Effect of Hubbard Interaction on Quadratic Band Touching (QBT) semi-metal in Bernal-stacked Honeycomb Bilayer

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Outline of the Talk

- History, The Big Picture, etc.
- Problem Statement
- Motivation
- Mean-Field Theory
- Previous Results on $N = 2$:
  1) Weak-coupling RG
  2) det-QMC
- Our Results on general $N$:
  1) Weak-coupling RG
  2) det-QMC
- Conclusion
The Big Picture: Condensed Matter Physics

- Physics is HUGE (screenshot from Wiki)

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- Condensed Matter is one of biggest sub-fields
- Affects our lives in a big way ...
- Synergies with Materials Science, Applied and Engg. Physics, and allied fields
The Big Picture: Various States of Matter

- One of the oldest philosophical questions

Today we focus on electronic states of quantum matter
The Big Picture: Approaches to Condensed Matter

- Theory
- Simulation
- Experiment
- Big Data

The diagram illustrates the interconnections between Theory, Simulation, Experiment, and Big Data, highlighting the cyclical nature of research and data analysis in condensed matter physics.
Going towards our Problem ... Some History

- 1920s: Classical Mechanics $\rightarrow$ Quantum Mechanics.
- Applied to electrons in solids immediately (Sommerfeld, Peierls, etc.)
- "Crystallized" into Free-Electron Theory or Band Theory
  - Bloch’s Theorem leads to Electronic band states for non-interacting electrons
  - Pauli’s Exclusion leads to filling of a certain fraction of bands
  - Fermi Surface with many low-energy excitations

Figure: 1) cartoon, 2) Silicon, 3) Copper

- Basically explains many metals ($Na$, $Al$), Insulators/Semiconductors ($Si$)
But what about electrons interactions?

Answer given by Landau .... Fermi Liquid Theory

Low energy quasiparticles “smoothly connected” to non-interacting electrons

They are well-defined fermions with long lifetimes

Due to Fermi surface and energy-momentum conservation, no phase space to scatter ...

BUT .. there are electronic states of matter where this breaks down

e.g. Mott Insulators, lower dimensions

This brings us to Interacting Electrons.. and our problem
Problem Statement

- **Hamiltonian:**
  - Lattice: Bernal Stack honeycomb bilayer
  - Nearest neighbour hopping on: \( \sum \langle i,j \rangle, \sigma \ c_i^\dagger \sigma c_j, \sigma \ + h.c. \)
  - On-site Hubbard Interaction: \( \sum_{i, \sigma \neq \sigma'} (n_{i, \sigma} - 0.5)(n_{i, \sigma'} - 0.5) \)
  - \( \sigma \) is spin/flavour index for \( SU(N) \)
  - Symmetries: Lattice, \( SU(N) \) flavour, Time Reversal

**Figure:** LEFT: Side view RIGHT: Top view
Motivation: The Quadratic Band Touching (QBT) semi-metal

- Relevant to Graphene Material

![Graphene Band Structure Diagram](image)

Figure: LEFT: Spectrum RIGHT: Brillouin Zone

- SEMI-METAL: Fermi Points instead of Fermi Surfaces
- Two Fermi Points in the Brillouin Zone
Motivation: Power Counting

- (Engineering) Dimensional Analysis of Effect of Interactions
- Also poor man’s RG
- Effective Low-Energy Continuum Action of QBT

\[
S_0 \sim \sum_{\sigma} \int d^d \vec{r} \, dt \, \Psi_\sigma^\dagger(\vec{r}, t) \left( \tau_0 \partial_t + \tau_1 \left( \partial_x^2 - \partial_y^2 \right) / m + \tau_2 \partial_x \partial_y / m \right) \Psi_\sigma(\vec{r}, t)
\]

- above \( S_0 \) gives the QBT dispersion
- under Space-time Rescaling: \( \vec{r} \rightarrow b\vec{r}, \ t \rightarrow b^2 t \) with \( b \gtrsim 1 \) and
- Field-Rescaling: \( \Psi_\sigma \rightarrow b^{-d/2} \Psi_\sigma \)
- \( S_0 \) scale-invariant
Motivation: Power Counting

- **(Local) Interaction Term**

\[ \int d^d \vec{r} \, dt \, U \left( \Psi^\dagger_\sigma (\vec{r}, t) \Psi_\sigma (\vec{r}, t) \Psi^\dagger_- \sigma (\vec{r}, t) \Psi_- \sigma (\vec{r}, t) \right) \]

- \( U \rightarrow b^{2-d} U \)
- \( d = 2 \), Local Interactions are marginal
- Can expect Instabilities for QBT semi-metal to Local Interactions
- What are possible ground states??
- **ASIDE** Dirac semi-metal, \( \vec{r} \rightarrow b \vec{r}, \ t \rightarrow bt \rightarrow U \rightarrow b^{1-d} U \rightarrow \)
  Interactions are irrelevant \( \rightarrow \) Stability
- Heuristically,
  - \( \sim 0 \) d.o.s. near Dirac Cones \( \rightarrow \) Irrelevance
  - finite d.o.s. near QBT points \( \rightarrow \) Possible Instabilities
Mean-Field Theory

- Antiferromagnet (AFM) and Valence Bond (VBS) Ansatzes

**Figure**: Left: AFM ansatz. Right: VBS ansatz

- AFM order at zero or $\Gamma$ wave-vector
- VBS order at QBT wave-vector
- Both open a gap $\rightarrow$ Not Semi-metallic
Mean-Field Theory

- Kékule Current Ansatz

- Current Order at QBT wave-vector
- Opens a gap $\rightarrow$ Not Semi-metallic
Mean-Field Theory

- **Method**: Self-consistent Hartree-Fock MFT

- **MFT** → QBT unstable to AFM order for all $N$ and $U$
  - AFM order opens a gap at QBT → Insulating state
Existing Results: weak-coupling RG

- Perturbative RG goes beyond MFT
- needs a small parameter \( \rightarrow \) useful in weak-coupling
- O. Vafek did the \( N = 2 \) calculation \( \text{Phys. Rev. B} \ 82, \ 205106 \ (2010) \)
- zeroth-order effective Action \( S_0 \) \( \rightarrow \) quadratic

\[
S_0 = \int \bar{\psi}(\mathbf{r}, \tau) \left( \partial_\tau + \frac{\partial_x^2 - \partial_y^2}{2m} \mathbb{I} \otimes \sigma_x \otimes \mathbb{I}_N - \frac{\partial_x \partial_y}{m} \tau_z \otimes \sigma_y \otimes \mathbb{I}_N \right) \psi(\mathbf{r}, \tau)
\]

- Internal Indices of field configurations:
  - Valley: \( \mathbb{I}_2, \tau_x, \tau_y, \tau_z \)
  - Layer: \( \mathbb{I}_2, \sigma_x, \sigma_y, \sigma_z \)
  - Spin/Flavour: \( \mathbb{I}_N \) above \( SU(N) \) symmetric
Existing Results: weak-coupling RG

- general local interaction $\to$ quartic

$$ S_{\text{int}} = \frac{1}{2} \sum_{S,T} g_{ST} \int d\tau d^2r \left( \bar{\psi}(r, \tau) S \otimes \mathbb{I}_N \psi(r, \tau) \right) \times $$

$$ \left( \bar{\psi}(r, \tau) T \otimes \mathbb{I}_N \psi(r, \tau) \right) $$

- $S, \ T$ are $4 \times 4$ matrices combining Valley and Layer indices
- $SU(N)$ spin/flavour symmetric $\to \mathbb{I}_N$ above
- Low energy projection of $U$ Hubbard term $\to$ 3 non-zero $g_{ST}$
- Do pert-RG calc to compute RG flows of $g_{ST}$s to lowest order
  - Integrate momentum shell high energy modes, apply Cumulant Expansion, Tree-level $O(g) = 0$ is same as marginality from Power counting, One-loop $O(g^2)$ corrections. R. Shankar, Rev. Mod. Phys. 66, 129 (1994)
- 6 new couplings generated
- Compute RG flows of Susceptibility to quadratic order sources
  \[ \propto \Delta^O \int d\tau d^2r \, \psi^\dagger(r, \tau) O \psi(r, \tau) \]
Existing Results: weak-coupling RG: $U \rightarrow 0$ instability

- Instability in Spin channel $\rightarrow$ magnetic
- Identity in Valley Index
- diagonal $\sigma_z$ in layer index $\rightarrow$ AFM is leading instability
Existing Results: det-QMC

- Det-QMC method for interacting fermions
  - Suzuki-Trotter, Hubbard-Stratonovich (HS) to decouple the Interaction term, MC sum over HS variables, Importance sample using detailed Balance, Weight of HS configurations has Determinantal structure, Measure Observables as a weighted-average in this ensemble, Assaad and Evertz, Volume 739 of Lecture Notes in Physics pp 277-356 (2008)
- $N = 2$ study by T. C. Lang et al
- AFM order for all $U$
- Single particle gap opens at QBT wavevector
- Zero spin gap at AFM wavevector due to Goldstone Modes
- Agreement with Vafek’s $N = 2$ RG prediction
Existing Results: det-QMC

- One example: AFM order parameter vs $1/L$

![Graph showing AFM order parameter vs $1/L$ for different values of $U/t$.]

**Figure**: from Lang et al, Phys. Rev. Lett. 109, 126402 (2012).
Our Results : weak-coupling RG : $U \to 0$ instability

- $N \geq 4$ : Instability in Charge channel $\to$ Non-magnetic
- $N \geq 4$ : Off-diagonal $\tau_x$ in Valley index $\to$ Order at QBT wavevector which joins the two valleys
- $N \geq 4$ : Off-diagonal $\sigma_y$ in Layer index $\to$ Odd under Time Reversal
- Consistent with Kékule Currents $\to$ look for them in det-QMC
Our Results: det-QMC

- Search for Order → Bragg Peaks in associated Structure Factors
- Quantify (presence or absence of) Bragg Peaks using Binder Ratios
- Look at Single Particle and Spin Gap
Our Results: det-QMC: structure factors

- \( N = 4 \) First look at AFM structure factor

![Diagram](image)

- No Bragg peak in Weak Coupling
- Consistent with Expectation of Kékule Currents
- AFM in Strong coupling: Peak size scales with system size
- Look for Currents in weak-coupling...
Our Results: det-QMC: structure factors

- $N = 4$ Now look for Current Structure Factor Bragg peak at QBT wavevector in weak-coupling..

There is no Bragg peak at QBT!!
- Where are the currents???

Figure: LEFT: Weak Coupling | RIGHT: Strong Coupling
Our Results: det-QMC: structure factors

- \( N = 6 \) AFM structure factor

![Graphs showing AFM structure factors for weak and strong coupling.](image)

**Figure:** LEFT: Weak Coupling       RIGHT: Strong Coupling

- No AFM order in weak-coupling as expected..
- No AFM order in strong-coupling unlike \( N = 4 \)..
- What is the order in strong coupling?
Our Results: det-QMC: structure factors

- $N = 6$ Dimer VBS structure factor

$$t_p = 1, \ t = 1, \ N = 6, \ L = 12, \ U = 20.$$  

- $N = 6$ strong coupling is VBS ordered.
- Are there Currents at weak coupling??
Our Results: det-QMC: structure factors

- $N = 6$ Current structure factor

![Graph](image)

Figure: LEFT: Weak Coupling  RIGHT: Strong Coupling

- No Bragg peak in weak coupling again!!
- What is this mysterious state??
Our Results: det-QMC: structure factors

- Revisit $N = 2$ AFM structure factor.. strange scaling of AFM order parameter in weak-coupling remarked earlier on pg. 15..

Figure: LEFT: Weak Coupling RIGHT: Strong Coupling

- No AFM Bragg peak in weak coupling again!
- Is the mysterious state perhaps a stable QBT semi-metal??
Our Results: det-QMC: Binder ratios

- Construct Binder Ratios $R$ to quantify Bragg peaks presence
- Construction: $R \rightarrow 1$ ordered, while $R \rightarrow 0$ not ordered
- $N = 4$ AFM Binder ratio

Figure: LEFT: Ratio Crossing  RIGHT: Crossing Drifts

- AFM in Strong Coupling as seen before
- No AFM order in Weak Coupling as seen before
Our Results: det-QMC: Binder ratios

- $N = 4$ VBS and Current Binder ratios

**Figure**: LEFT: VBS  RIGHT: Current

- No VBS order as expected
- No Current Order even in weak-coupling
Our Results: det-QMC: Binder ratios

- \( N = 2 \) AFM Binder ratio

![Graph showing Binder ratios](image)

**Figure**: LEFT: Ratio Crossing  RIGHT: Crossing Drifts

- No AFM order in Weak Coupling evidenced here too!
- AFM in Strong Coupling as seen before
Our Results: det-QMC: Binder ratios

- $N = 2$ VBS and Current Binder ratios

![Graphs showing VBS and Current results](image)

Figure: LEFT: VBS | RIGHT: Current

- No VBS or Current Order in weak-coupling
Our Results: det-QMC: Binder ratios

- $N = 6$ VBS Binder ratio

Figure: LEFT: Weak Coupling  RIGHT: Strong Coupling

- VBS in Strong Coupling as seen before
- No VBS in Weak Coupling as seen before
Our Results: det-QMC: Binder ratios

- $N = 6$ AFM and Current Binder ratios

![Graphs showing Binder ratios for AFM and Current](image)

**Figure:** LEFT: AFM  RIGHT: Current

- No AFM order as expected
- No Current Order even in weak-coupling
- What is this mysterious state in weak-coupling??
What about RG? : Hypothesis of Dirac phase

RG argument:

- QBT has no linear term in dispersion by definition
- IMP: Instead self-energy processes due to the interaction generate a linear term in dispersion!
- Linear term not disallowed by symmetries of the problem
- Once generated, they are RG relevant at the QBT fixed point
- Flow to a Dirac semi-metallic fixed point in weak-coupling
- Dirac semi-metal stable to weak local interactions
- Thus no weak-coupling instability of Bernal Stacked Honeycomb Bilayer Hubbard model
- Instead Dirac fermions form a stable weak-coupling phase
- IMP: Irrelevant cubic corrections to QBT are needed to generate the linear term
What about RG? : RG flows

How to verify this RG picture?
- Dynamical critical exponent: QBT $z = 2$ or Dirac $z = 1$ (Gross-Neveu)
- Look into Gap data
Our Results: det-QMC: Spin Gaps

- $N = 4$ Spin Gap at AFM wavevector

Figure: Strong and Weak shown together

- Strong Coupling: gapless spin excitations at AFM wavevector
- Consistent with AFM order with gapless Goldstone modes
- Weak Coupling: no gapless modes
- Consistent with no AFM order
Our Results: det-QMC: Spin Gaps

- $N = 2$ Spin Gap at AFM wavevector

![Graph showing spin gaps for different values of $U$ and $t_p$.]

**Figure**: Strong and Weak shown together

- **Strong $U$**: gapless spin excitations at AFM wavevector
- Consistent with AFM order with gapless Goldstone modes
- **Weak $U$**: no gapless modes
- Consistent with NO AFM order (IMP)
Our Results: det-QMC: Spin Gaps

- $N = 6$ Spin Gap at AFM wavevector

Figure: Strong and Weak shown together

- Strong and Weak $U$: no gapless modes
- Consistent with no AFM (no $SU(N)$ symm breaking)
Our Results: det-QMC: Single Particle Gaps

- $N = 4$ Single Particle Gap at QBT wavevector

![Graphs showing single particle gaps at QBT wavevector with $t_p = 1$, $t = 1$, $N = 4$, and $U = 10$, $U = 32$.]

**Figure:** LEFT: Strong and Weak  
RIGHT: Only Weak

- Strong Coupling: QBT is gapped out
- Consistent with insulating AFM order
- Weak Coupling: tending towards 0 (Note y-axis)
- Not Inconsistent with gapless state
Our Results: det-QMC: Single Particle Gaps

- \( N = 2 \) Single Particle Gap at QBT wavevector

**Figure**: LEFT: Strong and Weak  
RIGHT: Only Weak

- Strong Coupling: QBT is gapped out  
- Consistent with insulating AFM order  
- Weak Coupling: Tending towards 0 (Note y-axis again)  
- Not Inconsistent with gapless state
Our Results: det-QMC: Single Particle Gaps

- \( N = 6 \) Single Particle Gap at QBT wavevector

\[
\Delta_{sp} \text{ at QBT where } t_p = 1, t = 1, N = 6
\]

**Figure**: LEFT: Strong and Weak
RIGHT: Only Weak

- Strong Coupling: QBT is gapped out
- Consistent with insulating VBS order
- Weak Coupling: Tending towards 0 (Note y-axis again)
- Not Inconsistent with gapless state
Single Particle Gap scaling

- $U_c$ estimate of 2.65(10).
- Above scaling consistent with $z = 1$.
- Scaling form: $\Delta_{sp} = L^{-z} F_\Delta((U - U_c)L^{1/\nu})$
Our Results: det-QMC: AFM Order Parameter Scalings

- revisit strange Scaling of pg. 15

Figure: AFM Order parameter scalings

- It is not strange; rather no AFM order in weak-coupling for $N = 2$
AFM Order Parameter Scalings

- Smooth crossing in $R$ indicates at *continuous* transition $U_c \sim 2.6$

- Scaling Collapse $U_c = 2.65(10)$ $\nu = 0.90(5)$ $a = 0.22(15)$
- $U_c$ consistent with Gap scaling
- $R = \mathcal{F}_R((U - U_c)L^{1/\nu})$ $m^2 = L^a \mathcal{F}_{m^2}((U - U_c)L^{1/\nu})$
Conclusion: A Dirac phase for all $N = 2, 4, \ldots$

- No AFM for $N = 2$ in weak-coupling
  - Crossing in Binder Ratio
  - No gapless Goldstone modes seen at AFM wavevector
- QBT gives way to Dirac fermions for general $N$
  - None of the possible dominant weak-coupling instabilities observed
  - gapless single particle excitations
  - $z = 1$ scaling of single particle gap ... CRUCIAL
  - Also IMP Gap opening and Magnetic Transition at same $U_c$
- What about Experiments?
  - Experiments on suspended samples ... Amir Yacoby’s group
  - Insulating state is observed ..
  - Our comment: can not be weak short-range interactions
  - Perhaps long-range part of Coulomb interactions IMP
  - Can the Dirac phase be observed ??
Thank you!

Details in PRL 117, 086404 (2016), arxiv:1604.03876

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- NSF for financial support
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Introduction

Existing Results

Our Results

Conclusion

R map

Map of $R$ for $L = 12$
Self-Energy with Cubic Corrections to QBT
**det-QMC Extra 2 : Lang et al Plots**

**Figure**: For $N = 2$ figs from Phys. Rev. Lett. 109, 126402 (2012).

- **Note in Weak Coupling**:
  - AFM Order parm *goes towards zero* unlike strong coupling
  - Single Particle gap *goes towards zero* unlike strong coupling
  - Spin Gap *increases* unlike strong coupling.
det-QMC Extra 3 : 3D Structure Factor Plots $N = 4$

$t_p = 1. \ t = 1. \ N = 2 \ L = 12 \ U = 10.$

$t_p = 1. \ t = 1. \ N = 2 \ L = 12 \ U = 10.$

$t_p = 1. \ t = 1. \ N = 2 \ L = 12 \ U = 10.$

Figure : Top : Weak $U = 10.$  Bottom : Strong $U = 32.$
Left : Spin  Centre : Currents  Right : VBS
det-QMC Extra 4 : 3D Structure Factor Plots $N = 2$

$t_p = 1$, $t = 1$, $N = 2$, $L = 12$, $U = 1.6$

Figure: Top: Weak $U = 1.6$
Left: Spin  Centre: Currents

Bottom: Strong $U = 3.8$
Right: VBS
det-QMC Extra 5 : 3D Structure Factor Plots $N = 6$

$t_p = 1. \; t = 1. \; N = 6 \; L = 12 \; U = 20.$

$t_p = 1. \; t = 1. \; N = 6 \; L = 12 \; U = 20.$

$t_p = 1. \; t = 1. \; N = 6 \; L = 12 \; U = 20.$

$t_p = 1. \; t = 1. \; N = 6 \; L = 12 \; U = 60.0$

$t_p = 1. \; t = 1. \; N = 6 \; L = 12 \; U = 60.0$

$t_p = 1. \; t = 1. \; N = 6 \; L = 12 \; U = 60.0$

Figure : Top : Weak $U = 1.6$
Left : Spin Centre : Currents Right : VBS

Bottom : Strong $U = 3.8$
Technical: weak-coupling RG 1

- RG goes beyond MFT
- needs a small parameter → useful in weak-coupling
- O. Vafek did the $N = 2$ calculation
- Steps of RG:
  - zeroth-order effective quadratic Action $S_0$

$$S_0 = \int d\tau d^2r \bar{\psi}(r, \tau) \left( \partial_\tau + \frac{\partial_x^2 - \partial_y^2}{2m} \mathbb{I} \otimes \sigma_x - \frac{\partial_x \partial_y}{m} \tau_z \otimes \sigma_y \right) \psi(r, \tau)$$

- Internal Indices of field configurations:
  - Valley: $\tau_x, \tau_y, \tau_z$
  - Layer: $\sigma_x, \sigma_y, \sigma_z$
  - Spin/Flavour
Technical : weak-coupling RG 2

Steps of RG cont.:

- local spin $SU(N)$ symmetric quartic interaction

$$S_{\text{int}} = \frac{1}{2} \sum_{S,T} g_{ST} \int d\tau d^2r \left( \bar{\psi}(r, \tau) S \otimes \mathbb{I}_N \psi(r, \tau) \right) \times$$

$$\left( \bar{\psi}(r, \tau) T \otimes \mathbb{I}_N \psi(r, \tau) \right)$$

- Valley and Layer combine to give an $SU(4)$ index
- $S$ and $T$ above chosen as $SU(4)$ generators
- No. of coupling constants $g_{ST}$ ? Naively, $16 + 16 \times 15/2 = 136$
- Apply symmetries to reduce: a) Lattice, b) Time Reversal
- Final no. of couplings : 9 $g_{ST}$s !!!
- Low energy projection of $U$ Hubbard term
- 3 out of 9 coupling constants are non-zero
Steps of RG cont.:

- **RG step**: Integrate out high energy modes in a thin momentum shell
- **apply Cumulant expansion perturbatively in** $g_{ST}$

$$S_< = S_0 + \langle \delta S \rangle_0 + \frac{1}{2}(\langle \delta S^2 \rangle_0 - \langle \delta S \rangle_0^2) + \ldots$$

- **Tree Level** $O(g)$: $\langle \delta S \rangle_0 = 0 \rightarrow$ Marginality
- **One-Loop** $O(g^2)$: $(\langle \delta S^2 \rangle_0 - \langle \delta S \rangle_0^2) \rightarrow$ RG flows of coupling constants
- **Given above, compute RG flows of infinitesimal source quadratic “mass” terms** $\propto \Delta^0 \int d\tau d^2r \psi^\dagger(r, \tau) O\psi(r, \tau)$
- **both in Charge and Spin channel to get RG prediction** ...
Technical: det-QMC 1

- QMC method for Interacting Fermions
- Do Suzuki-Trotter Decomposition (gives controllable systematic errors)

\[
Z = \text{Tr} \left[ e^{-\beta (H_U + H_t)} \right] = \text{Tr} \left[ (e^{-\Delta \tau H_U} e^{-\Delta \tau H_t})^m \right] + O(\Delta^2) 
\]

- \(\Delta \tau\) like an imaginary time; \(m = \beta/\Delta \tau\)
- Apply (discrete) Hubbard-Stratonovich (HS) Transformation to \(U\) Hubbard term

\[
e^{-\Delta \tau U \sum_i (n_{i,\uparrow} - 1/2)(n_{i,\downarrow} - 1/2)} = C \sum_{\{s_i\}=\pm1} e^{\alpha \sum_i s_i (n_{i,\uparrow} - n_{i,\downarrow})} 
\]

- \(\cosh(\alpha) = \exp(\Delta \tau U/2)\)
- Decouples Interacting problem to a non-interacting one
Technical: det-QMC 2

- Have to *sum* over the HS variables \( \{s_i\} \) to compute for the interacting problem.
- Do this sum as a Monte-Carlo sum.
- One MC configuration corresponds to one realization of the HS variables \( \{s_i\} \).
- MC step: Importance sample over the configurations with weights \( W(\{s_i\}) \).
- Usual way: Detailed Balance

\[
W(\{s_i\}_1) \ T(\{s_i\}_1 \rightarrow \{s_i\}_2) = W(\{s_i\}_2) \ T(\{s_i\}_2 \rightarrow \{s_i\}_1)
\]
Weight of configurations has determinantal structure

\[ Z \sim C^m \sum_{\{s_i\}=\pm1} \text{Tr} \left( (e^{\alpha c^\dagger V(\{s_i\})} e^{-\Delta_T c^\dagger T c})^\beta / \Delta_T \right) \]

\[ = C^m \sum_{\{s_i\}=\pm1} \det \left[ I + e^{\alpha V(\{s_i\}_1)} e^{-\Delta_T T} e^{\alpha V(\{s_i\}_2)} e^{-\Delta_T T} \ldots \right] \]

Above is the heavy-lifting step

Easier to see the determinant structure with Grassman variables
Technical: det-QMC 4

- Measure various observables of interest

\[
\langle O \rangle = \frac{\text{Tr} O e^{-\beta (H_U + H_t)}}{\text{Tr} e^{-\beta (H_U + H_t)}}
\]

- As a MC average

- Projector version of det-QMC also there ...

\[
\langle O \rangle_0 = \frac{\langle \psi_0 | O | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle} = \lim_{\Theta \to \infty} \frac{\langle \psi_{\text{trial}} | e^{-\Theta H} O e^{-\Theta H} | \psi_{\text{trial}} \rangle}{\langle \psi_{\text{trial}} | e^{-2\Theta H} | \psi_{\text{trial}} \rangle}
\]

- Sign-Problem free guaranteed by Particle-Hole Symmetry
  - bipartite hoppings at half-filling
  - Repulsive Hubbard Interactions favouring half-filling
Defn: $\Theta S \Theta^\dagger = -S$

Requires anti-unitarity of $\Theta$ time-reversal operator For spin-1/2 fermionic operators, we get ...

$\Theta c_{\uparrow} \rightarrow -c_{\downarrow}^\dagger \quad \Theta c_{\downarrow} \rightarrow c_{\uparrow}^\dagger$

Current operators is $I = \sum_\sigma i(c_{i,\sigma}^\dagger c_{j,\sigma} - c_{j,\sigma}^\dagger c_{i,\sigma})$

$\Theta I \Theta^\dagger = -I$
Our Results 13 : OLD Hypothesis of stable QBT

- Can the QBT semi-metal be stable to Hubbard Interactions?
- Hypothesis contrary to RG : let’s go on ...
- Non-magnetic \(\implies\) no gapless Goldstone spin modes at AFM wavector
- \(\implies\) gapless single particle excitations at QBT wavector
Fermi-Liquid: Phase Space argument

This result can be obtained from a simple phase space argument. Consider the process where a particle above the Fermi sea \((k > k_F)\) is scattered into the state \(k + q, |k + q| > k_F\) by creating a particle-hole pair \((k', k' - q, |k'| < k_F\) and \(|k' - q| > k_F\)). Because of energy conservation, \(\omega = \epsilon_k - \epsilon_{k'} = -\epsilon_{k' - q} + \epsilon_{k + q}\), the phase space available for this scattering process is proportional to \((|k| - k_F)^2\). This result can be seen by evaluating the integral \(\int d^3k' d^3q' \delta((k_{k'q'} + \epsilon_{\nu_+}\nu_+ - \epsilon_k + \epsilon_{q'})\)

where the momenta satisfied the above mentioned constraints. Higher-order processes, involving multi-pair excitations, are more strongly suppressed as the corresponding phase space is smaller.

More precisely, for the notion of quasi-particles (or quasi-holes) to make sense, their life-time \(\tau_k\) and excitation energy \(\xi_k = \epsilon_k - \mu\) should satisfy

\[
\frac{1}{\tau_k} \ll |\xi_k|, \tag{4.11}
\]

since \(1/|\xi_k|\) is the minimum time required to observe (or create with an external field) the quasi-particle. We shall see in section 4.4.1 that in a three-dimensional Fermi liquid\(6\)

\[
\frac{1}{\tau_k} = \mathcal{O}\left((|k| - k_F)^2\right) \tag{4.12}
\]

at zero temperature, so that the condition (4.11) is satisfied in the vicinity of the Fermi surface (recall that \(\xi_k = \mathcal{O}(|k| - k_F)\)). Suppose that the interaction is switched on within a characteristic time \(\eta^{-1}: \tilde{H}_{\text{int}}(t) = \tilde{H}_{\text{int}}(t \equiv 0) e^{\eta t}\). Quasi-particles can be observed if their life-time is larger than \(\eta^{-1}\) and \(1/|\xi_k|\) smaller than \(\eta^{-1}\), i.e.

\[
\frac{1}{\tau_k} \ll \eta \ll |\xi_k|, \tag{4.13}
\]
**det-QMC Extra 1: Ratio Crossing Drifts**

**Figure:** LEFT: $N = 2$  
RIGHT: $N = 4$

- Both $N = 2$ and $N = 4$ extrapolate to finite $U_c$