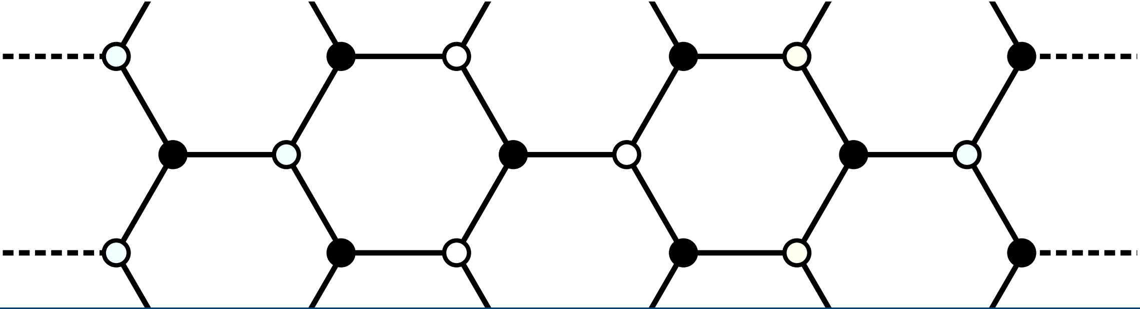


HUBBARD INTERACTION AT FINITE T
on a hexagonal lattice

July 30, 2024 | **Lado Razmadze**, Tom Luu | Forschungszentrum Jülich

Introduction

Motivation

- Characteristic temperature $\sim$ Energy of the lowest modes $\mathcal{E}$
- LQCD:
  - $m_\pi \approx 150\text{MeV}$
  - For $T \ll m_\pi$ assume $T = 0 \Rightarrow$ no temporal finite volume effects
  - At $T \approx m_\pi$ thermal field theory is applicable
  - TFT is used to study nuclear matter, quark-gluon plasma [Le Bellac ’96, Kapusta ’06]
- Physical lattices:
  - Usually $T \approx \mathcal{E}$
  - Graphene K-points, Topological insulators...
    - Vanishing dispersion i.e. $\mathcal{E} = 0 \Rightarrow$ TFT relevant for all T.
    - Perturbative treatment is tricky
- Preferable to work with inverse temperature $\beta = 1/T$

Introduction

Hubbard Model

- Hubbard at half-filling

$$H = -\kappa \sum_{\langle x,y \rangle s} c^\dagger_{xs} c_{ys} - \frac{U}{2} \sum_x (c^\dagger_{x\uparrow} c_{x\uparrow} - c^\dagger_{x\downarrow} c_{x\downarrow})^2$$

  - κ - Hopping strength
  - U - On site Hubbard interaction
  - $s = \uparrow, \downarrow$ - Spin

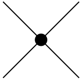
Introduction

Hubbard Model cont'd

- Momentum basis

$$H = H_0 + H_1 + H_2$$

$$= -\sum \sigma \mathcal{E}_k \phi^\dagger_{k\sigma s}\phi_{k\sigma s} + \underbrace{-\frac{U}{2}\sum \phi^\dagger_{k\sigma s}\phi_{k\sigma s}}_{\sim} + \underbrace{\sum V^{\rho'\sigma'\rho\sigma}_{k'l'kl}\phi^\dagger_{k'\rho'\uparrow}\phi^\dagger_{l'\sigma'\downarrow}\phi_{k\rho\downarrow}\phi_{l\sigma\uparrow}}_{\sim}$$



  - $V^{\rho'\sigma'\rho\sigma}_{k'l'kl} \propto U$
  - ρ, σ - Bands ($\pm 1 \rightarrow$ particle/hole)
  - k, l - Momenta in Brillouin Zone

- H_0 - Non-interacting system
- $H_1 + H_2 \overset{!}{=} H_I$ - Perturbing interaction

Perturbation

Propagator

- Thermal expectation value $\Rightarrow$ Physical quantities

$$\langle \hat{\mathcal{O}} \rangle_0 = Z_0^{-1} \mathrm{Tr}\left[e^{-\beta H_0} \hat{\mathcal{O}}\right], \quad Z_0 = \mathrm{Tr}\left[e^{-\beta H_0}\right]$$ – Partition function

Perturbation

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- Non-interacting (Bare) propagator

$$G^0_{k\sigma s}(i\omega) = -\int_0^\beta d\tau\, e^{i\omega\tau}\left\langle T_\tau[\phi_{k\sigma s}(\tau)\phi^\dagger_{k\sigma s}(0)]\right\rangle_0 = \frac{1}{i\omega - \sigma\mathcal{E}_k} \sim$$

  - Imaginary time $\tau = it \Rightarrow$ imaginary frequencies $i\omega = i\frac{\pi(2n+1)}{\beta}$, $n \in \mathbb{Z}$
  - T_τ - time ordering operator, arranging operators in decreasing order of τ

Perturbation

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- Fermi-Dirac distribution

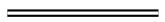
$$n_{k\sigma} \stackrel{!}{=} \frac{1}{\beta} \sum_{i\omega} G^0_{k\sigma s}(i\omega) = \frac{1}{e^{\sigma\beta\mathcal{E}_k} + 1}$$

Perturbation

Propagator

- Interacting (Full) propagator

$$G_{k\sigma s}(i\omega) = -\int_0^\beta d\tau\; e^{i\omega\tau} \frac{\left\langle T_\tau \left[S(\beta)\phi_{k\sigma s}(\tau)\phi^\dagger_{k\sigma s} \right] \right\rangle_0}{\langle T_\tau\, [S(\beta)] \rangle_0} \quad \sim$$



- *S*-matrix is defined as

$$S(\beta) = T_\tau \exp\left\{ -\int_0^\beta H_I(\tau')d\tau' \right\}$$

Perturbation

Propagator

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$$\xrightarrow{\text{Expand in } U} = \sum_{m=0}^{\infty} \frac{(-)^m}{m!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_m T_\tau [H_I(\tau_1) \cdots H_I(\tau_m)]$$

Perturbation

Wick Contraction

- S-matrix expansion $\Rightarrow$ Thermal average of the field products

$$\left\langle T_\tau[H_I(\tau_1)\cdots H_I(\tau_m)\phi(\tau)\phi^\dagger]\right\rangle_0 \propto \left\langle T_\tau[\phi_1\,\phi_2\ \cdots\phi^\dagger_{1'}\phi^\dagger_{2'}\cdots]\right\rangle_0$$

- Define Wick contraction

$$\overline{\phi_1\,\phi^\dagger_{1'}} \stackrel{!}{=} \left\langle T_\tau[\phi_1\,\phi^\dagger_{1'}]\right\rangle_0 = -G^0_1\delta_{1\,1'}$$

- Then one can write

$$\left\langle T_\tau[\phi_1\,\phi_2\ \cdots\phi^\dagger_{1'}\phi^\dagger_{2'}\cdots]\right\rangle_0 = \wick{\c1\phi_1\,\c2\phi_2\ \cdots\c1\phi^\dagger_{1'}\c2\phi^\dagger_{2'}}\cdots + \wick{\c1\phi_1\,\c2\phi_2\ \cdots\c2\phi^\dagger_{1'}\c1\phi^\dagger_{2'}}\cdots$$

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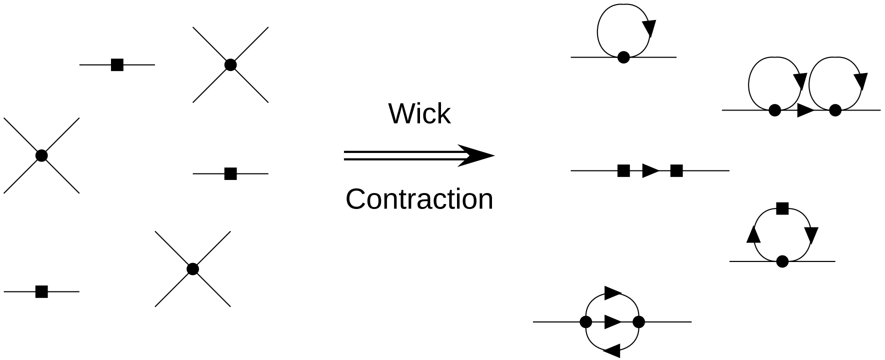
Perturbation

Diagrams



Self-Energy

Dyson Equation

- 1-PI diagram cannot be separated by removing one propagator.
  - Denote the sum of all 1-PI diagrams with Σ

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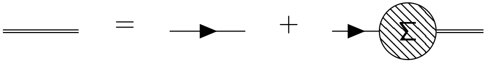
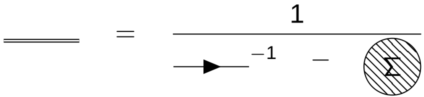


  - Solve for G



$$= \frac{1}{i\omega - \mathcal{E} - \Sigma(i\omega)}$$

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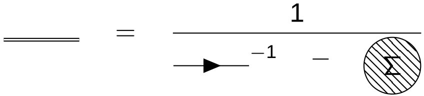


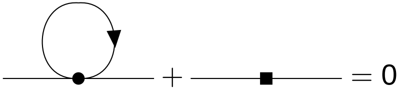
$$= \frac{1}{i\omega - \mathcal{E} - \Sigma(i\omega)}$$

- Pole of the full propagator $\Rightarrow$ Interacting self-energy $\mathcal{E}^*$

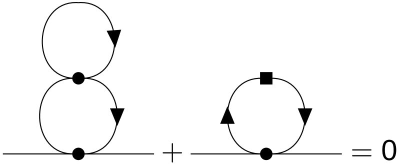
$$\mathcal{E}^* - \mathcal{E} - \Sigma(\mathcal{E}^*) = 0$$ – Quantization condition

Self-Energy
Vanishing Diagrams

- $\mathcal{O}(U)$: Linear correction vanishes at half-filling

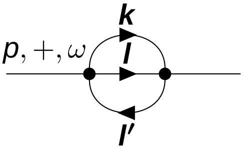


- $\mathcal{O}(U^2)$: Similar diagrams vanish for the second order



Self-Energy

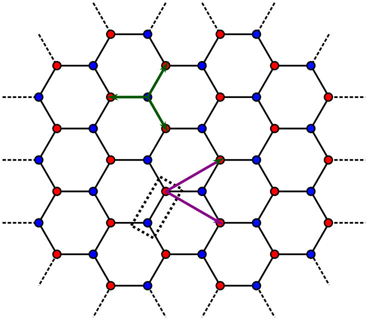
General Lattice



$$\sim \sum_{\boldsymbol{l}'\boldsymbol{k}\boldsymbol{l}} |V_{p\boldsymbol{l}'\boldsymbol{k}\boldsymbol{l}}|^2 \frac{n_{-\boldsymbol{l}'}n_{\boldsymbol{k}} + (n_{\boldsymbol{l}'} - n_{\boldsymbol{k}})n_{-\boldsymbol{l}}}{i\omega - (\mathcal{E}_{\boldsymbol{k}} - \mathcal{E}_{\boldsymbol{l}'} + \mathcal{E}_{\boldsymbol{l}})}$$

- We have used shorthand
  - $\pm\boldsymbol{k} = (k, \pm\rho)$
  - $\mathcal{E}_{\boldsymbol{k}} = \rho\mathcal{E}_k$
- Only momentum conservation was assumed
- Exact form of $\mathcal{E}$ and V depends on the lattice

Graphene



- Graphene:
  - Dashed rectangle - Unit cell
  - 2-sites per cell - A/B
  - $m \times n$ graphene $\Rightarrow 2mn$ sites

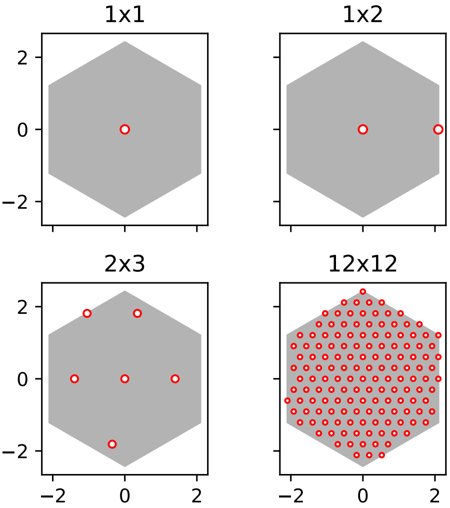


Figure: Brillouin Zone for $m \times n$

Self-Energy

2-site, 1x1 Graphene

- For 2-sites only one momentum in BZ - $\Gamma = (0, 0)$

$$\Sigma(i\omega) = \frac{U^2}{4}\left(\frac{3n_{\Gamma+}n_{\Gamma-}}{i\omega - \mathcal{E}_\Gamma} + \frac{1 - 3n_{\Gamma+}n_{\Gamma-}}{i\omega + 3\mathcal{E}_\Gamma}\right), \quad n_{\Gamma+}n_{\Gamma-} \xrightarrow{\beta\to\infty} e^{-\beta\mathcal{E}_\Gamma}$$

- Dyson equation

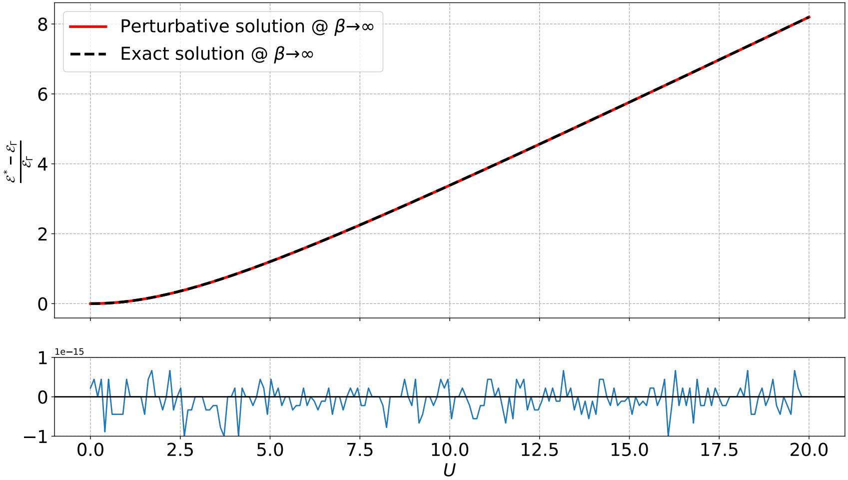
$$(i\omega - \mathcal{E}_\Gamma)^2(i\omega + 3\mathcal{E}_\Gamma) - \frac{U^2}{4}(i\omega - \mathcal{E}_\Gamma + 12n_{\Gamma+}n_{\Gamma-}\mathcal{E}_\Gamma) = 0$$

- Cubic polynomial in $i\omega \Rightarrow$ can be solved exactly

Self-Energy

2-sites

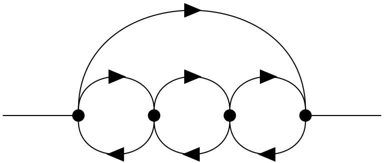
$\beta \to \infty$



Self-Energy

2-sites

$\beta \to \infty$

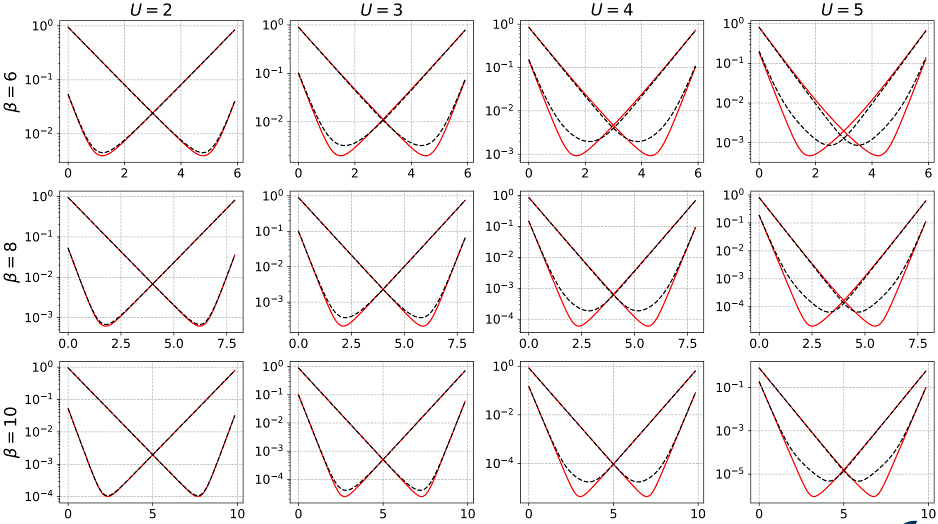


- Each loop $\sim e^{-\beta \mathcal{E}_\Gamma}$
- For $\beta \to \infty$ higher order terms vanish

Self-Energy

2-sites

$\beta < \infty$



Self-Energy

4-site, 1x2 Graphene

- For 4-sites 2 momenta
  - $\Gamma = (0, 0)$
  - $M = \left(\frac{2\pi}{3}, 0\right)$
- For finite β

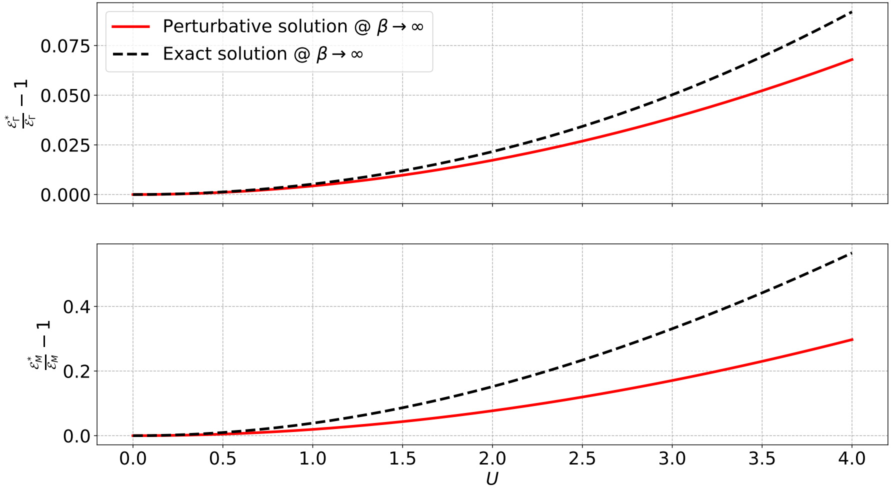
$$\Sigma(i\omega) = \text{Quintic Polynomial}$$

- For $\beta \to \infty$ $\Sigma(i\omega)$ becomes a *Cubic* again

Self-Energy

4-sites

$\beta \to \infty$



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Summary & Outlook

- In summary:
  - We found LO correction to the 2-site model
    - For $\beta \to \infty$ perturbative solution was exact
    - For finite β correlators are in good agreement with the exact solution
  - We found LO correction to the 4-site model
- Outlook:
  - Do HMC simulations for various geometries
    - Larger graphene sheets
    - Graphene nanoribbon
    - Graphene nanotube
  - Find $\beta \to \infty$ dependence and match with perturbative solutions
  - Find general expression for higher order contributions
  - Find general finite temporal volume effects and match them to calculations

Thank You!