

HUBBARD INTERACTION AT FINITE T on a hexagonal lattice

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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

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

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

Introduction

Hubbard Model cont'd

- Momentum basis

$$H = H_0 + H_1 + H_2$$

$$= - \sum \sigma \mathcal{E}_k \phi_{k\sigma}^\dagger \phi_{k\sigma} + \underbrace{-\frac{U}{2} \sum \phi_{k\sigma}^\dagger \phi_{k\sigma}}_{\sim \blacksquare} + \underbrace{\sum V_{k'l'kl}^{\rho'\sigma'\rho\sigma} \phi_{k'\rho'\uparrow}^\dagger \phi_{l'\sigma'\downarrow}^\dagger \phi_{k\rho\downarrow} \phi_{l\sigma\uparrow}}_{\sim \times}$$

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

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

Perturbation

Propagator

- Thermal expectation value \Rightarrow Physical quantities

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

Perturbation

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- Non-interacting (Bare) propagator

$$G_{k\sigma S}^0(i\omega) = - \int_0^\beta d\tau e^{i\omega\tau} \left\langle T_\tau [\phi_{k\sigma S}(\tau) \phi_{k\sigma S}^\dagger(0)] \right\rangle_0 = \frac{1}{i\omega - \sigma \mathcal{E}_k} \sim \longrightarrow$$

- 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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- T_τ - time ordering operator, arranging operators in decreasing order of τ
- Fermi-Dirac distribution

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

Perturbation

Propagator

- Interacting (Full) propagator

$$G_{k\sigma S}(i\omega) = - \int_0^\beta d\tau e^{i\omega\tau} \frac{\langle T_\tau [S(\beta)\phi_{k\sigma S}(\tau)\phi_{k\sigma S}^\dagger] \rangle_0}{\langle T_\tau [S(\beta)] \rangle_0} \sim \underline{\underline{\hspace{2cm}}}$$

- 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

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

- Define Wick contraction

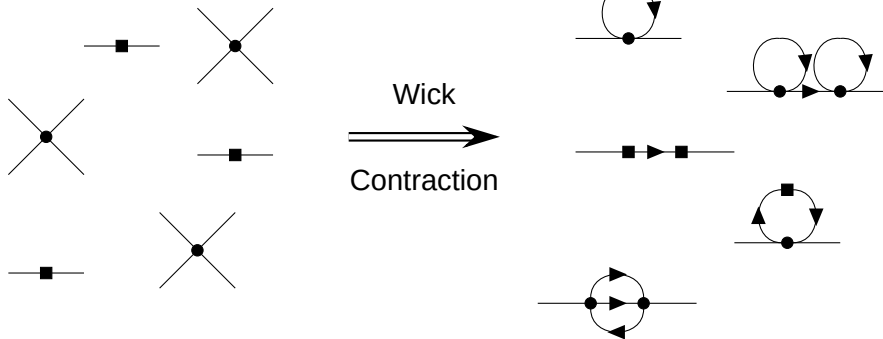
$$\overbrace{\phi_1 \phi_{1'}^{\dagger}} \stackrel{!}{=} \left\langle T_{\tau}[\phi_1 \phi_{1'}^{\dagger}] \right\rangle_0 = -G_1^0 \delta_{1 1'}$$

- Then one can write

$$\left\langle T_{\tau}[\phi_1 \phi_2 \cdots \phi_{1'}^{\dagger} \phi_{2'}^{\dagger} \cdots] \right\rangle_0 = \overbrace{\phi_1 \phi_2 \cdots \phi_{1'}^{\dagger} \phi_{2'}^{\dagger} \cdots} + \overbrace{\phi_1 \phi_2 \cdots \phi_{1'}^{\dagger} \phi_{2'}^{\dagger} \cdots}$$

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

Self-Energy

Dyson Equation

- 1-PI diagram cannot be separated by removing one propagator.
 - Denote the sum of all 1-PI diagrams with Σ
 - Dyson equation relates G to G^0 and Σ

The diagram illustrates the Dyson equation in a diagrammatic form. On the left, a double horizontal line represents the full propagator G . This is set equal to the sum of two terms. The first term is a single horizontal line with an arrow pointing to the right, representing the free propagator G^0 . The second term is a single horizontal line with an arrow pointing to the right that enters a shaded circle containing the Greek letter Σ , representing the self-energy. From the right side of the Σ circle, a double horizontal line exits, representing the full propagator G again. This visualizes the equation $G = G^0 + G^0 \Sigma G$.

Self-Energy

Dyson Equation

- 1-PI diagram cannot be separated by removing one propagator.
 - Denote the sum of all 1-PI diagrams with Σ
 - Dyson equation relates G to G^0 and Σ



- Solve for G

The diagram shows the Dyson equation in algebraic form. On the left is a double horizontal line representing G . This is equal to the fraction $\frac{1}{\text{single line with arrow and } -1 \text{ minus shaded circle } \Sigma}$. The denominator consists of a single horizontal line with an arrow pointing to the right and a -1 below it, followed by a minus sign and a shaded circle containing Σ . This is equal to the fraction $\frac{1}{i\omega - \mathcal{E} - \Sigma(i\omega)}$.

Self-Energy

Dyson Equation

- 1-PI diagram cannot be separated by removing one propagator.
 - Denote the sum of all 1-PI diagrams with Σ
 - Dyson equation relates G to G^0 and Σ

The diagrammatic Dyson equation shows a double line (representing the full propagator G) is equal to a single line with an arrow (representing the free propagator G^0) plus a single line with an arrow entering a shaded circle labeled Σ (representing the self-energy).

- Solve for G

The algebraic Dyson equation is shown as: a double line equals $\frac{1}{\text{single line with arrow and } -1} \times \text{shaded circle labeled } \Sigma$, which is equal to $\frac{1}{i\omega - \mathcal{E} - \Sigma(i\omega)}$.

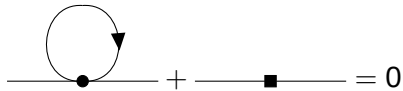
- Pole of the full propagator \Rightarrow Interacting self-energy \mathcal{E}^*

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

Self-Energy

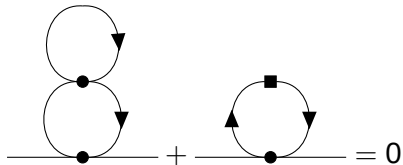
Vanishing Diagrams

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



A Feynman diagram representing the linear order $\mathcal{O}(U)$. It consists of a horizontal line with a dot at its center. A circle is drawn above the line, starting and ending at the dot, with an arrow pointing clockwise. This is followed by a plus sign, then a horizontal line with a square at its center, and finally an equals sign followed by a zero.

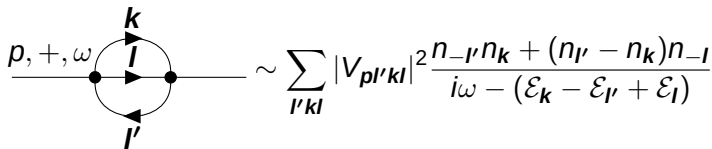
- $\mathcal{O}(U^2)$: Similar diagrams vanish for the second order



Two Feynman diagrams representing the second order $\mathcal{O}(U^2)$. The first diagram shows a horizontal line with two dots. Two circles are stacked vertically, each starting and ending at a dot, with arrows pointing clockwise. The second diagram shows a horizontal line with a dot and a square above it. A circle is drawn around the square, starting and ending at the dot, with arrows pointing clockwise. This is followed by a plus sign, then a horizontal line with a dot, and finally an equals sign followed by a zero.

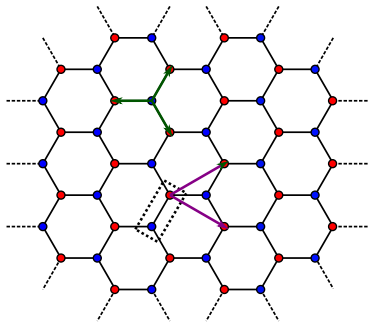
Self-Energy

General Lattice


$$\rho, +, \omega \quad \sim \sum_{l'k} |V_{pl'l}|^2 \frac{n_{-l'} n_k + (n_{l'} - n_k) n_{-l}}{i\omega - (\mathcal{E}_k - \mathcal{E}_{l'} + \mathcal{E}_l)}$$

- We have used shorthand
 - $\pm \mathbf{k} = (k, \pm \rho)$
 - $\mathcal{E}_k = \rho \mathcal{E}_k$
- 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

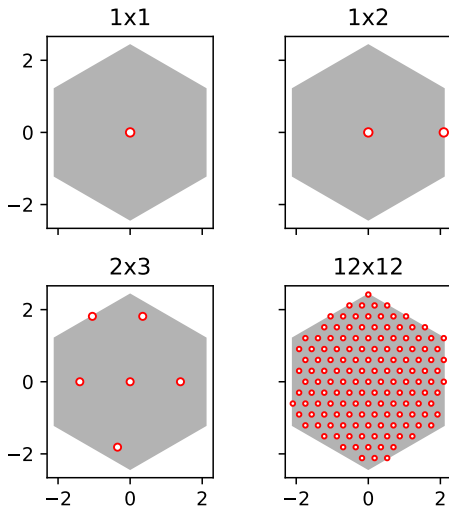


Figure: Brillouin Zone for $m \times n$

Self-Energy

2-site, 1x1 Graphene

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

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

- Dyson equation

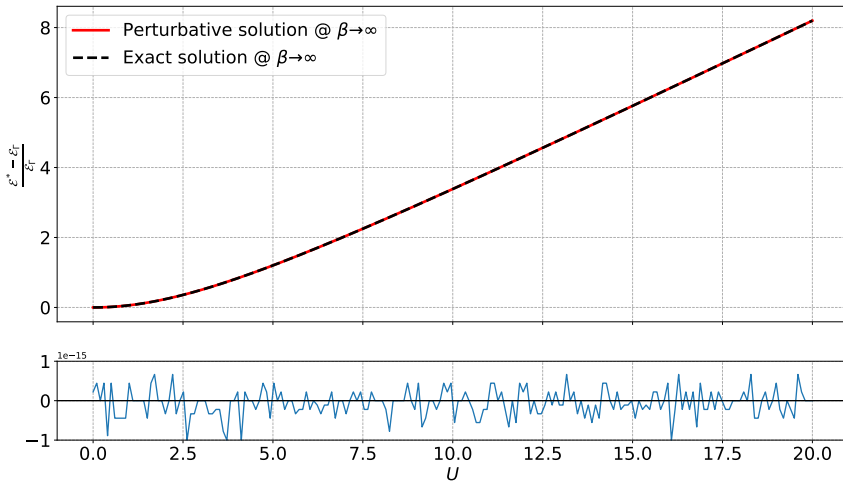
$$(i\omega - \mathcal{E}_{\Gamma})^2(i\omega + 3\mathcal{E}_{\Gamma}) - \frac{U^2}{4}(i\omega - \mathcal{E}_{\Gamma} + 12n_{\Gamma+}n_{\Gamma-}\mathcal{E}_{\Gamma}) = 0$$

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

Self-Energy

2-sites

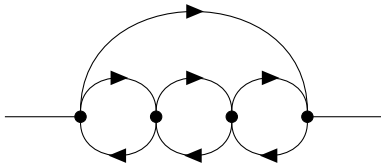
$\beta \rightarrow \infty$



Self-Energy

2-sites

$\beta \rightarrow \infty$

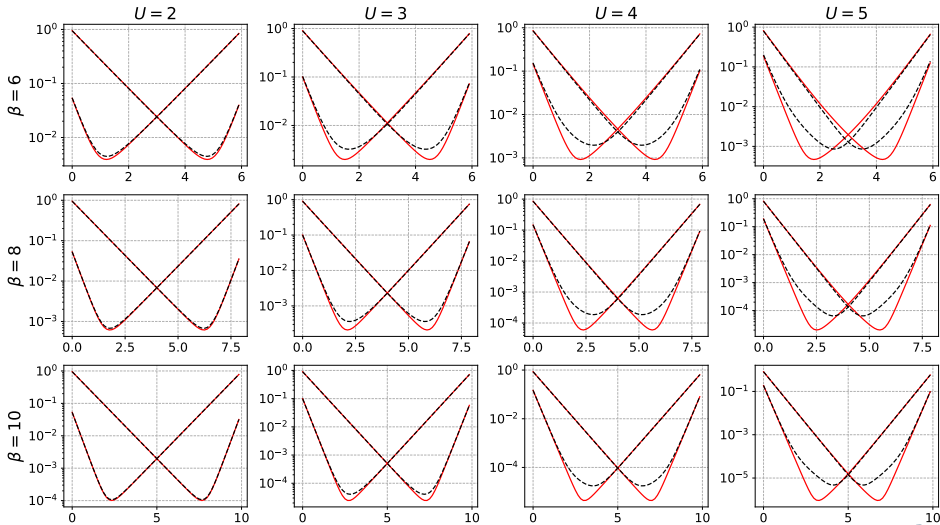


- Each loop $\sim e^{-\beta \mathcal{E}_T}$
- For $\beta \rightarrow \infty$ higher order terms vanish

Self-Energy

2-sites

$\beta < \infty$



Self-Energy

4-site, 1x2 Graphene

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

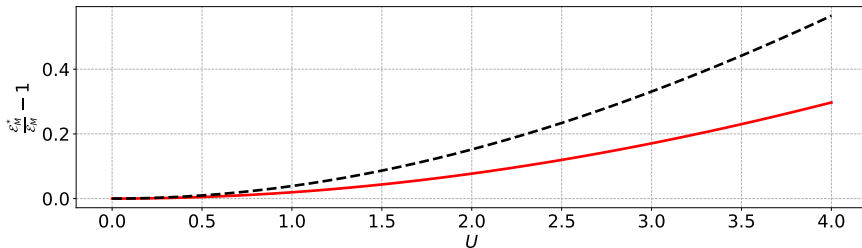
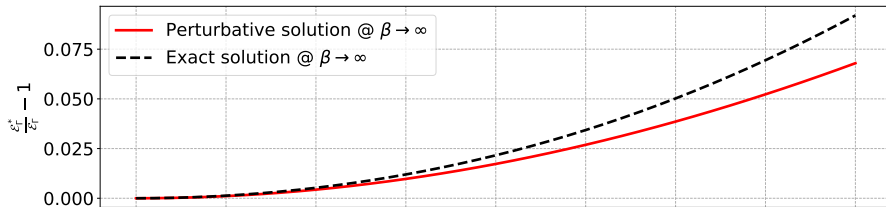
$\Sigma(i\omega) = \text{Quintic Polynomial}$

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

Self-Energy

4-sites

$\beta \rightarrow \infty$



Summary & Outlook

- In summary:
 - We found LO correction to the 2-site model
 - For $\beta \rightarrow \infty$ 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 $\beta \rightarrow \infty$ 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!