Tight-binding model of graphene with Coulomb interactions

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Dedicated to the memory of Professor Mikhail Polikarpov

Introduction

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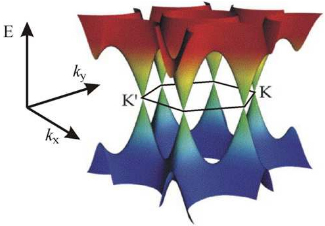
Many properties of graphene are well understood in extreme weak coupling limit.

$$H = \sum_{\langle x,y \rangle, s} (-\kappa)(a^\dagger_{x,s} a_{y,s} + a^\dagger_{y,s} a_{x,s}) \quad , \ \{a_\mu, a_\nu\} = \{a^\dagger_\mu, a^\dagger_\nu\} = 0 \quad , \ \{a^\dagger_\mu, a_\nu\} = \delta_{\mu\nu}$$

- Well described by tight-binding theory.
- Conical dispersion at low energies.
- Low energy effective Dirac theory.
- Van Hove singularity at saddle points.
- Semi-metallic behavior (no band gap).
- ...



Include electromagnetic interaction: Low energy theory becomes QED_{2+1}.

Simulated with staggered Fermions.

Drut, Lähde, Phys.Rev.Lett. 102, 026802 (2009)

Armour, Hands, Strouthos, Phys.Rev.B81:125105, 2010

Buividovich et al. (ITEP), Phys. Rev. B 86 (2012), 045107

Presently: Go beyond low energies. $\rightarrow$ **Simulate hexagons directly**.

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First derivation of path-integral for hexagonal lattice: — Brower,Rebbi,Schaich, PoS(Lattice 2011)056

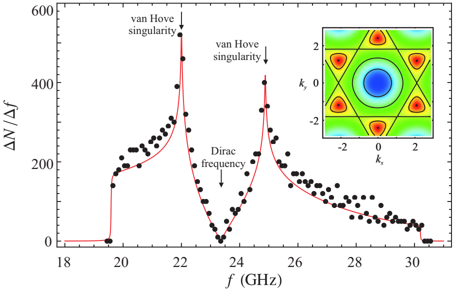
Currently:

- Tight-binding with gauge-links. — Buividovich, Polikarpov, Phys. Rev. B 86 (2012) 245117
- **Tight-binding with instantaneous interactions.** — Ulybyshev et al. (ITEP), arXiv:1304.3660

Our goal: Investigate effect of interactions on Van Hove singularity.

Dietz,Smekal et al. arXiv:1304.4764

Status: CUDA code operational and producing. Plausibility checks (find α_c) and cross-checks (ITEP).



Outline

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- Interacting tight-binding model with normal-ordering terms (non-compact Hubbard field).
- Introducing the compact Hubbard field $\longrightarrow$ **results**.
- Improved Fermion discretization (ITEP) $\longrightarrow$ **comparison**.

Interacting tight-binding theory

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Since $v_F \approx c/300 \ll c$, model interactions by non-local potential (Brower et al.):

$$H = \sum_{\langle x,y\rangle,s} (-\kappa)(a^\dagger_{x,s}a_{y,s} + a^\dagger_{y,s}a_{x,s}) + \sum_{x,y} e^2\, q_x V_{xy} q_y \ , \quad q_x = a^\dagger_{x,1}a_{x,1} + a^\dagger_{x,-1}a_{x,-1} - 1$$

Introduce hole operators $b^\dagger_x, b_x$ for spin -1 particles:

$$b^\dagger_x = a_{x,-1}\ ,\ b_x = a^\dagger_{x,-1}\ ,\ a^\dagger_x = a^\dagger_{x,+1}\ ,\ a_x = a_{x,+1} \qquad \longrightarrow \qquad q_x = a^\dagger_x a_x - b^\dagger_x b_x\ .$$

Apply normal ordering $\rightarrow$ extra term from potential. Flip sign of $b^\dagger_x, b_x$ on one sub-lattice.

$$H = \sum_{\langle x,y\rangle,s} (-\kappa)(a^\dagger_x a_y + b^\dagger_y b_x + \mathrm{h.c.}) + \sum_{x,y} e^2 :q_x V_{xy} q_y: + \sum_x e^2 V_{xx}(a^\dagger_x a_x + b^\dagger_x b_x)$$

Add “staggered” mass to break-sublattice symmetry:

$$H \rightarrow H + \sum_x m_S(a^\dagger_x a_x + b^\dagger_x b_x) \quad (m_S \pm m, x \in A, B)$$

Functional-integral for interacting theory

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Factor the exponential: $e^{-\beta H} \approx e^{-\delta H} e^{-\delta H} \dots e^{-\delta H}$ $\qquad \delta = \beta / N_t$.

Express partition function using **coherent states** $|\psi_t, \eta_t\rangle$, $\langle \psi_t, \eta_t|$:

$$\mathrm{Tr}\, e^{-\beta H} = \int \prod_{t=0}^{N_t - 1} \left[\prod_x d\psi^*_{x,t}\, d\psi_{x,t}\, d\eta^*_{x,t}\, d\eta_{x,t} \right] \; e^{-\sum_x (\psi^*_{x,t+1}\psi_{x,t+1} + \eta^*_{x,t+1}\eta_{x,t+1})} \langle \psi_{t+1}, \eta_{t+1} | e^{-\delta H} | \psi_t, \eta_t \rangle \; .$$

Using $\langle \xi | F(a^\dagger_\lambda, a_\lambda) | \xi' \rangle = F(\xi^*_\lambda, \xi'_\lambda)\, e^{\sum_\lambda \xi^*_\lambda \xi'_\lambda}$, obtain

$$\mathrm{Tr}\, e^{-\beta H} = \int \prod_{t=0}^{N_t - 1} \left[\prod_x d\psi^*_{x,t}\, d\psi_{x,t}\, d\eta^*_{x,t}\, d\eta_{x,t} \right] \exp \Bigg\{ -\delta \Bigg[\sum_{x,y} e^2 Q_{x,t+1,t} V_{xy} Q_{y,t+1,t}$$

$$- \sum_{\langle x,y \rangle} \kappa (\psi^*_{x,t+1}\psi_{y,t} + \psi^*_{y,t+1}\psi_{x,t} + \eta^*_{y,t+1}\eta_{x,t} + \eta^*_{x,t+1}\eta_{y,t}) + \sum_x m_S (\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t})$$

$$+ \sum_x e^2 V_{xx} (\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t}) \Bigg] - \sum_x \left[\psi^*_{x,t+1}(\psi_{x,t+1} - \psi_{x,t}) + \eta^*_{x,t+1}(\eta_{x,t+1} - \eta_{x,t}) \right] \Bigg\} \; .$$

where $Q_{x,t,t'} = \psi^*_{x,t}\psi_{x,t'} - \eta^*_{x,t}\eta_{x,t'}$. Antiperiodic in time! **Leading error is $\mathcal{O}(\delta)$.**

The Hubbard field

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Hubbard-Stratonovich transformation eliminates fourth powers:

$$\exp\left(-\delta e^2 \sum_{x,y} Q_{x,t+1,t} V_{xy} Q_{y,t+1,t}\right) = [\det(\ldots)]^{1/2}$$

$$\times \int \prod_x \left[\prod_{t=0}^{N_t-1} d\phi_{x,t}\right] \exp\left(-\frac{\delta}{4}\sum_{t=0}^{N_t-1}\sum_{x,y}\phi_{x,t}V_{xy}^{-1}\phi_{y,t} - i\,e\,\delta\sum_{t=0}^{N_t-1}\sum_x \phi_{x,t}Q_{x,t+1,t}\right).$$

Gaussian integral can be carried out to obtain Fermion determinant

$$\mathrm{Tr}\, e^{-\beta H} = \int \left[\prod_{t=0}^{N_t-1}\prod_x d\phi_{x,t}\right] \exp\left\{-\frac{\delta}{4}\sum_{t=0}^{N_t-1}\sum_{x,y}\phi_{x,t}V_{xy}^{-1}\phi_{y,t}\right\} \left|\det\left(M + ie\frac{\beta}{N_t}\phi_{x,t}\delta_{xy}\delta_{t-1,t'}\right)\right|^2$$

$$M_{(x,t)(y,t')} = \delta_{xy}(\delta_{tt'} - \delta_{t-1,t'}) - \frac{\beta}{N_t}\kappa\sum_{\vec{n}}\delta_{y,x+\vec{n}}\delta_{t-1,t'} + \frac{\beta}{N_t}m_S\delta_{xy}\delta_{t-1,t'} + \frac{\beta}{N_t}e^2 V_{xx}\delta_{xy}\delta_{t-1,t'}$$

Suitable for HMC simulations! No sign problem!

Hybrid Monte-Carlo for non-compact Hubbard field

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Force terms for Hubbard field ϕ and momentum p:

$$\frac{d}{d\tau}\phi_{x,t} = p_{x,t}\,, \quad -\frac{d}{d\tau}p_{x,t} = \frac{\beta}{2N_t}(V^{-1}\phi)_{x,t} - 2\frac{\beta}{N_t}e\,\mathrm{Im}\left(\chi^*_{x,t+1}(B^{-1}\chi)_{x,t}\right)$$

Order parameter for sub-lattice symmetry breaking (“chiral condensate”)

$$\langle\Delta_N\rangle = \mathrm{Tr}\left[\widehat{\Delta}_N e^{-\beta H}\right] \qquad \left(B = M + ie\frac{\beta}{N_t}\phi_{x,t}\delta_{xy}\delta_{t-1,t'}\right)$$

$$= \frac{1}{ZN_t}\int \mathcal{D}\psi\mathcal{D}\psi^*\mathcal{D}\eta\mathcal{D}\eta^*\left[\sum_{x_A,t}\left(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t}\right) - \sum_{x_B,t}\left(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t}\right)\right]e^{-\beta H}$$

$$= \frac{-1}{\beta Z}\int\mathcal{D}\phi\left[\frac{\partial}{\partial m}\det\left(BB^\dagger\right)\right]e^{-S[\phi]} = \frac{-2}{\beta Z}\int\mathcal{D}\phi\det\left(BB^\dagger\right)\mathrm{Re\,Tr}\left(B^{-1}\frac{dB}{dm}\right)e^{-S[\phi]}$$

$$= \frac{-2}{N_t}\sum_{t=0}^{N_t-1}\langle\sum_{x\in A}B^{-1}_{(x,t+1)(x,t)} - \sum_{x\in B}B^{-1}_{(x,t+1)(x,t)}\rangle$$

Doesn’t work (no symmetry breaking)! **Why??**

The compact Hubbard field

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No sub-lattice symmetry breaking observed. Possible reason: Non-compact Hubbard field ϕ in Fermion determinant (thanks Maksim Ulybyshev!)

The determinant of $\left(M + ie\frac{\beta}{N_t}\phi_{x,t}\delta_{xy}\delta_{t-1,t'}\right)$ is $\sim \phi^V \longrightarrow$ uncontrollable errors from floating point rounding.

Solution: Use **compact** Hubbard field instead!

Brower,Rebbi,Schaich, PoS(Lattice 2011)056

Replacement: $\left(\frac{\beta}{N_t}e^2 V_{xx}\delta_{xy}\delta_{t-1,t'} + ie\frac{\beta}{N_t}\phi_{x,t}\delta_{xy}\delta_{t-1,t'}\right) \longrightarrow \exp\left(ie\frac{\beta}{N_t}\phi_{x,t}\right)\delta_{xy}\delta_{t-1,t'}$

Changes Fermion force term:

$$-\frac{d}{d\tau}p_{x,t} = \frac{\beta}{2N_t}(V^{-1}\phi)_{x,t} - 2\frac{\beta}{N_t}e\,\mathrm{Im}\left(\chi^*_{x,t+1}\exp\left(ie\frac{\beta}{N_t}\phi_{x,t}\right)(B^{-1}\chi)_{x,t}\right)$$

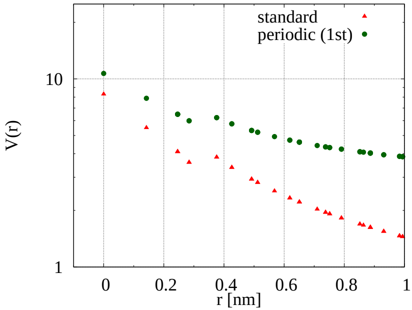
Sub-lattice symmetry breaks!

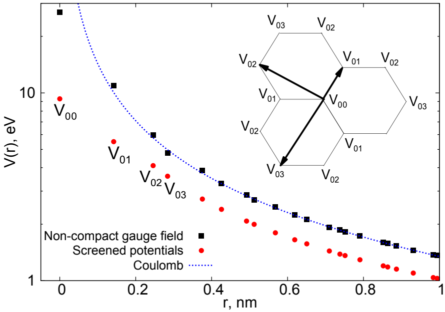
The potential

Constructed piecewise: Constrained random phase approximation (cRPA) at short distances (Wehling et al. PRL 106, 236805 (2011)), Coulomb otherwise. Corrected for periodic boundary (one image in each direction). **Differs from ITEP.**

$$e^2 V(r) = \begin{cases} V_{00}, V_{01}, V_{02}, V_{03} & : r \leq 2a \\ e^2/r & : r > 2a \end{cases}$$

Ulybyshev et al. (ITEP), arXiv:1304.3660





Results

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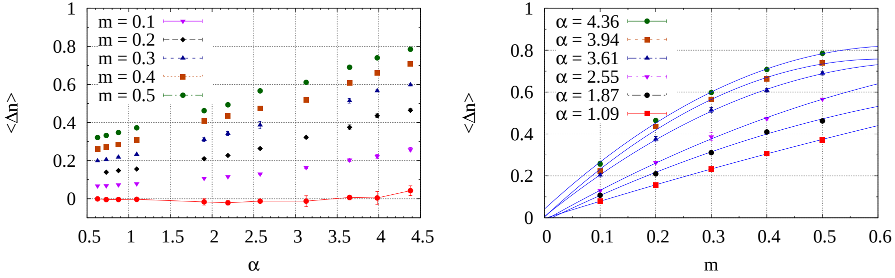
Simulating at $\beta = 2.0$ on $N_x = 6$. Extrapolating $N_t \to \infty$ from $N_t = 8, 10, 12, 14, 16$. Several hundreds of independent measurements for each set (N_t, α, m).



Limit $m \to 0$ from $\langle \Delta_N \rangle = a_0 + a_1 m + a_2 m^2$. Probably large finite-volume errors! (In progress: Improve V_{xy}^{-1} computation $\to$ larger N_x will be feasible.)

Improved discretization

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Error of standard Fermion operator is $\mathcal{O}(\delta)$. Strategy for improvement: **split Hamiltonian** (ITEP).

$$\mathrm{Tr}\, e^{-\beta H} \approx Tr\left[e^{-\beta H_{TB}} e^{-\beta H_C}\right] = \int \left[\prod_{t=0}^{2N_t-1} \prod_x d\psi^*_{x,t}\, d\psi_{x,t}\, d\eta^*_{x,t}\, d\eta_{x,t}\right]$$

$$\times \left\{ \prod_{t=0}^{N_t-1} e^{-\sum_x (\psi^*_{x,2t}\psi_{x,2t}+\eta^*_{x,2t}\eta_{x,2t}+\psi^*_{x,2t+1}\psi_{x,2t+1}+\eta^*_{x,2t+1}\eta_{x,2t+1})}\right.$$

$$\left. \times \langle \psi_{2t}, \eta_{2t} | e^{-\delta H_{TB}} | \psi_{2t+1}, \eta_{2t+1} \rangle \langle \psi_{2t+1}, \eta_{2t+1} | e^{-\delta H_C} | \psi_{2t+2}, \eta_{2t+2} \rangle \right\} .$$

Leads to 2nd-order Fermion action:

$$S_F[\phi] = \sum_{t=0}^{N_t-1} \left[\sum_x \psi^*_{x,2t} \left(\psi_{x,2t} - \psi_{x,2t+1}\right) - \delta\, \kappa \sum_{<x,y>} \left(\psi^*_{x,2t}\psi_{y,2t+1} + \psi^*_{y,2t}\psi_{x,2t+1}\right)\right.$$

$$\left. + \sum_x \psi^*_{x,2t+1} \left(\psi_{x,2t+1} - e^{-i\delta\, \phi_{x,t}} \psi_{x,2t+2}\right) + \delta \sum_x \pm m \psi^*_{x,2t}\psi_{x,2t+1} \right] .$$

Improved discretization (II)

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Improved Fermion matrix:

$$M_{(x,t)(y,t')} = \begin{cases} \delta_{xy}(\delta_{tt'} - \delta_{t+1,t'}) - \frac{\beta}{N_t}\kappa \sum_{\vec{n}} \delta_{y,x+\vec{n}}\delta_{t+1,t'} + \frac{\beta}{N_t} m_S \delta_{xy}\delta_{t+1,t'} & : t \text{ even} \\ \delta_{xy}\delta_{tt'} - \delta_{xy}\delta_{t+1,t'} \exp(-i\frac{\beta}{N_t} e \phi_{x,(t-1)/2}) & : t \text{ odd} \end{cases}$$

Hubbard field only on odd timeslices!

HMC force: $-\frac{d}{d\tau} p_{x,k} = \frac{\beta}{2N_t}(V^{-1}\phi)_{x,k} - \frac{2\beta}{N_t} e \,\mathrm{Im}\left(\chi^*_{x,2k+1} \exp\left(i\frac{\beta}{N_t} e \phi_{x,k}\right)(M^{-1}\chi)_{x,2k+2}\right)$

Order parameter:

$$\langle \Delta_N \rangle \propto \int \mathcal{D}\psi\mathcal{D}\psi^*\mathcal{D}\eta\mathcal{D}\eta^* \left[\sum_{X_A,t}\left(\psi^*_{x,2t}\psi_{x,2t+1} + \eta^*_{x,2t}\eta_{x,2t+1}\right) - \sum_{X_B,t}\left(\psi^*_{x,2t}\psi_{x,2t+1} + \eta^*_{x,2t}\eta_{x,2t+1}\right)\right] e^{-\beta H}$$

$$= \frac{-1}{\beta Z}\int \mathcal{D}\phi \left[\frac{\partial}{\partial m} \det\left(MM^\dagger\right)\right] e^{-S[\phi]} = \frac{-2}{N_t}\sum_{t=0}^{N_t-1}\langle \sum_{x\in A} M^{-1}_{(x,2t)(x,2t+1)} - \sum_{x\in B} M^{-1}_{(x,2t)(x,2t+1)}\rangle$$

Operator inserted only on even timeslices! Perhaps a problem...

Comparison

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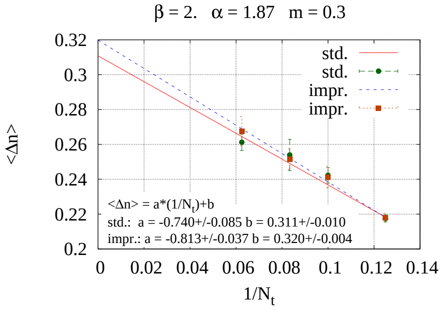
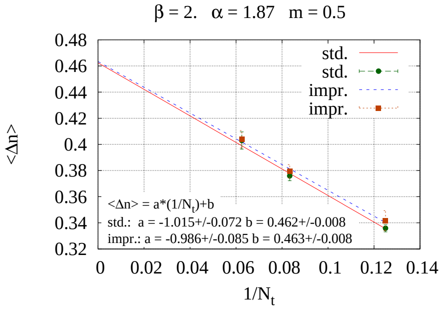
$N_t \to \infty$ extrapolation for naive and improved Fermion operators.

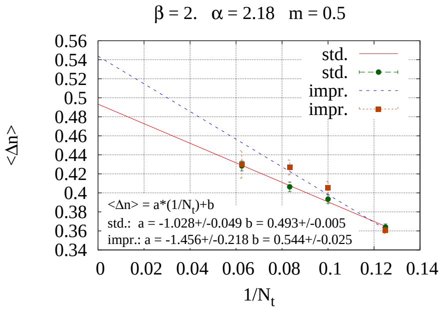


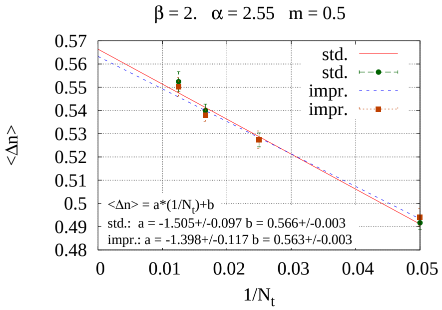


Within errors no difference. $\mathcal{O}(\delta)$ behavior in both cases. Reason currently unknown. Coulomb energy shows similar behavior.

Comparison (II)

Similar results for different α. Self-consistency is confirmed, but no improvement...





Conclusion: Much work ahead.