. Test of another approximations is needed?

2) Short-range interactions influence the numbers even at small momenta, but this influence is limited.

3) We observe the effects of proximity to the AFM transition in the spectral function at the Dirac point

4) Strong scattering at $E \sim 0.3 \ldots 0.4 \kappa$, which is definitely connected to the long-range Coulomb tail. More detailed predictions for experiment?