Fermion positivity and the QMC sign problem

Congjun Wu

Department of Physics, UC San Diego

References
1. C. Wu, and S. C. Zhang, Phys. Rev. B 71, 155115 (2005).
2. Z. C. Wei, C. Wu , Y. Li, S. W. Zhang, T. Xiang, Phys. Rev. Lett. 116, 250601 (2016).
3. S. Xu, Y. Li, and C. Wu, Phys. Rev. X 5, 021032, (2015).

INT- Workshop March 21, 2017

Collaborators:

Shou-Cheng Zhang	(Stanford)
Tao Xiang	(IOP, Chinese Academy of Sciences)
Shi-Wei Zhang	(William & Mary)
Zhong-chao Wei	(IOP, Chinese Academy of Sciences)
Yi Li	(Johns Hopkins)

Thank Z. Cai, S. Capponi, T. X. Ma, D. Wang, L. Wang, Y. Wang, S. L. Xu, G. M. Zhang, D. Zheng, Z. C. Zhou for QMC collaborations.

Thank J. Hirsch, J. Kuti for helpful discussions

Supported by NSF, AFOSR

Outline

- Early efforts: solving the sign problem by factorization.

- Kramers positivity (Dirac and Majorana).

- Reflection positivity (Majorana)

QMC: stochastic method to tame the large Hilbert space

- Importance sampling over very small but representative portions.
- Fermion and frustrated spin systems → sign problem
- Auxiliary field QMC for fermions:

Blankenbecler, Scalapino, and Sugar, PRD 24, 2278 (1981)

Hubbard-Stratonovich(HS) → path integral over space-time HS fields

$$Z = \mathrm{Tr} e^{-\beta H} = \lim_{M \to \infty} \sum_{P} \rho_P$$

$$\rho_P = \mathrm{Tr} \prod_{k=1}^{M} e^{-\Delta\tau H_0} \, e^{-\Delta\tau H_I(\tau_k)} = \det(\mathrm{I} + \prod_{k=1}^{M} e^{-\Delta\tau h_0} e^{-\Delta\tau h_I(\tau_k)})$$

Sign problem: determinant not positive-definite

J. E. Hirsch, PRB 28, 4059 (1983)

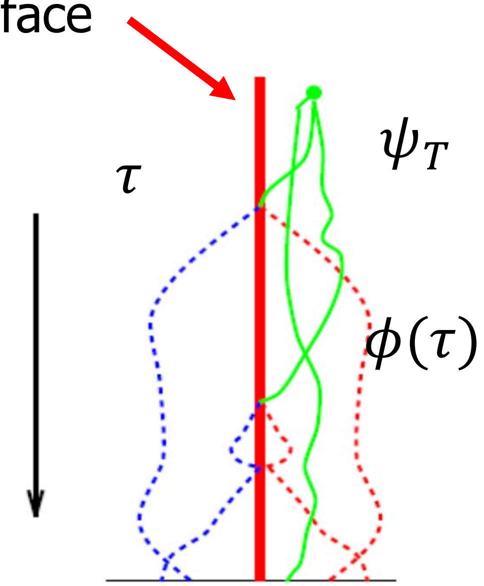
Early efforts in taming the sign-problem

- Meron-cluster method for path-integral QMC.

A config. of word-line is decomposed to clusters.
A cluster flipping sign is a meron.
Only meron-free configs. contribute to the partition function.

Chandrasekharan, Wiese, PRL 83, 3116 (1999).

- Constrained path QMC.



Random walks of Slater determinant states $\phi(\tau)$
Only keep paths with $\langle \phi(\tau) | \psi_T \rangle \geq 0$

S. W. Zhang, "QMC methods in Physics and Chemistry", Kluwer Academic, Dordrecht,1999.

The Hubbard model – factorization

$$H=-t\sum_{\langle ij\rangle}\{c_{i\sigma}^{+}c_{j\sigma}+h.c.\}-\mu\sum_{i}\hat{n}_{i}+U\sum_{i}(\hat{n}_{i\uparrow}-\tfrac{1}{2})\,(\hat{n}_{i\downarrow}-\tfrac{1}{2})$$

- U<0: density channel decomposition

$$\rho_P=\det(\mathrm{I}+\mathrm{B}),\;\; B=\prod_{k=1}^{M}\quad e^{-\Delta\tau h_0}e^{-\Delta\tau h_I(\eta_k)}=B_{\uparrow}\otimes B_{\downarrow}$$

$$\det(1+B_{\uparrow})=\det\left(1+B_{\downarrow}\ \right)\Rightarrow\;\rho_P\geq 0$$

-- no sign-problem.

- U>0: spin channel decomp. $B_{\uparrow}\neq B_{\downarrow}$ J. E. Hirsch, PRB 31, 4403, (1985).

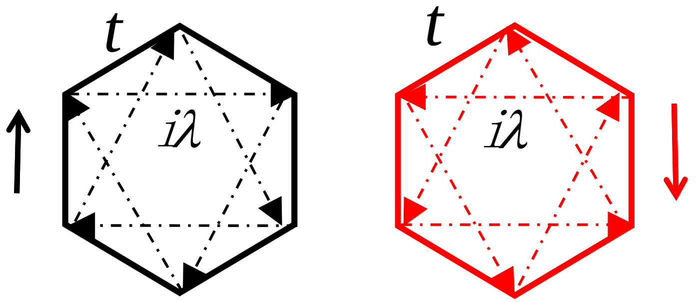
Half-filling (μ=0), bipartite lattice.

partial particle-hole (p-h) transformation: $c_{i\downarrow}\rightarrow(-)^{i}c_{i\downarrow}^{+}$

$$\det(1+B_{\uparrow})=const*\det\left(1+B_{\downarrow}\ \right)\Rightarrow\;\rho_P\geq 0$$

-- no sign-problem.

Kane-Mele-Hubbard – interacting topo-insulator



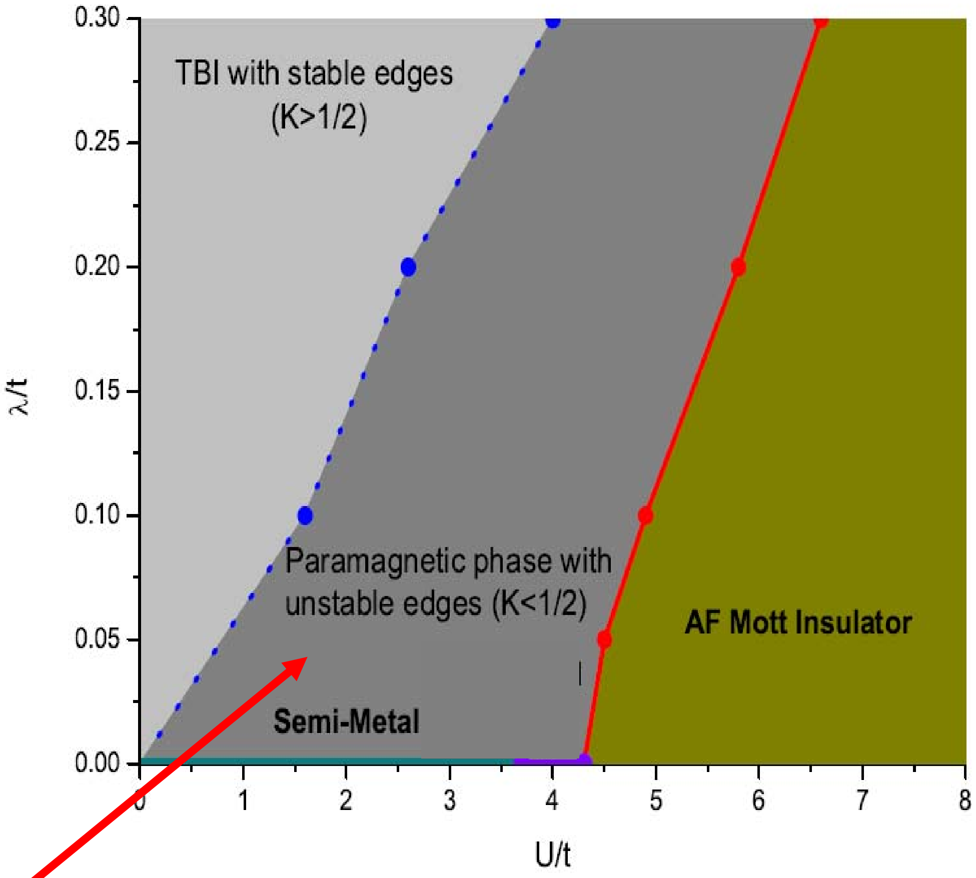
- Non-bipartite, complex hopping, S_z conserved.

- $\det(1 + B_\uparrow) = \det(1 + B_\downarrow\ )^*$

- Helical Luttinger edge liquid – Luttinger parameter K extracted.

- Destabilized edge but bulk remains non-magnetic.

C. Wu, Bernevig, S. C. Zhang PRL 96, 106401 (2006).



D. Zheng, G. M. Zhang, C.Wu, PRB 84, 205121 (2011).

Hohenadler, Lang, Assaad, PRL 106, 100403 (2011).

New principles needed!

- General solution is NP-hard!   Troyer and Wiese, PRL 94, 170201 (2005).

- Q: For a given model, what are the **sufficient and necessary** conditions that its sign problem can be eliminated?

- c.f. Algebraic equation root-finding.

Quintic equations and higher do not have **general solutions** using radicals.

New math: group theory

$$x^5 = a$$

Criterion that a ***given*** quintic or higher equation to be solvable:

Its **Galois group** is solvable.

- Sign problem → positivity problem → stimulate new math application and research?

Criteria for the absence of the sign problem

- Kramers positivity (Dirac)

S. Hands, et al, Eur. Phys. J. C 17, 285 (2000).
C. Wu and S. C. Zhang, Phys. Rev. B 71, 155115 (2005);

- Kramers positivity (Majorana)

Z. X. Li, Y. F. Jiang, H. Yao, PRB91, 24117 (2015)
Z. Wei, C. Wu, Y. Li, S. W. Zhang, and T. Xiang, PRL 116, 250601 (2016).

- Reflection positivity (Majorana)

Z. Wei, C. Wu, Y. Li, S. W. Zhang, and T. Xiang, PRL 116, 250601 (2016).

- Orthogonal split group L. Wang, M. Troyer et al, PRL 115, 250601 (2015).

- Topological aspect of the sign problem.

M. Lazzi, A. A. Soluyanov, M. Troyer et al, PRB 2016.

Kramers positivity (Dirac)

C. Wu and S. C. Zhang, PRB 2005; S. Hands, et al, Eur. Phys. J. C 17, 285 (2000).

- **Theorem 1**: For any HS field config., if there exists an anti-unitary *T*,

$$T^2 = -1, \qquad T h_0 T^{-1} = h_0, \qquad T h_I(\tau) T^{-1} = h_I(\tau)$$

then $\rho_P = \det(\mathrm{I} + B) \geq 0$, where $B = \prod_{k=1}^{M} e^{-\Delta\tau h_0} e^{-\Delta\tau h_I(\tau_k)}$

Proof:
- I+B may not be diagonalizable.
- Eigenvalues complex-conjugate pairwised (λ, λ^*).
- Real λ → double degeneracy.

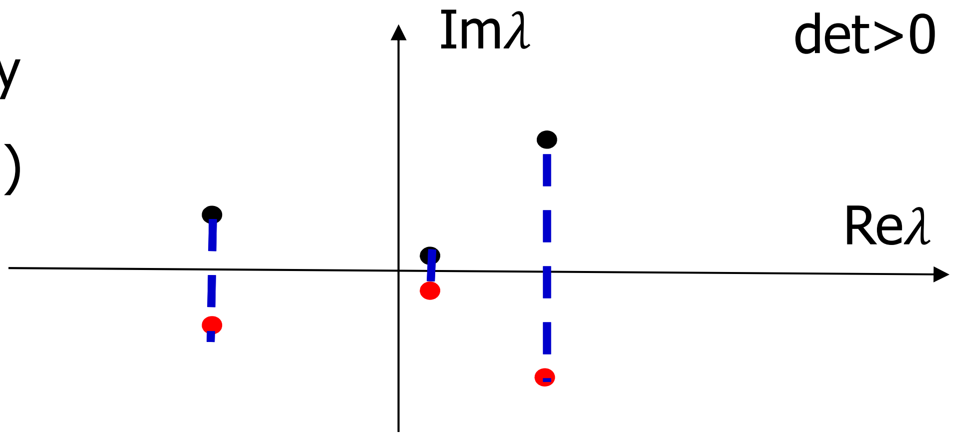
$$\det(I + B) = (\lambda_1 \lambda_1^*)(\lambda_2 \lambda_2^*) \cdots (\lambda_n \lambda_n^*) \geq 0$$

- T needs not be the physical time reversal (TR)-operator.

Eigenvalue distribution – random matrices

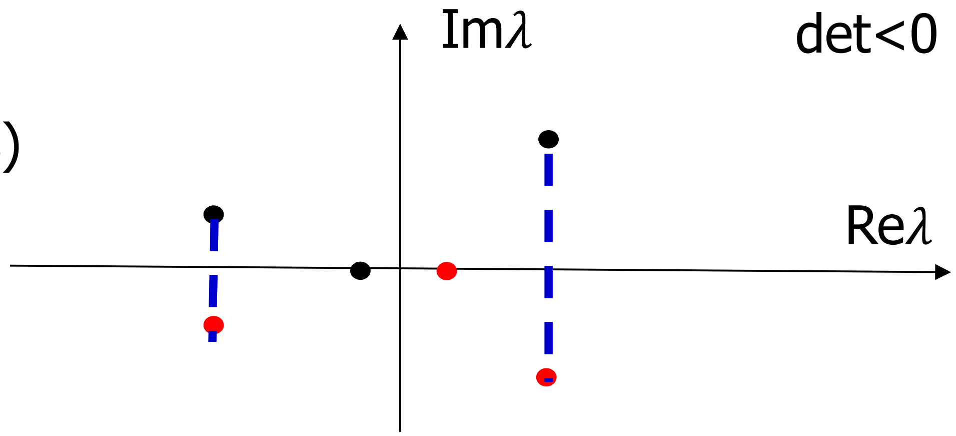
Kramers' positivity

(symplectic class)



Real decomp.

(orthogonal class)



A general criterion: symmetry principle

- Re-check the spin-1/2 Hubbard model.

$$T n T^{-1} = n, \quad T \vec{S} T^{-1} = -\vec{S}$$

- U<0: density decomp.→ Kramers positivity → no sign problem

- U>0: spin decomp. → T-odd → sign problem.

- Applicable in a wide class of large-spin and multi-band models at any doping level and lattice geometry.

The factorizibility of determinants is not required

Sp(4)-symmetry: spin-3/2 Hubbard model

$$H_0 = \sum_{\alpha=\pm\frac{3}{2},\pm\frac{1}{2}} - t\{c^+_{i,\alpha} c_{j,\alpha} + h.c.\} - \mu \sum_i c^+_{i,\alpha} c_{i,\alpha}$$

$$H_I = U_0 \sum_i P^+_{00}(i) P_{00}(i) + U_2 \sum_{i,m=\pm 2,\pm 1,0} P^+_{2m}(\vec{r}) P_{2m}(\vec{r})$$

Singlet (S=0) and quintet (S=2): $P^+_{sm}(i) = \sum_{\alpha\beta} \left\langle Sm \middle| \frac{3}{2}\frac{3}{2}\alpha\beta \right\rangle c^+_{i,\alpha}\, c^+_{i,\beta}$

- Γ-matrices: $\{\Gamma^a, \Gamma^b\} = 2\delta_{ab}$, $\Gamma^{ab} = \frac{i}{2}[\Gamma^a, \Gamma^b]$, $(1 \leq a < b \leq 5)$

$n = c^+ c$ $\qquad$ $n_a = c^+ \Gamma^a c$

density $\qquad$ spin-quadrupole

TR even

$L_{ab} = c^+ \Gamma^{ab} c$

Sp(4): 3 spin + 7 spin-octupole:

TR odd

C. Wu, J. Hu and S. C. Zhang, PRL91, 186402 (2003).

Sign-problem free QMC away from half-filling

- Express H_I by TR invariant operators.

$$H_I = - \sum_{i,1\le a\le 5} \{V(n(i) - 2)^2 + W n_a^2(i)\}$$

- Sign-problem free at V, W>0

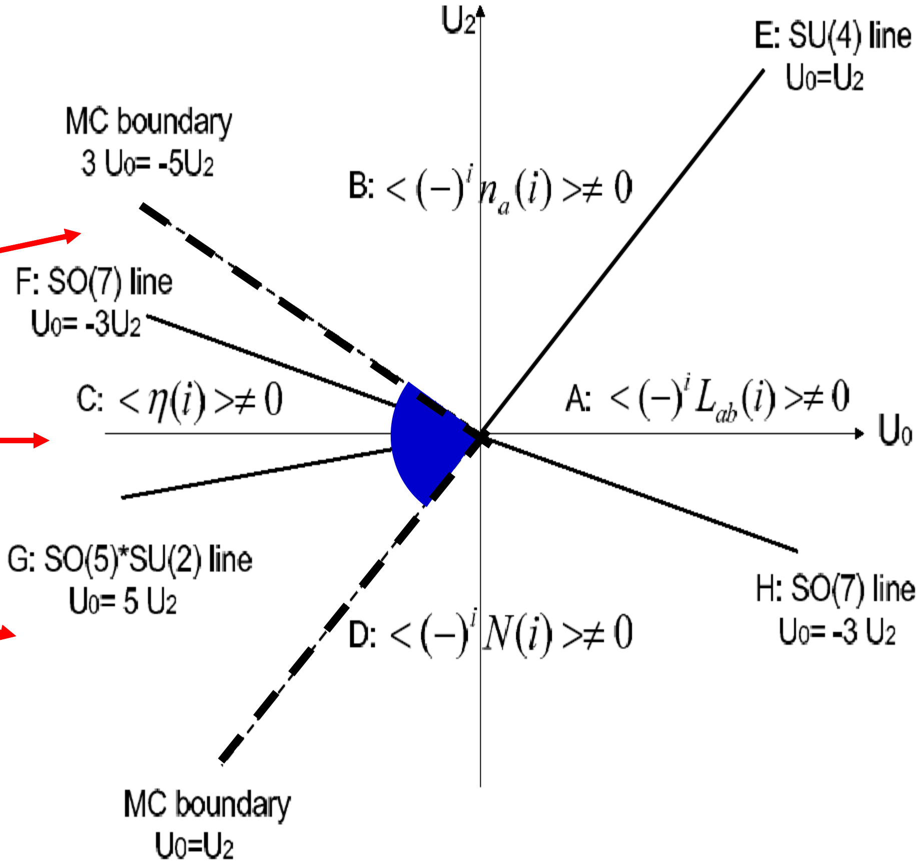
antiferro-spin-quadrapole (AFQ)

supercond. (SC)

charge-density-wave (CDW)

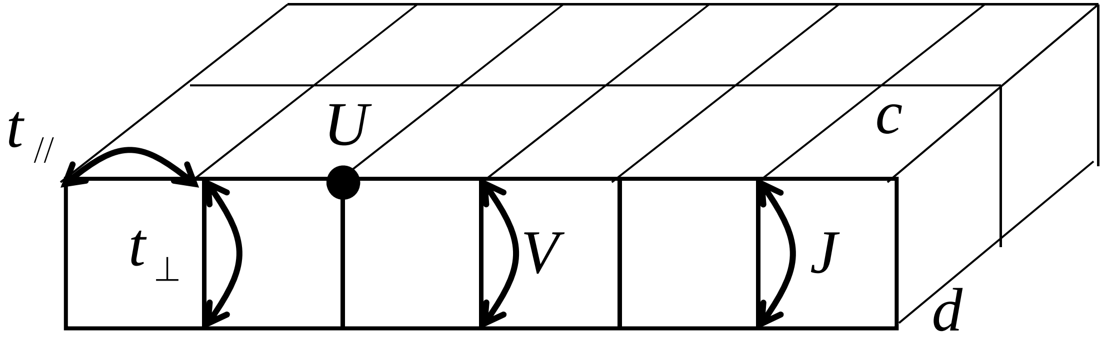
- Away from half-filling → AFQ, SC, CDW, and quartetting (α-**particle-like**).

phase diagram



C. Wu, Hu and Zhang, PRL91, 186402 (2003).

Spin-$\frac{3}{2}$ system mapped to spin $\frac{1}{2}$ bilayer



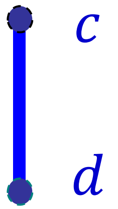
Scalapino-Zhang-Hanke model, PRB 1998.

$$H = -t_{//}\sum_{\langle ij\rangle}\{c^{+}_{i\sigma}c_{j\sigma} + d^{+}_{i\sigma}d_{j\sigma} + h.c\} - t_{\perp}\sum_{i}\{c^{+}_{i\sigma}d_{j\sigma} + h.c\} - \mu\sum_{i} n(i)$$

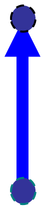
$$+J\sum_{\langle ij\rangle}\vec{S}_{ic}\cdot\vec{S}_{id} + U\sum_{i}(n_{i,\uparrow,c} - \tfrac{1}{2})(n_{i,\downarrow,c} - \tfrac{1}{2}) + (c\rightarrow d) + V\sum_{i}(n_{i,c} - 1)(n_{i,d} - 1)$$

- T=Time reversal × layer flip T-even operators

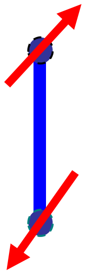
$$n_{bd}(i) = \frac{1}{2}(c^{+}_{i,\sigma}d_{i,\sigma} + d^{+}_{i,\sigma}c_{i,\sigma})$$



$$n_{cur}(i) = \frac{i}{2}(c^{+}_{i,\sigma}d_{i,\sigma} - d^{+}_{i,\sigma}c_{i,\sigma})$$



$$n_{AFM}(i) = \frac{i}{2}(c^{+}_{i}\vec{\sigma}c_{i} - d^{+}_{i}\vec{\sigma}d_{i}\ )$$



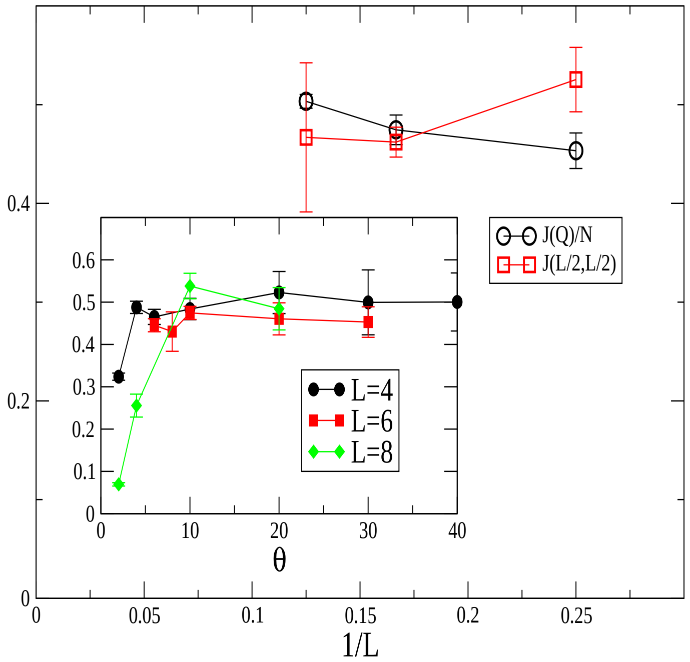
S. Capponi, C. Wu and S. C. Zhang, PRB 70, 220505 (R) (2004).

Staggered inter-layer current phase

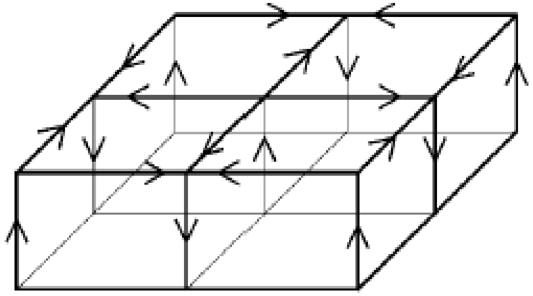
- High Tc, heavy fermion……

Long-range staggered current order:

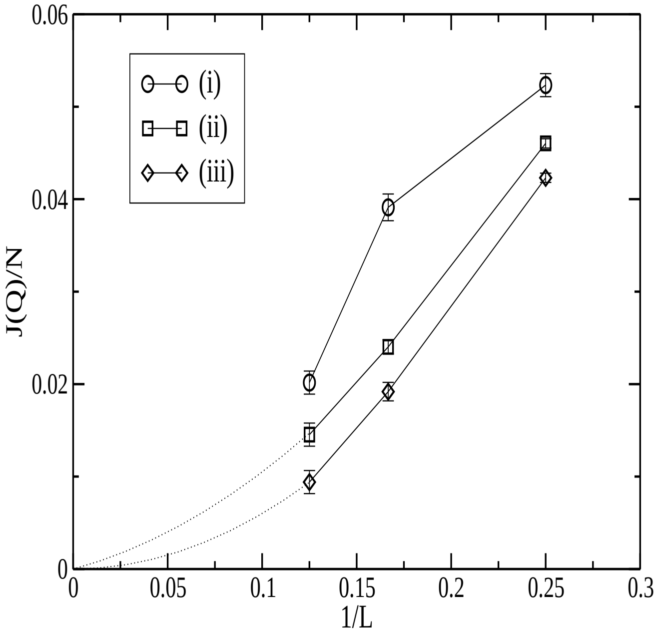
$t_\perp = 0.1, U = 0, V = 0.5,\ J = 2.$



S. Capponi, C. Wu and S. C. Zhang, PRB 70, 220505 (R) (2004).



suppression of order

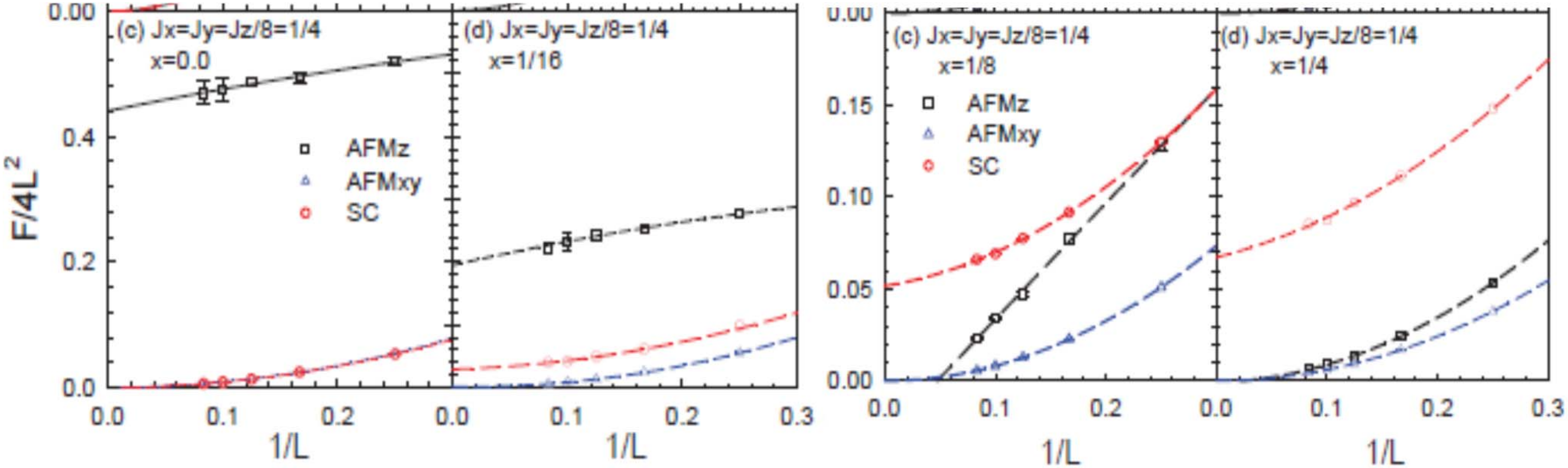


i) $t_\perp = 0.5$ ii) $U = V = 0.3, J = 1.6$

iii) 1/8-doping

Superconductivity from doping antiferromagnetism

$t_\perp = 0, U = 1, V = 0, J_z = 2.$



AFM order: $n_{AFM}(i) = \frac{i}{2}(c_i^+\vec{\sigma}c_i - d_i^+\vec{\sigma}d_i)$

SC order: $\Delta(i) = c_{i\uparrow}^+ d_{i\downarrow}^+ - c_{i\downarrow}^+ d_{i\uparrow}^+$

T. X. Ma, D. Wang, C. Wu,
in preparation (2017)

- Half-filling: AFM insulator.
- SC (extended s-wave) appears after doping.
- Microscopic model with 4-fermion interaction, no bosonic modes.

Other examples based on Kramers positivity

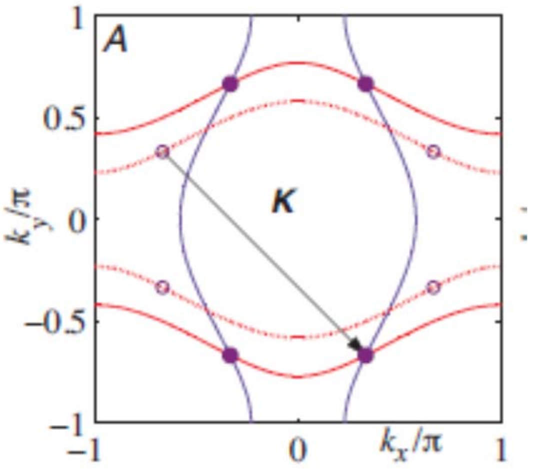
- Spin-orbit coupled negative-U Hubbard model. Spin-↑ and ↓ mixed → non-factorizable.

S.W. Zhang et al, PRL 2016.

- Another two-band model for SC and AFM. Interaction from coupling to bosonic mode. Invariant under time-reversal × $(\psi_y \rightarrow -\psi_y)$.

$$L_F = \sum_{i,j,\alpha=x,y} \psi^\dagger_{\alpha i}\left[(\partial_\tau - \mu)\,\delta_{ij} - t_{\alpha,ij}\right]\psi_{\alpha j} + \lambda \sum_i \psi^\dagger_{xi}\,(\vec{s}\cdot\vec{\varphi}_i)\,\psi_{yi} + H.c.,$$

$$L_\varphi = \frac{1}{2}\sum_i \frac{1}{c^2}\left(\frac{d\vec{\varphi}_i}{d\tau}\right)^2 + \frac{1}{2}\sum_{\langle i,j\rangle}(\vec{\varphi}_i - \vec{\varphi}_j)^2 + \sum_i \left(\frac{r}{2}\vec{\varphi}_i^2 + \frac{u}{4}(\vec{\varphi}_i^2)^2\right).$$



- Fermion coupled to gauge fields, or, local moments.

Assaad, Grover, PRX 2016. ……..

Gazit et al, Nat. Phys. 2016.

Berg, et al, Science 2012. .

Majorana representation

- Fermions bilinears: N fermion → 2N Majorana fermion

$$H_0 = \gamma^T V_0 \gamma, \quad H_I(\tau) = \gamma^T V_I(\tau)\gamma$$

Matrix kernels antisymm. $2N \times 2N$

$$O = \prod_{k=1}^{M} e^{-\Delta\tau V_0} e^{-\Delta\tau V_I(\tau_k)}$$

SO(2N,C) eigenvalues pairwised $(\Lambda_i, \Lambda_i^{-1})$

Z. X. Li, Y. F. Jiang, H. Yao, PRB91, 24117 (2015)

$$\rho_P = \mathrm{tr}O = \prod_{i=1}^{N}(\Lambda_i + \Lambda_i^{-1})$$

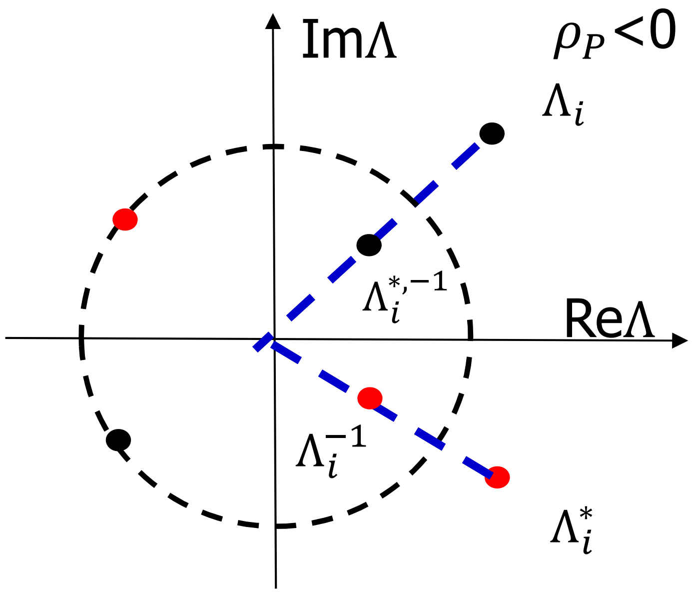
- Majorana Kramers symmetry: $T^{-1}VT = V$, and $T^2 = -1$, where $T = SK$.

- No guarantee for positivity!

$$(\Lambda_i, \Lambda_i^{-1}) \quad \Leftrightarrow (\Lambda_i^*, \Lambda_i^{*,-1})$$

Eigenvalues on the unit circle ➔

$$\Lambda \quad + \Lambda^{-1} = \Lambda \quad + \Lambda^* \quad < 0$$



Z. Wei, C. Wu, Y. Li, S. W. Zhang, and T. Xiang, PRL 116, 250601 (2016).

Majorana Kramers symmetry

- Theorem 2: In addition to the Kramers symmetry $T = SK$, if there exists a parity symmetry P satisfying

$$PVP^{-1} = V, \qquad PS = -SP$$

$P^2 = 1$: Hermitian

antisymmetic imaginary

or symmetric real

then $\rho_P \geq 0$.

- Case I: P is antisym. and imaginary → Dirac Kramers positivity

$Q = \frac{1}{4}\gamma^T P\gamma$ conserved as particle number.

- Case II: P is sym. and real, all V's are factorizable to complex conjugate pairs.

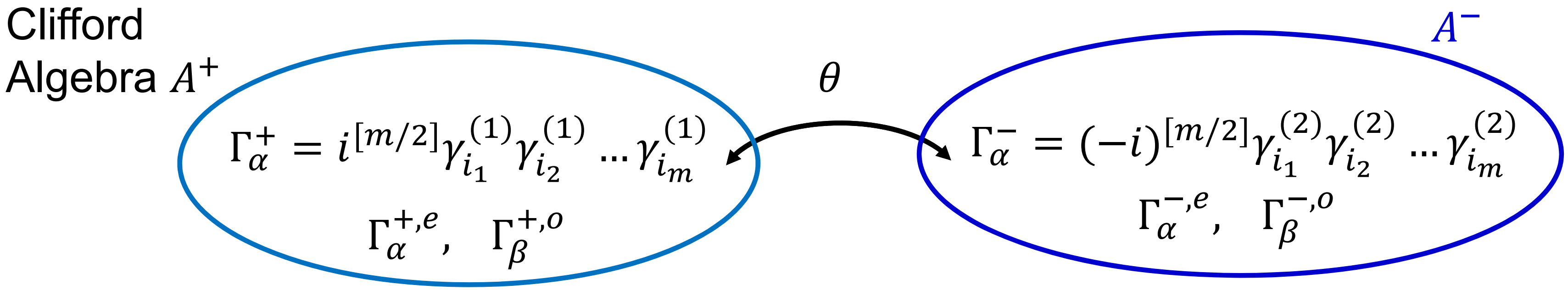
$$O^T V O = \begin{pmatrix} X & 0 \\ 0 & X^* \end{pmatrix}$$

Z. Wei, C. Wu, Y. Li, S. W. Zhang, and T. Xiang, PRL 116, 250601 (2016).

Majorana(MJ) reflection positivity

A. Jaffe and B. Janssens, arxiv 1506.04197

- Antilinear: $\theta(i) = -i,\ \theta\left(\gamma_i^{(1)}\right) = \gamma_i^{(2)},\ \theta\left(\gamma_i^{(2)}\right) = \gamma_i^{(1)},\ \ (i = 1, \ldots N).$



Clifford Algebra A^+

A^-

θ

$$\Gamma_\alpha^+ = i^{[m/2]}\gamma_{i_1}^{(1)}\gamma_{i_2}^{(1)} \ldots \gamma_{i_m}^{(1)}$$

$$\Gamma_\alpha^{+,e},\quad \Gamma_\beta^{+,o}$$

$$\Gamma_\alpha^- = (-i)^{[m/2]}\gamma_{i_1}^{(2)}\gamma_{i_2}^{(2)} \ldots \gamma_{i_m}^{(2)}$$

$$\Gamma_\alpha^{-,e},\quad \Gamma_\beta^{-,o}$$

- Physical operator $O \in A^+ \otimes A^-$ is reflection symmetric if $\theta(O) = O$.

- Inner product: $\langle Q|O|Q\rangle = Tr[Q^\circ\theta(Q)O]$

$$Q = \sum\nolimits_{\alpha\epsilon even} t_\alpha^e\,\Gamma_\alpha^{e,+} + \sum\nolimits_{\alpha\epsilon odd} t_\alpha^o\,\Gamma_\alpha^{o,+} \qquad Q \in A^+, \theta(Q) \in A^-$$

$$Q^\circ\theta(Q) = \sum\nolimits_{\alpha\beta} t_\alpha^e t_\beta^{e,*}\,\Gamma_\alpha^{+,e}\Gamma_\beta^{-,e} + i\sum\nolimits_{\alpha\beta} t_\alpha^o t_\beta^{o,*}\,\Gamma_\alpha^{+,o}\Gamma_\beta^{-,o}$$

- O is MJ-reflection-positive iff $\boldsymbol{\langle Q|O|Q\rangle \geq 0}$ **for all** $\boldsymbol{Q \in A^+ \Rightarrow Tr[O] \geq 0.}$

MJ-reflection-positive decomposition

- Time-evolution for a HS field config.: $O = \prod_{k=1}^{M} e^{-\Delta\tau H_0} e^{-\Delta\tau H_I(\tau_k)}$
- Fermion bilinears: $H_0 = \gamma^T V_0 \gamma,\ H_I(\tau) = \gamma^T V_I(\tau)\gamma$ with $\gamma^T = (\gamma_i^{(1)}, \gamma_i^{(2)})^T$
- Theorem 3: $\rho_P \geq 0$ if all V's can be expressed as

$$V = \begin{pmatrix} A & iB \\ -iB^T & A^* \end{pmatrix}$$

A, B $N \times N$ complex matrices.

A: antisymmetric $A^T = -A$

B: Hermitian, positive or negative definite

Proof: 1. $e^{-\Delta\tau H_0}$ and $e^{-\Delta\tau H_I}$ are MJ-reflection-positive

2. MJ-reflection-positive operators form a ring ➔
O is also MJ-refection-positive.

3. $\rho_P = Tr[O] \geq 0.$

Z. Wei, C. Wu, Y. Li, S. W. Zhang, and
T. Xiang, PRL 116, 250601 (2016).

Applicability

$$V = \begin{array}{c|c} \begin{array}{cc} \gamma_i^{(1)} & \gamma_i^{(2)} \end{array} & \\ \hline \begin{pmatrix} A & iB \\ -iB^T & A^* \end{pmatrix} & \begin{array}{c} \gamma_i^{(1)} \\ \gamma_i^{(2)} \end{array} \end{array}$$

A: antisymmetric $A^T = -A$

B: Hermitian, positive or negative definite

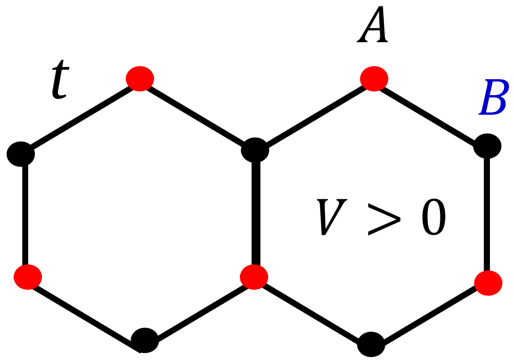
B=0:
1. factorizable Hubbard models: $\gamma_i^{(1)}$for spin-↑, $\gamma_i^{(2)}$ for spin-↓
2. spinless fermion models based on Majorana Reps, and orthogonal split group

   – Case II of the Kramers (Majorana) positivity

B≠0:
1. Particle-hole symmetry breaking
2. Kramers symmetry breaking

Particle-hole symmetry breaking

S. L. Xu, T. Xiang, C. Wu, in preparation.

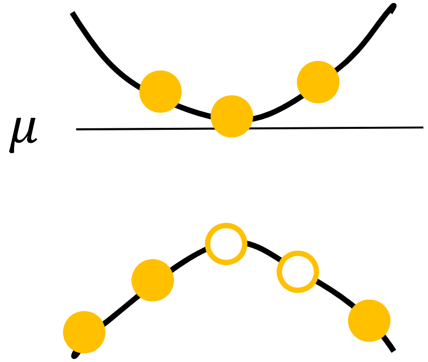


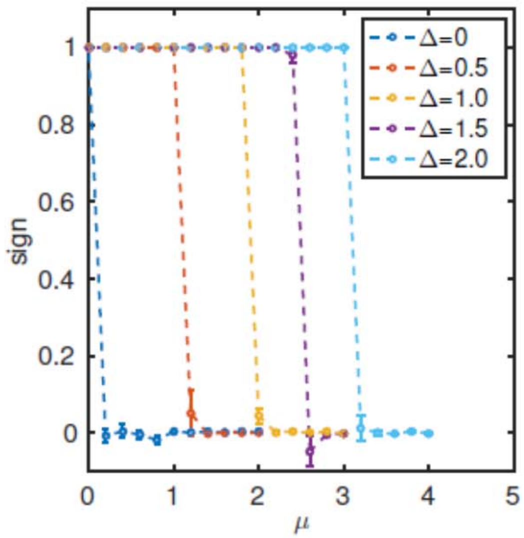
$$H_I = V \sum_{\langle ij\rangle}(n_i - \tfrac{1}{2})\,(n_j - \tfrac{1}{2})$$

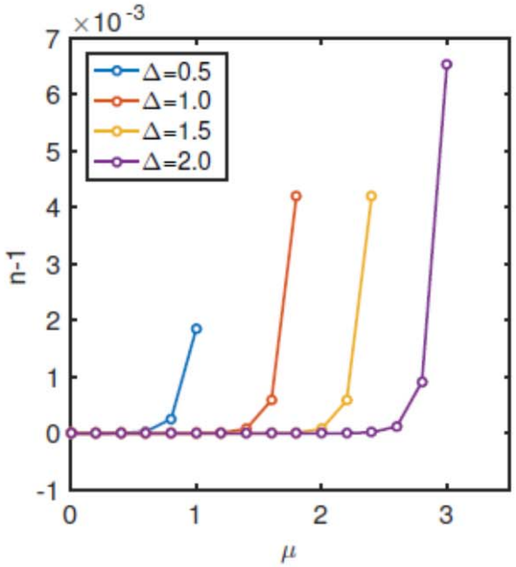
$$H_0 = \sum_{i\in A}(\Delta - \mu)c_i^+ c_i + \sum_{i\in B}(-\Delta - \mu)c_i^+ c_i - t\sum_{\langle ij\rangle}(c_i^+ c_j + h.c.)$$

$$B = \begin{pmatrix} \Delta + \mu & 0 \\ 0 & \Delta - \mu \end{pmatrix}$$ positive-definite at $\mu \leq \Delta$.

thermally excited particles from vacuum







β=10, t=V=1

QMC: itinerant ferromagnetism and Curie-Weiss (CW) metal

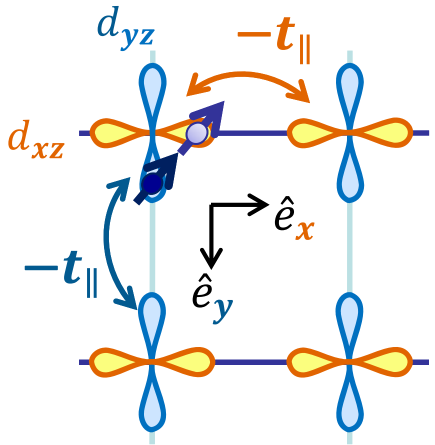
- Strong correlation physics – magnetism with Fermi surface, failure of Stoner criterion

- Proof to a stable itinerant FM phase, and QMC simulations – the first time to our knowledge.

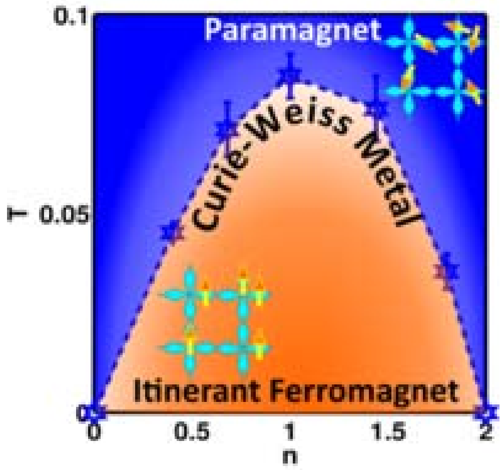
- 1D kinetic energy + 2D multi-orbital interactions – no-local moments.

- Peron-Frobenius sign structure → sign problem free.

1. CW-metal phase – dichotomy of charge coherence and spin incoherence.
2. Critical scaling near Curie temperatures.
3. Fermi distribution in the CW-metal phase.



Y. Li, E. H. Lieb and C. Wu PRL 2014.



S. Xu, Y. Li and C. Wu PRX 2015.

Summary: the positivity structure of the QMC sign problem

- Theorem 1: Kramers-positivity (Dirac)

$$T^2 = -1, \quad Th_0T^{-1} = h_0, \quad Th_I(\tau)T^{-1} = h_I(\tau)$$

- Theorem 2: Kramers-positivity (Majorana)

$$S^TVS = V^*, PVP^{-1} = V, PS = -SP$$

$S^2 = -1$: real antisymmetric,

$P^2 = 1$: Hermitian

- Theorem 3: Reflection positivity (Majorana)

$$V = \begin{pmatrix} A & iB \\ -iB^T & A^* \end{pmatrix}$$

A, B $N \times N$ complex matrices.

A: antisymmetric $A^T = -A$

B: Hermitian, positive or negative definite