Structure of the Lefschetz thimbles decomposition of lattice fermion models

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Motivation (1)

Path integral is usually treated in Quantum Monte Carlo (QMC) in condensed matter physics as «black box»: once we have an algorithm for sampling, we are not looking into the details of the structure of path integral. Also, formulations with discrete fields in path integrals make such analysis more difficult (no theorems of calculus).

In Lattice Quantum Field theory, we have more knowledge on quasi-classical objects as special field configurations appearing in path integrals (monopoles, instantons, etc), but still some improvement is possible after several algorithmic developments.

The structure of path integrals (saddle points) is connected to the complexity of the sign problem through the Lefschetz thimbles decomposition. Lefschetz thimbles decomposition (1)



Questions to answer:

- 1) Scaling of the number of thimbles in the thermodynamic limit: one- or many-thimble regime?
- 2) Connection of the thimbles decomposition to the physics, in particular its reaction on the phase transition.

Lefschetz thimbles decomposition (2)



a) μ =0; b...d) increasing μ

Motivation (2)

Cond-mat algorithms:

Exact evaluation of fermionic forces and fermionic determinant (BSS-QMC)

Lattice field theory:

Gradient flow equations for continuous auxiliary fields

Ultimate goal is twofold:



Better understanding of the structure of path integral

 Better understanding of the Lefschetz thimbles decomposition for large enough lattices, which factors influence its complexity, and if it's possible to weaken the residual sign problem.
 to formulate some approximate theory which might be applicable to the regions of the phase diagram, where lattice simulations are not working (e.g. at non-zero chemical potential, lattice models with frustration, etc)

Exact calculation of fermonic forces (1)

 $\operatorname{Re} \varphi$

 $S = S_b + \ln \det M$

Staggered fermions:

$$\begin{split} M_{i,j}^{st} &= 2am\delta_{i,j} + \left(\eta_{i,1}e^{\mu a}U_{i,1}\delta_{i+\hat{1},j} - \eta_{j,1}U_{j,1}^{\dagger}e^{-\mu a}\delta_{i-\hat{1},j}\right) + \sum_{\nu=2}^{4} \left(\eta_{i,\nu}U_{i,\nu}\delta_{i+\hat{\nu},j} - \eta_{j,\nu}U_{j,\nu}^{\dagger}\delta_{i-\hat{\nu},j}\right) \\ M^{st}(U) &= & \eta_{i,\nu} = \left(-1\right)^{i_1+\ldots+i_{\nu-1}} \\ \begin{pmatrix} B_1 & e^{\mu a}[U_{(1,x),1}] & 0 & 0 & 0 & \ldots & e^{-\mu a}[U_{(N_{\tau},x),1}^{\dagger}] \\ -e^{-\mu a}[U_{(1,x),1}^{\dagger}] & B_2 & e^{\mu a}[U_{(2,x),1}] & 0 & 0 & \ldots & 0 \\ 0 & -e^{-\mu a}[U_{(2,x),1}^{\dagger}] & B_3 & \ddots & 0 & \ldots & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & \ddots & \ldots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \ldots & 0 & -e^{-\mu a}[U_{(N_{\tau-1},x),1}^{\dagger}] & B_{N_{\tau}} - e^{\mu a}[U_{(N_{\tau-1},x),1}] \\ -e^{\mu a}[U_{(N_{\tau},x),1}] & 0 & \ldots & 0 & 0 & -e^{-\mu a}[U_{(N_{\tau-1},x),1}^{\dagger}] & B_{N_{\tau}} \end{pmatrix} \end{split}$$

(in terms of spatial $N_s \times N_s$ blocks)

Exact calculation of fermonic forces (2)

Following A. Hasenfratz and D. Toussaint, Nuclear Physics B 371, 539 (1992)

$$\overline{M}^{st}(U) = \begin{pmatrix} 1 & D_1 & 0 & 0 & 0 & \dots \\ 0 & 1 & D_2 & 0 & 0 & \dots \\ 0 & 0 & 1 & D_3 & 0 & \dots \\ 0 & 0 & 0 & 1 & D_4 & \dots \\ \vdots & & & \ddots & \\ -D_{2N_{\tau}} & 0 & 0 & & \dots & 1 \end{pmatrix}$$

Inverse fermionic operator:

$$\overline{M}^{st^{-1}}(U) = \begin{pmatrix} g_1 & \dots & \dots & \overline{g}_{2N_{\tau}} \\ \overline{g}_1 & g_2 & \dots & \dots & \dots \\ \dots & \overline{g}_2 & g_3 & \dots & \dots \\ \dots & \dots & \overline{g}_3 & g_4 & \dots & \dots \\ \vdots & & \ddots & \vdots & & \ddots \\ \dots & \dots & \dots & \dots & g_{2N_{\tau}} \end{pmatrix}$$

$$D_{2k} = \begin{pmatrix} e^{\mu a} [U_{(k,x),1}] & 0 \\ 0 & e^{\mu a} [U_{(k,x),1}] \end{pmatrix}$$
$$D_{2k-1} = \begin{pmatrix} B_k & I \\ I & 0 \end{pmatrix}, \ k = 1...N_{\tau}$$

$$\frac{\partial \ln \det M}{\partial \Phi} = \operatorname{Tr} \left(M^{-1} \frac{\partial M}{\partial \Phi} \right)$$

Iterations for blocks of fermonic propagator:

$$\bar{g}_{i+1} = D_{i+1}^{-1} \bar{g}_i D_i$$
 $N_s^3 N_{\tau}$ - scaling

«seed» blocks for iterations - from Schur complement solver [arXiv 1803.05478]

Recovering the saddle points from Hybrid Monte Carlo data



Flow time

S

reetern





Dispersio energy (C)





gnetic orderir introduce

ws that over a rticle gap me ks the stagge strong indica the only relev directly the s r ith the histace ynomial extr so obtained, ormed. H_t

an unusual 1 1 0

in graphene. The situation resembles the chiral symmetry breaking in QCD. Recently the Hybrid Monte-Carlo method wa for a studying of graphene electronic properties. Several types of mass term are possible due to several kinds transitions. Sign problem appears in fermionic determinant in case of mass term which corresponds to the excitor transition. A brief discussion concerning ways to solve this problem is presented.

:tronic properties:

miltonian for the electrons at p₋ orbitals:

$$(\hat{a}_{y,s}^+ \hat{a}_{x,s} + \hat{a}_{x,s}^+ \hat{a}_{y,s})$$

the electron at the site x with spin $s=\pm 1$,

$$n = 2.7e^{-1}$$

K and K' points in Brillouine zone. Due to this fact the lownponent massless Dirac fermions:

Chiral (sublattice) symmetry breaking in graphene

There are several possible channels of the «chiral symmetry» breaking in graphene. These channels correspond to appearance of different condensates. The following condensate are in the focus of research at the moment:

$$ar{\psi}_{m{a}}\sigma_3^{m{a}b}\psi_b$$
 - antiferromagnetic condensate

excitonic condensate



From microscopic point of view, antiferromagnetic condensate corresponds to opposite spins of electrons at different sublatt Excitonic condensate corresponds to opposite charge excess at different sublattices.

Hybrid Monte-Carlo simulations of graphene

After the standart Suzuki-Trotter decomposition we arrive at the following representation of the euc partition function: \bigcirc

$$\operatorname{Tr}(e^{-(H_{tb}+H_{C})\beta}) \approx \operatorname{Tr}(e^{-H_{tb}\delta}Ie^{-H_{C}\delta}Ie^{-H_{tb}\delta}Ie^{-H_{C}\delta}Ie^{-H_{C}\delta}I.....)$$

$$\bigcup_{\mathrm{Tr}} e^{-\beta\hat{H}} = \int \mathcal{D}\varphi_{r,p} \mathcal{D}\psi_{\mathbf{p}p} \mathcal{D}\eta_{x,n} \mathcal{D}\bar{\psi}_{x,n} \mathcal{D}\eta_{x,n} e^{-\frac{\delta}{2}\sum_{x,y,n}\varphi_{x,n}V_{xy}^{-1}\varphi_{y,n} - \sum_{x,y,n,n'}(\bar{\eta}_{x,n}M_{x,y,n,n'}^{el}\eta_{y,n'} + \bar{\psi}_{x,n})}$$

We need to introduce artificial mass gap in fermionic operator in order to make it invertible. Usually this mas correspond to the condensate which behaviour we want to study. Crucial point in the calculations is the operators for electrons $M^{el.}$ and holes $M^{h.}$ are comlex conjugated to each other only in antiferromagnetic mass term.

Therefore, if we want to study excitonic condensate, the sign problem appears due to the corresponding mass term in fermionic operator. $S_{QUAFE} = U_{U} + U_{U} +$

We may simulate the theory without

We introduce «electrons» and «holes»:

Dispersion relation c

energy excitations ca

 $H = \int e^{i \frac{\widehat{\psi}}{\widehat{q}}} \frac{0.6}{0.4}$ $\hat{D} = -iv \qquad 0$

$$\hat{a}_x = \hat{a}_{x,1} \qquad \hat{b}_x = \begin{cases} \hat{a}_{x,-1}^+, x \in \text{sublattice } 0\\ -\hat{a}_{x,-1}^+, x \in \text{sublattice } 1 \end{cases}$$

Free fermions with only nearest-neighbor hoppings:

0.8

0.6

 $V_{\rm F} \sim 1/300 \ c$. So the effective coupling constant is

 $\alpha = 300/137 \sim 2$. We have a theory with very

strong instantaneous Coulomb interaction

-3 -2

-10 1 2 3

Density of States, Honeycomb

O After it the Hamiltonian takes the form: $\hat{H} = \hat{H}_C + \hat{H}_{th}$

$$\mathcal{R}_{\hat{H}_{tb}} = -\kappa \sum_{\langle x,y \rangle} \left(\hat{a}_y^+ \hat{a}_x + \hat{b}_y^+ \hat{b}_x + h.c. \right)$$

where
$$\hat{q}_x = \mathcal{R}_x^+ \hat{a}_x - \hat{b}_x^+ \hat{b}_x$$
 is electric charge at site x.

Interaction takes the form:
$$\hat{H}_C = \frac{1}{2} \sum_{xy} V_{xy} \hat{q}_x \hat{q}_y$$

Hubbard model on bipartite lattice (2) $\mathcal{Z} = \operatorname{Tr} e^{-\beta \hat{H}} \approx \operatorname{Tr} \left(e^{-\delta \hat{H}_{(2)}} e^{-\delta \hat{H}_{(4)}} e^{-\delta \hat{H}_{(2)}} e^{-\delta \hat{H}_{(4)}} ... \right)$

Discrete auxiliary fields (BSS-QMC):

Continuous auxiliary fields:

$$\frac{U}{2}(\hat{n}_{el.} - \hat{n}_{h.})^{2} = \frac{\alpha U}{2}(\hat{n}_{el.} - \hat{n}_{h.})^{2} - \frac{(1 - \alpha)U}{2}(\hat{n}_{el.} + \hat{n}_{h.})^{2} + (1 - \alpha)U(\hat{n}_{el.} + \hat{n}_{h.})$$

$$e^{-\frac{\delta}{2}\sum_{x,y}U_{x,y}\hat{n}_{x}\hat{n}_{y}} \cong \int D\phi_{x}e^{-\frac{1}{2\delta}\sum_{x,y}\phi_{x}U_{xy}^{-1}\phi_{y}}e^{i\sum_{x}\phi_{x}\hat{n}_{x}}, \quad \text{Fierz identities:}$$

$$\alpha = 0...1 e^{\frac{\delta}{2}\sum_{x,y}U_{x,y}\hat{n}_{x}\hat{n}_{y}} \cong \int D\phi_{x}e^{-\frac{1}{2\delta}\sum_{x,y}\phi_{x}U_{xy}^{-1}\phi_{y}}e^{\sum_{x}\phi_{x}\hat{n}_{x}} \quad \delta_{b}^{a}\delta_{d}^{c} = \frac{1}{2}\delta_{d}^{a}\delta_{b}^{c} + \frac{1}{2}\sum_{i}\sigma^{(i)a}\sigma^{(i)c}_{b}$$

$$(\bar{a}O_{i}b)(\bar{c}O^{i}d) = \sum_{k}C_{ik}(\bar{a}O_{k}d)(\bar{c}O^{k}b)$$

$$\mathcal{Z}_{c} = \int \mathcal{D}\phi_{x,\tau}\mathcal{D}\chi_{x,\tau}e^{-S_{\alpha}}\det M_{el.}\det M_{h.},$$

$$S_{\alpha}[\phi_{x,\tau},\chi_{x,\tau}] = \sum_{x,\tau} \left[\frac{\phi_{x,\tau}^{2}}{2\alpha\delta U} + \frac{(\chi_{x,\tau} - (1 - \alpha)\delta U)^{2}}{2(1 - \alpha)\delta U}\right] \quad M_{el.,h.} = I + \prod_{\tau=1}^{N_{\tau}} \left[e^{-\delta(h\pm\mu)}\operatorname{diag}\left(e^{\pm i\phi_{x,\tau} + \chi_{x,\tau}}\right)\right]$$

Examples of the thimbles decomposition for the Hubbard model on hexagonal lattice(2)



Spin-coupled auxiliary field

Examples of the thimbles decomposition for the Hubbard model on hexagonal lattice(2)



Examples of the thimbles decomposition for the Hubbard model on hexagonal lattice(2)

Mixed regime: both field are present. One-thimble regime possible even at strong coupling.



It means that we can use unphysical degrees of freedom in the path integral representation to optimize the structure of thimbles decomposition.

Connection to the sign problem(1)



Spin-coupled field: only real saddle points (due to fermionic determinant being real)

Connection to the sign problem(2)

 $\mu = 0$



thimble1 (+) thimble2 (+)(both charge-, and spin-Mixed case coupled fields): complex saddle points. general scheme <u>of</u>_{det M}the search a) algorithm; b) c) examples of iterations

-- det M_h

 $- - \det M_e$

0.8

0.6

0.4

0.2

0.0





a) *α*=0.9; b) *a*=0.8

Summary(1)

Using non-iterative solvers we can compute exact derivatives of the fermonic determinant with respect to bosonic fields. It allows us to solve the gradient flow equations for relatively large lattices taking into account the fermonic back reaction on bosonic fields.

Thus, we can find both real and complex saddle points and describe the structure of the thimbles decomposition approaching thermodynamic limit.

Using this information we can optimize the structure of the thimbles decomposition, which is actually formulation-dependent.

In particular, we demonstrated that at least in one example of strongly correlated model with lattice fermions, we can find the representation where only one thimble survives in thermodynamic limit even at the phase transition or in the strong coupling regime.

TODO algorithms for sampling following curved manifolds in complex space

Instantons for charge-coupled auxiliary field



Saddle point field configurations are localised both in space and Euclidean time, hence many-instanton saddles are equidistant in action

Analytical description of instantons
with fermonic back reaction (1)

$$S = \frac{\sum_{x,\tau} (P_{x}^{\tau})^{2}}{2U_{A}\tau} - \ln \det \left(I + \prod e^{-a\tau H} e^{ip_{x}^{\tau}} \right) - - \ln \det \left(I + \prod e^{-a\tau H} \left\{ e^{-ip_{x}^{\tau}} \right\} \right) - \ln \det \left(I + \prod e^{-a\tau H} \left\{ e^{-ip_{x}^{\tau}} \right\} \right)$$

$$\frac{S}{p_{x}^{\tau}} = \frac{P_{x}^{\tau}}{U_{A}\tau} - \left[\overline{g}_{xx}^{\tau} e^{ip_{x}^{\tau}} - i \left(\overline{g}_{xx}^{\tau} \right)^{*} e^{-ip_{x}^{\tau}} \right] = 0 \quad \text{(saddle point)}$$

$$= \sum \text{ we need to add equations for } \overline{g}_{xx}^{\tau} \quad \text{(saddle point)}$$

$$\overline{g}_{x}^{\tau+1} = \left\{ e^{-ip_{x}^{\tau+1}} \right\} e^{a\tau H} \overline{g}_{x}^{\tau} \left\{ e^{ip_{x}^{\tau}} \right\} e^{-a\tau H}$$

$$= \sum p_{x}^{\tau} - U \operatorname{Im} \overline{g}_{xx}^{\tau}$$

Analytical description of instantons with fermonic back reaction (2) Final system of equations for propagator in continuous time: $\varphi_x^T = -\mathcal{U} \operatorname{Im} \overline{g}_{2\pi}^T$ $\begin{cases} \overline{g}_{xx}^{(T)} = -\partial \overline{g}_{xy}^{(T)} (\overline{g}_{xy} - \overline{g}_{yx}) \\ c_{x,y}^{(T)} (\overline{g}_{xy} - \overline{g}_{yx}) \end{cases}$ $\frac{1}{9} \frac{1}{2} \frac{1$ $\frac{d(\hat{a}_{x}^{\dagger}\hat{a}_{x})}{d\tau} = -\mathcal{R}\sum_{x,y} \left(\hat{a}_{y}^{\dagger}\hat{a}_{x} - \hat{a}_{x}^{\dagger}\hat{a}_{y}\right)$ $d(\hat{a}_{x}^{\dagger}\hat{a}_{y})$ $\frac{d(\hat{a}_{x}^{\dagger}\hat{d}_{y})}{d\tau} = (\hat{\lambda}\hat{a}_{y}^{\dagger}\hat{d}_{x}(\hat{b}_{x}^{\dagger}\hat{b}_{x}-\hat{b}_{y}^{\dagger}\hat{b}_{y})-\mathcal{R}\left(\sum_{\substack{x = 1 \\ z \neq y}}^{z}\hat{a}_{x}^{\dagger}-\sum_{\substack{x \neq 1 \\ z \neq x}}^{z}\hat{a}_{y}\hat{d}_{z}\right)$ Mean field approximation: $\langle \hat{a}_{x}^{\dagger}\hat{a}_{y}\hat{b}_{x}\hat{b}_{x}\rangle = g_{xy}g_{yy}^{\dagger}$

Hessians and continuum limit Degenerate saddle: 7 ly lr f3 m Tcenter Tcenter continuous symmetry: Zero mode in hessian H Tcenter $L = \mathcal{N}_{\tau} \left| \overline{\varphi}(\tau_c) - \overline{\varphi}(\tau_{c+1}) \right| = >$ dependent on st However: -hessian for fluctuations in perpendicular ìS directions 07-independent det Miss dependent on AT

Simple analytic partition function for non-interacting instantons (1)

All N-instanton saddle points + gaussian fluctuations around them.



Simple analytic partition function for non-interacting instantons (2) $\frac{2}{2} = 1 + \sum_{k=1}^{l} \frac{\beta N_s (\beta N_s - \beta \beta X) \dots (\beta N_s - (k-1) \beta X) x}{\kappa!}$ quantum of action of instantons Volume factors Svacuum $\times 2^{2\kappa} \mathcal{C}^{-S_{0}\kappa} \left(\left(\frac{\det \mathcal{H}_{0}}{2^{3\nu}} \right)^{\frac{1}{2}} \frac{L}{B} \right)^{\kappa} = \operatorname{length} \operatorname{of} \operatorname{orBit} \operatorname{in configura-tion space}_{\operatorname{tion space}}$ combinatorial factor: Sublattice + (instanton-anti-instanton) $K_{ma} \stackrel{\simeq}{\to} \frac{3^{3}}{43^{3}} \frac{N_{s}}{\chi} = \int f = f_{0} - \frac{1}{43^{3}} \ln\left(1 + \frac{4e^{-3}}{3^{3}} \frac{1}{2} \ln\left(1 + \frac{4e^{-3}}{3^{3}} \frac{1}{2} \ln\left(1 + \frac{4e^{-3}}{3^{3}} \frac{1}{2} \ln\left(1 + \frac{4e^{-3}}{3^{3}} \frac{1}{2} \ln\left(1 + \frac{1}{3^{3}} \frac{1}{3^{3}} \ln\left(1 + \frac{1}{3^{3}} \frac{1}{3^{3}} + \frac{1}{3^{3}} + \frac{1}{3^{3}} + \frac{1}{3^{3}} + \frac{1}{3^{3}} \ln\left(1 + \frac{1}{3^{3}} \frac{1}{3^{3}} + \frac{1}{3^{3}} + \frac{1}{3^{3}} + \frac{1}{3^{3}} + \frac{1}{3^{3}} + \frac{1}{3^{3}} \ln\left(1 + \frac{1}{3^{3}} + \frac{$ Vacuum

Double occupancy from noninteracting instantons model



Double occupancy as the derivative of the free energy over U

Benchmark: density of instantons

AFM susceptibility from noninteracting instantons model



10

n

5

10

15

20

25

30

35

-5

-6

-7

We really described spin localization, but local spins are still in paramagnetic phase

Interaction of instantons: various factors



Example of interaction curves



Instanton and anti-instanton at nearestneighbour lattice sites Two instantons at the same lattice site

Summary (2)

The solution of gradient flow equations with fermions provided us with knowledge on both real and complex saddle points of the full action. This information can be used to construct quasi-classical approximation on the basis of saddle points field configurations and gaussian fluctuations around them.

Here we present example of such study for Hubbard model, where the detailed knowledge on the saddle points leads to the formulation of instantons gas model with either interacting or non-interacting instantons. Even simple non-interacting model already features at least some important properties of the initial quantum Hamiltonian: spin localization and growth of magnetic susceptibility. Since the saddle points do not change qualitatively away of half-filling, we can try to expand this model to non-zero chemical potential, where QMC doesn't work due to the sign problem.

Further directions: many-body interaction of instantons, tunnelling between different instanton sectors, another lattice models (QCD?)