Graphene physics within the Hubbard model

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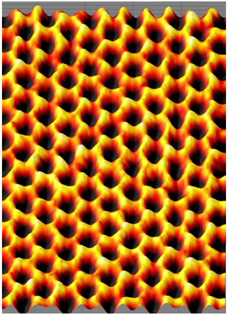
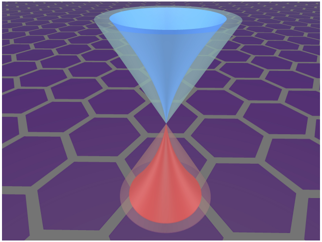
ITEP Lattice



(a) Full spectrum

$\Longrightarrow$



(b) Dirac cones free/reshaped

$$E(\vec{k}) = v_F|\vec{k} - \vec{k}_F|, \text{ where } v_F \sim 1/300.$$

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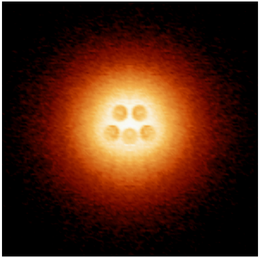
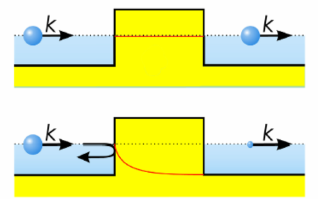
- Low energy excitations — massless 4-component Dirac fermions $\Longrightarrow$ playground to study various quantum relativistic effects — "CERN on ones desk": relativistic collapse at a supercritical charge, Klein tunnelling, etc.



(a) An artificial atomic nucleus made up of five charged calcium dimers is centered in an atomic-collapse electron cloud.



(b) Klein tunnelling: ultrarelativistic and nonrelativistic cases.

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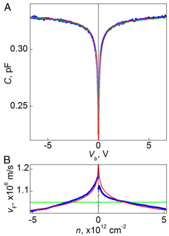

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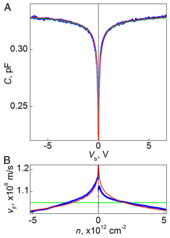

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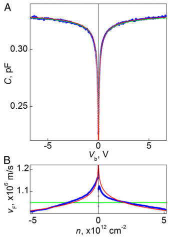

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- Analytically (at least in the high ϵ limit).

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2. But the linear spectrum approximation sometimes leads to nasty divergences.
3. Moreover, the bare interaction deviates from the Coulomb law dramatically at small distances (due to σ-electrons screening that were not accounted we modify only 3 nearest potentials), this deviation *plays the crucial role* in shifting the phase transition ϵ value to non-physical $\epsilon \sim 0.7$ and other properties.

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Supercomputer simulations within the Hubbard model became a fruitful and developing approach for getting non-perturbative results. This is why it is extremely important to explore it analytically in order *to check HMC simulations* and explain some observations.

Hamiltonian

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We start from a pretty-simple Hubbard Hamiltonian

$$\hat{H} = \underbrace{-\kappa \sum_{(x,y),\sigma} \left(\hat{a}^\dagger_{\sigma,\,x}\hat{a}_{\sigma,\,y} + \hat{a}^\dagger_{\sigma,\,y}\hat{a}_{\sigma,\,x}\right) \pm m \sum_{x} \hat{a}^\dagger_{\sigma,\,x}\hat{a}_{\sigma,\,x}}_{\text{tight binding}} + \underbrace{\frac{1}{2}\sum_{x,y} V(x,y)\hat{q}_x\hat{q}_y}_{\text{interaction}},$$

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2. massive term, explicitly breaking the sublattice "chiral" symmetry — used in simulations (that's why we have to keep it) to avoid zero eigenvalues,
3. the electrostatic instantaneous interaction (must be a Coulomb law screened at small distances to accound σ-electrons).

Partition function

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After applying the Hubbard-Stratonovich transformation to decompose the four-fermion interaction term, the partition function becomes:

$$\mathcal{Z} = \int \mathcal{D}\varphi\, \mathcal{D}\bar{\eta}\mathcal{D}\eta\, \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-\mathcal{S}_{em}(\varphi) - \sum\limits_{\sigma,x,y} \bar{\eta}(x)\mathcal{M}_{x,y}(\varphi)\eta(y) - \sum\limits_{\sigma,x,y} \bar{\psi}(x)\bar{\mathcal{M}}_{x,y}(\varphi)\psi(y)},$$

where $\mathcal{M}_{l_1,l_2,\sigma}(x,y)$ is some (nasty-looking) fermion action matrix.

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where $\mathcal{M}_{l_1,l_2,\sigma}(x,y)$ is some (nasty-looking) fermion action matrix.
The main point is that in the analogue to QED three particles emerge: electron, hole and scalar "photon", carrying the interaction.

Self-energy function

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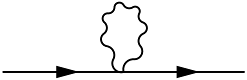
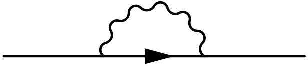
One-loop self-energy function $\Sigma_e^{(1)}$:

$\Sigma_e^{(1)} =$  $+$ 

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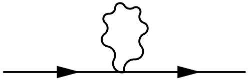
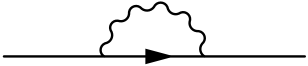
$\Sigma_e^{(1)} =$  $+$ 

$$\Sigma_e^{(1)}(p) = \underbrace{\cancel{\frac{1}{2}\delta\tau \begin{pmatrix} V_{00} & 0 \\ 0 & V_{00} \end{pmatrix} e^{ip^0\delta\tau}}}_{\Sigma_1(p)} -$$

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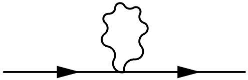
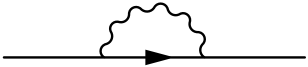
$\Sigma_e^{(1)} =$  $+$ 

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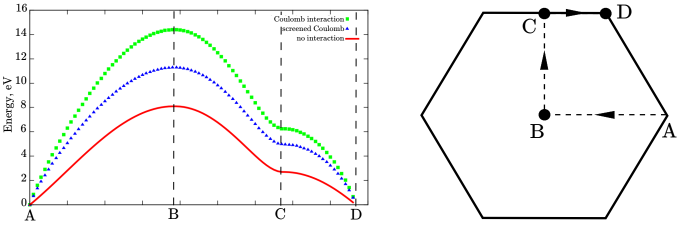
This cancellation is typical for lattice calculations and preserves $\Sigma_{xx} = 0$, conserving the charge. The structure of this correction preserves the propagator form, leading to its parameters renormalization.

Spectrum function

Given the Σ_e formula, one can renormalize the energy spectrum $\varphi(\vec{k})$ $(E_R^2(\vec{k}) = m_R^2 + \varphi_R^2(\vec{k}))$:



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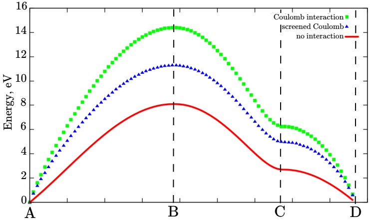

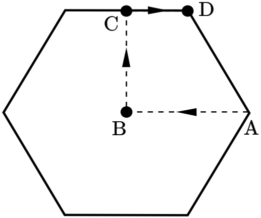

Figure : Energy spectrum profile: non-interacting, Coulomb and screened Coulomb cases. Very sensitive to modifications of the potential at small distances!

In the limit $a \to 0$, $\vec{k} \to \vec{k}_F$ the effective theory result is reproduced at the leading logarithmic accuracy

$$v_F^R = v_F \left[1 + \tfrac{1}{4}\alpha_g \left[\log\left(\tfrac{\Lambda}{2T}\right) + \gamma - \log \pi/4 + \mathcal{O}(\Lambda^{-1})\right]\right],$$

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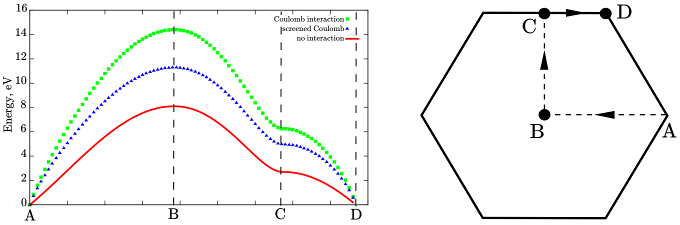

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But we have renormalized the whole spectrum!

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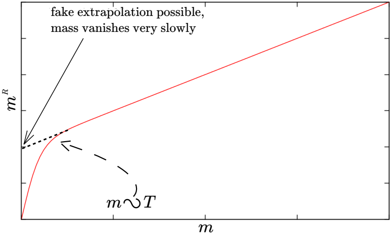
Similarly to φ function, the information on mass m_R can be extracted. The most exciting thing is its dependence on the bare mass m.



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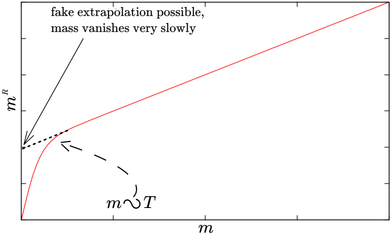

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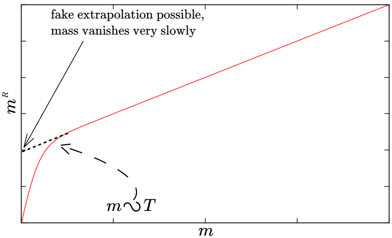
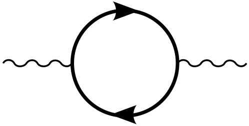


Such behaviour has recently been observed numerically by our colleagues and other lattice groups: they extrapolated mass and got non-zero result.
Now the analytical explanation obtained! One has to account this behaviour during simulations in order to achieve massless limit (answer to the question "How small the bare mass should be to get almost massless limit?" is "Smaller than expected. ").

Interaction itself renormalized

The "photon" self-energy function (polarisation operator) $\mathcal{P}_\gamma^{(1)}(\vec{k})$ is simply:



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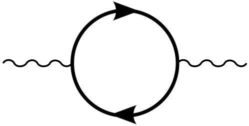

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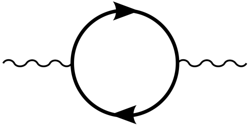

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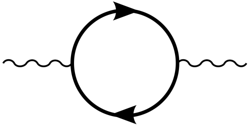

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In the presence of the temperature, the spectrum $\tilde{V}(\vec{k})$ modifies $\frac{1}{|\vec{k}|} \to \frac{1}{|\vec{k}|+m_D}$ by the Debye mass — also well-known result.

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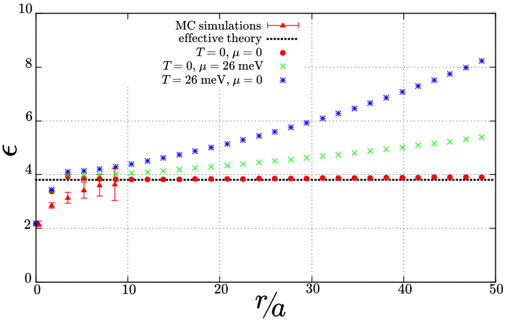

Figure : Potential renormalization in suspended graphene: effective model (dashed), HMC (red triangles) and one-loop calculation (bullets, circles and stars).

It was found out that one-loop potential describes simulation results pretty-well (massive comparison coming soon...), that is a question to answer.

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There is an experimental evidence that the conductivity $\sigma(\omega)$ (the same diagram, but easier to measure) does not feel higher order corrections — why?
There must be a symmetry or other explanation to this fact.

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- The sensitivity to the form of bare potential V_{xy} was shown, but to account it, one has to use the Hubbard model.
- Surprisingly, even when $\epsilon = 1$ (meaning $\alpha_G \sim 2.2$) one-loop interaction is very close to HMC results, implying that higher-order correction are somehow suppressed.

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- *The Hubbard graphene model* is widely used for computer HMC simulations, giving very precise non-perturbative results.
- In order to check them, the perturbative approach was developed, it will work for sure at least in $\epsilon \gg 1$ limit.
- The obtained analytic approach reproduces well-known effective field theory results and, most importantly, gives a good approximation to numerical simulations. Thus, it can be easily used to check any subsequent HMC results.
- The sensitivity to the form of bare potential V_{xy} was shown, but to account it, one has to use the Hubbard model.
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- Thank you for your attention, for details please visit arXiv-1506.00026.