Quantum Monte Carlo Methods for Fermion-Boson problems

Fakher F. Assaad (Autumn School on Correlated Electrons, Jülich 20th September 2018)

Outline:

- Fermion-Boson problems
  - Electron-Phonon, Su-Schrieffer-Heeger (SSH)
  - Unconstrained Gauge theories
  - "De-signer" Hamiltonians
- Auxiliary field Quantum Monte Carlo (QMC), Generalities
- Application of the Auxiliary field QMC to the SSH model
  - Sign-free formulation
  - Sampling, Hybrid Monte Carlo
- Conclusions

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Many thanks to

M. Hohenadler

J. Hofmann

S. Beyl

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Z. Wang

T. Sato

M. Ulybyshev

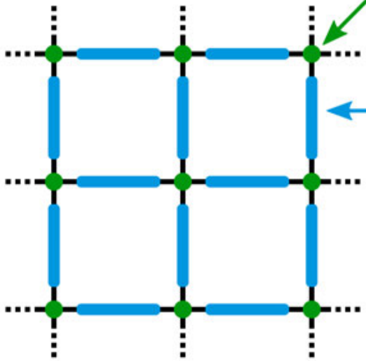
F. Parisen Toldin

J. Schwab

E. Huffman

Fermion-Boson problems: The Su-Schrieffer-Heeger (SSH) model

$$\boxed{\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \right) + g \sum_{\langle i,j\rangle,\sigma} \hat{X}_{\langle i,j\rangle} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \right) + \sum_{\langle i,j\rangle} \left[\frac{\hat{P}^2_{\langle i,j\rangle}}{2m} + \frac{k}{2}\hat{X}^2_{\langle i,j\rangle} \right]}$$



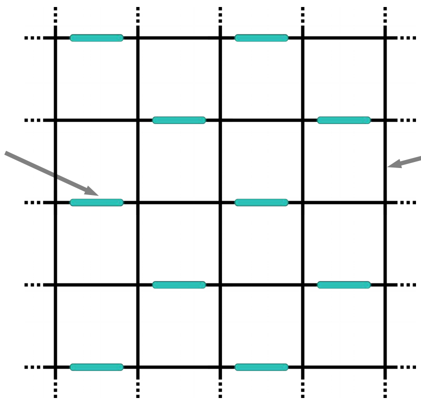
$$\boxed{\omega_0 = \sqrt{\frac{k}{m}}} \qquad \boxed{\left[\hat{X}_b, \hat{P}'_b\right] = i\hbar\, \delta_{b,b'}}$$

Limiting cases

$$\omega_0 = 0$$

Perfect nesting and Van-Hove singularity

$$\chi\left(\boldsymbol{Q}, i\Omega_m = 0\right) \propto \ln^2\left(\frac{W}{k_B T}\right)$$



Valence Bond Solid

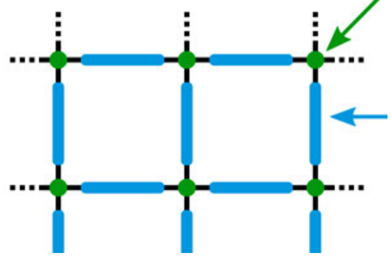
$$\omega_0 \rightarrow \infty$$

$$\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \right) \underbrace{- \frac{g^2}{4k} \sum_{\langle i,j\rangle} \left(\sum_{\sigma} \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \right)^2}_{\frac{g^2}{k}\sum_{\langle i,j\rangle} \hat{\boldsymbol{S}}_i \hat{\boldsymbol{S}}_j + \hat{\boldsymbol{\eta}}_i \hat{\boldsymbol{\eta}}_j}$$

Quantum antiferromagnet/ SSC + CDW

Fermion-Boson problems: The Su-Schrieffer-Heeger (SSH) model

$$\boxed{\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \right) + g \sum_{\langle i,j\rangle,\sigma} \hat{X}_{\langle i,j\rangle} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \right) + \sum_{\langle i,j\rangle} \left[\frac{\hat{P}^2_{\langle i,j\rangle}}{2m} + \frac{k}{2}\hat{X}^2_{\langle i,j\rangle} \right]}$$



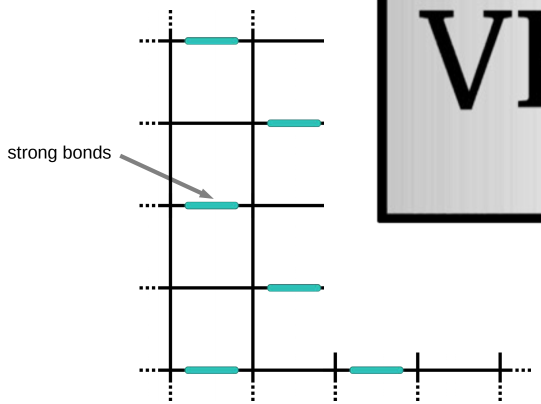
$$\boxed{\omega_0 = \sqrt{\frac{k}{m}}} \qquad \boxed{\left[\hat{X}_b, \hat{P}'_b\right] = i\hbar\, \delta_{b,b'}}$$

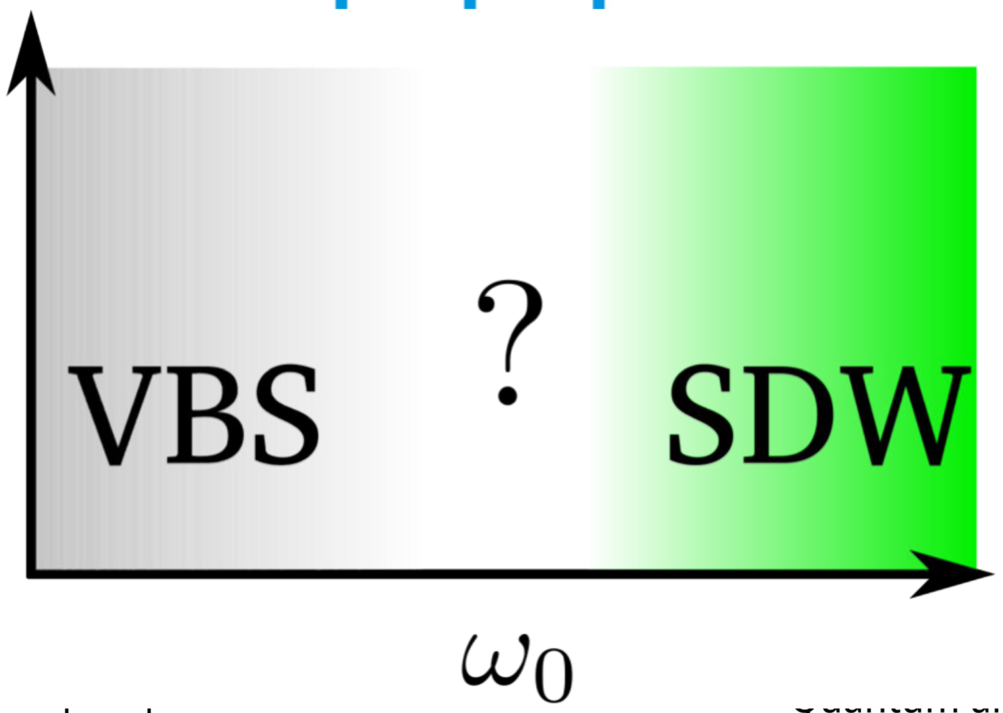
Limiting cases

$\omega_0 = 0$

Perfect nesting and Va

$\chi\left(\boldsymbol{Q}, i\Omega_m = 0\right) \propto \mathrm{l}$





∞

$_{\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \Big)$

$$\underbrace{\Big(\sum_{\sigma} \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \Big)^2}_{\sum_{\langle i,j\rangle} \hat{\boldsymbol{S}}_i\hat{\boldsymbol{S}}_j + \hat{\boldsymbol{\eta}}_i\hat{\boldsymbol{\eta}}_j}$$

Quantum antiferromagnet/ SSC + CDW

Fermion-Boson problems: The Su-Schrieffer-Heeger (SSH) model

Symmetries

$$\boxed{\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + g \sum_{\langle i,j \rangle,\sigma} \hat{X}_{\langle i,j \rangle} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right]}$$

Partial particle-hole symmetry

$$\hat{P}^{-1}_{\alpha} \hat{c}^{\dagger}_{\boldsymbol{i},\beta} \hat{P}_{\alpha} = \delta_{\alpha,\beta} e^{i\boldsymbol{Q}\cdot\boldsymbol{i}} \hat{c}_{\boldsymbol{i},\beta} + (1 - \delta_{\alpha,\beta}) \, \hat{c}^{\dagger}_{\boldsymbol{i},\beta}$$

$$\left[\hat{P}_{\alpha}, \hat{H} \right] = 0$$

$$\hat{P}^{-1}_{\uparrow} \hat{\boldsymbol{S}}_i \hat{P}_{\uparrow} = \hat{\boldsymbol{\eta}}_i$$

Time reversal symmetry

(Survives finite doping and and hence allows simulations at finite chemical potential)

$$\hat{T}^{-1} \alpha \begin{pmatrix} \hat{c}_{\uparrow} \\ \hat{c}_{\downarrow} \end{pmatrix} \hat{T} = \overline{\alpha} \begin{pmatrix} -\hat{c}_{\downarrow} \\ \hat{c}_{\uparrow} \end{pmatrix}$$

with

$$\hat{T}^2 = -1$$

Fermion-Boson problems: The Su-Schrieffer-Heeger (SSH) model

Symmetries

$$\boxed{\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + g \sum_{\langle i,j \rangle, \sigma} \hat{X}_{\langle i,j \rangle} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right]}$$

U(N) symmetry is manifest

$$\begin{pmatrix} \hat{c}_{i,1} \\ \vdots \\ \hat{c}_{i,N} \end{pmatrix} \rightarrow U \begin{pmatrix} \hat{c}_{i,1} \\ \vdots \\ \hat{c}_{i,N} \end{pmatrix}, \quad U^{\dagger} U = 1$$

Majorana fermions

$$\boldsymbol{i} \in A : \gamma_{\boldsymbol{i},1,\sigma} = \left(\hat{c}_{\boldsymbol{i},\sigma} + \hat{c}^{\dagger}_{\boldsymbol{i},\sigma} \right), \quad \gamma_{\boldsymbol{i},2,\sigma} = -i \left(\hat{c}_{\boldsymbol{i},\sigma} - \hat{c}^{\dagger}_{\boldsymbol{i},\sigma} \right)$$

$$\boldsymbol{i} \in B : \gamma_{\boldsymbol{i},2,\sigma} = - \left(\hat{c}_{\boldsymbol{i},\sigma} + \hat{c}^{\dagger}_{\boldsymbol{i},\sigma} \right), \quad \gamma_{\boldsymbol{i},1,\sigma} = -i \left(\hat{c}_{\boldsymbol{i},\sigma} - \hat{c}^{\dagger}_{\boldsymbol{i},\sigma} \right)$$

$$\{ \hat{\gamma}_{j,\alpha,\sigma}, \hat{\gamma}_{i,\beta,\sigma'} \} = 2 \delta_{i,j} \delta_{\alpha,\beta} \delta_{\sigma,\sigma'}$$

$$\boxed{\hat{H} = \sum_{\langle i,j \rangle, \alpha=1, \sigma}^{N,2} \frac{1}{2} \left(-t + g \hat{X}_{\langle i,j \rangle} \right) i \hat{\gamma}_{i,\alpha,\sigma} \hat{\gamma}_{j,\alpha,\sigma} + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right]}$$

O(2N) symmetry is now manifest

$$\begin{pmatrix} \hat{\gamma}_{i,1,1} \\ \vdots \\ \hat{\gamma}_{i,i,N} \\ \hat{\gamma}_{i,2,1} \\ \vdots \\ \hat{\gamma}_{i,2,N} \end{pmatrix} \rightarrow O \begin{pmatrix} \hat{\gamma}_{i,1,1} \\ \vdots \\ \hat{\gamma}_{i,i,N} \\ \hat{\gamma}_{i,2,1} \\ \vdots \\ \hat{\gamma}_{i,2,N} \end{pmatrix}, \quad O^T O = 1$$

Fermion-Boson problems: Unconstrained gauge theories

$$\hat{H} = \cancel{-t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right)} + g \sum_{\langle i,j\rangle,\sigma} \hat{X}_{\langle i,j\rangle} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + \sum_{\langle i,j\rangle} \left[\frac{\hat{P}^2_{\langle i,j\rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j\rangle} \right]$$

Bosonic variables. $\hat{b}^{\dagger}_{\langle i,j\rangle} = \dfrac{\omega m \hat{X}_{\langle i,j\rangle} - i\hat{P}_{\langle i,j\rangle}}{\sqrt{2\omega m}}$ $\qquad \omega_0 = \sqrt{\dfrac{k}{m}}$

$$\hat{H} = \sum_{\langle i,j\rangle} g \sqrt{\frac{1}{2\omega_0 m}} \left(\hat{b}^{\dagger}_{\langle i,j\rangle} + \hat{b}_{\langle i,j\rangle} \right) \sum_{\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + \omega_0 \sum_{b} \hat{b}^{\dagger}_{\langle i,j\rangle} \hat{b}_{\langle i,j\rangle}$$

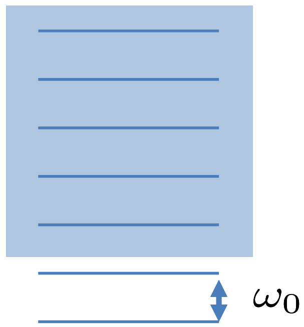
Local Z_2 conservation law

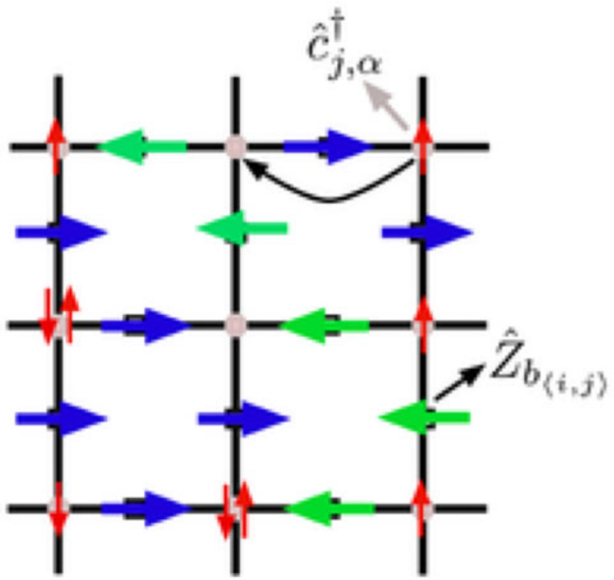
$$\hat{Q}_i = \underbrace{(-1)^{\hat{n}^b_{\langle i,i+a_x\rangle} + \hat{n}^b_{\langle i,i-a_x\rangle} + \hat{n}^b_{\langle i,i+a_y\rangle} + \hat{n}^b_{\langle i,i-a_y\rangle}}}_{\text{Boson parity on star}} \underbrace{(-1)^{\hat{n}^c_i}}_{\text{Fermion parity on site}} \qquad \left[\hat{H}, \hat{Q}_i \right] = 0$$

Fermion-Boson problems: Unconstrained gauge theories

$$\hat{H} = \sum_{\langle i,j \rangle} g \sqrt{\frac{1}{2\omega_0 m}} \left(\hat{b}^{\dagger}_{\langle i,j \rangle} + \hat{b}_{\langle i,j \rangle} \right) \sum_{\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + \omega_0 \sum_{b} \hat{b}^{\dagger}_{\langle i,j \rangle} \hat{b}_{\langle i,j \rangle}$$

Retain only one phonon excitation per bond, float $\sigma : 1 \cdots N$





$$\hat{H} = \sum_{\langle i,j \rangle} \hat{Z}_{\langle i,j \rangle} \left(\sum_{\alpha=1}^{N} \hat{c}^{\dagger}_{i,\alpha} \hat{c}_{j,\alpha} + \mathrm{H.c.} \right) - Nh \sum_{\langle i,j \rangle} \hat{X}_{\langle i,j \rangle}.$$

$h \rightarrow \omega_0$:

PHYSICAL REVIEW X **6,** 041049 (2016)

Simple Fermionic Model of Deconfined Phases and Phase Transitions

F. F. Assaad[1] and Tarun Grover[2,3]

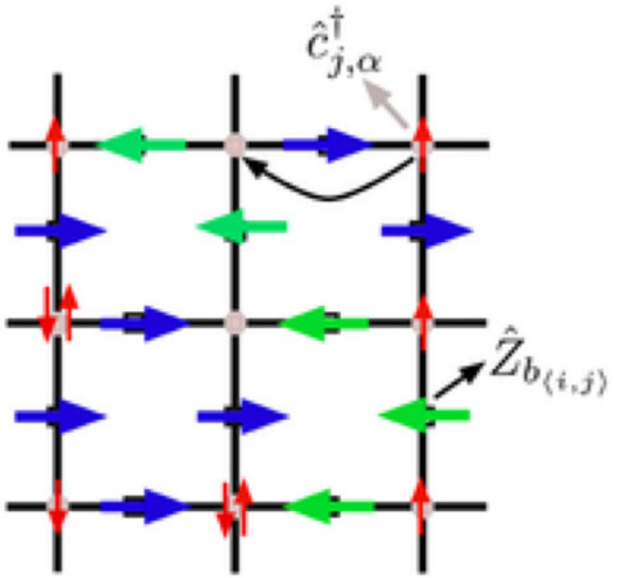
Fermion-Boson problems: Unconstrained gauge theories

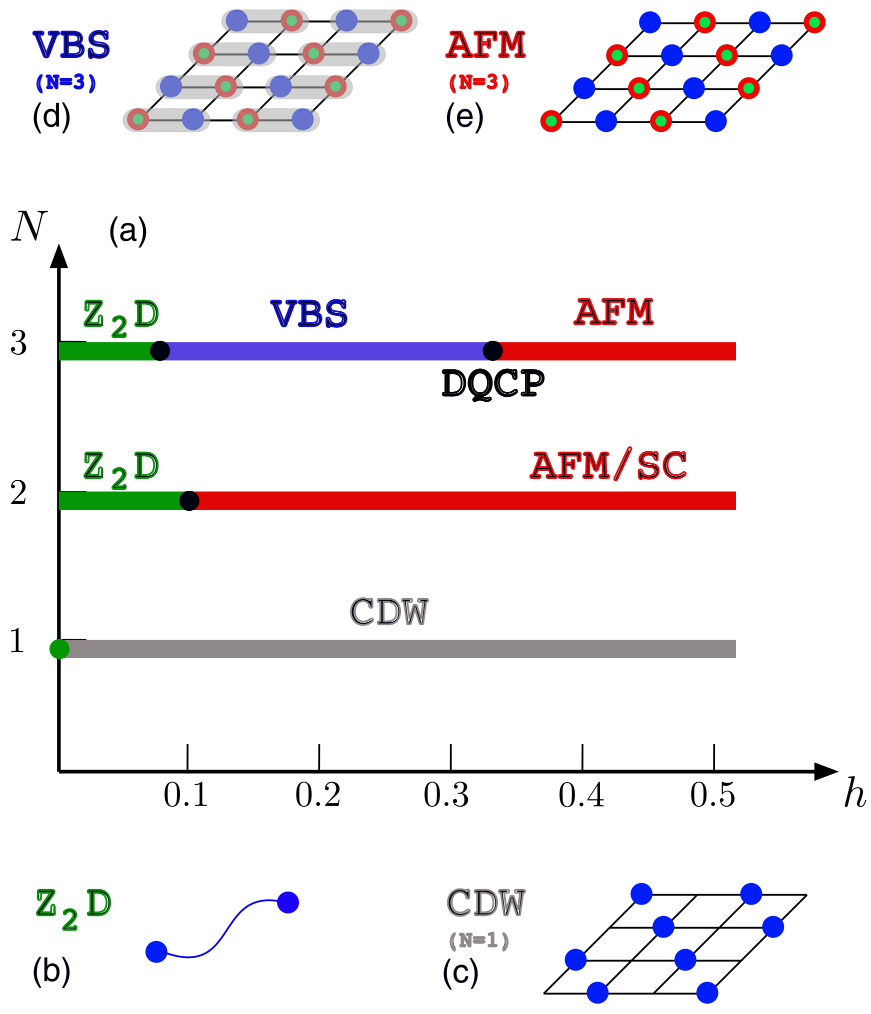
$$\hat{H} = \sum_{\langle i,j \rangle} \hat{Z}_{\langle i,j \rangle} \left(\sum_{\alpha=1}^{N} \hat{c}^{\dagger}_{i,\alpha} \hat{c}_{j,\alpha} + \text{H.c.} \right) - Nh \sum_{\langle i,j \rangle} \hat{X}_{\langle i,j \rangle}.$$

Sign free for all values of N.

N=2n   Antiunitary symmetry squaring to -1

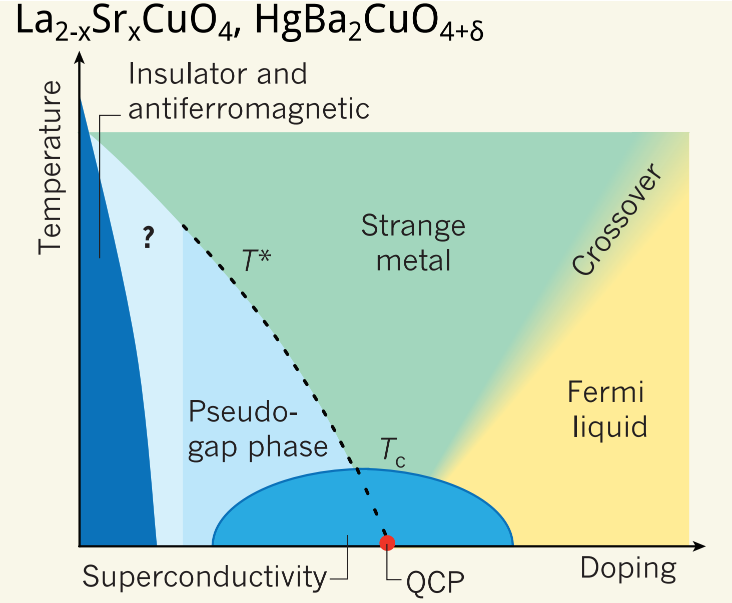
N=2n+1 Majonara representation → O(2N)





F. F. Assaad and Tarun Grover, Phys. Rev. X 6 (2016), 041049.
S. Gazit, F. F. Assaad, S. Sachdev, A. Vishwanath, and C. Wang, PNAS, (2018)

Fermion-Boson problems: "De-signer" Hamiltonians



C. Varma, Nature 468 (2010).

$$\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \right) + U \sum_{i} \left(\hat{n}_{i,\uparrow} - 1/2\right)\left(\hat{n}_{i,\downarrow} - 1/2\right) - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma}$$

Fractionalization → Emergent gauge theories
Spin liquids (Z_2 gauge theory in deconfined phase)

Intertwined orders → Superconductivity versus stripes
Superconductivity versus antiferromagnetism

Quantum phase transitions → Nematic transitions
(See also heavy fermions)

→ Designer models: are numerically tractable and capture aspects of the above physics

Fermion-Boson problems: "De-signer" Hamiltonians

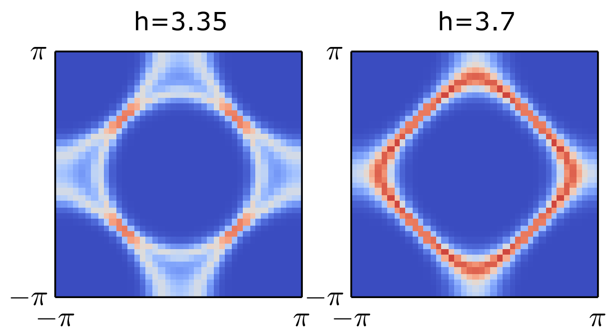
Ising nematic quantum critical point in a metal: a Monte Carlo study

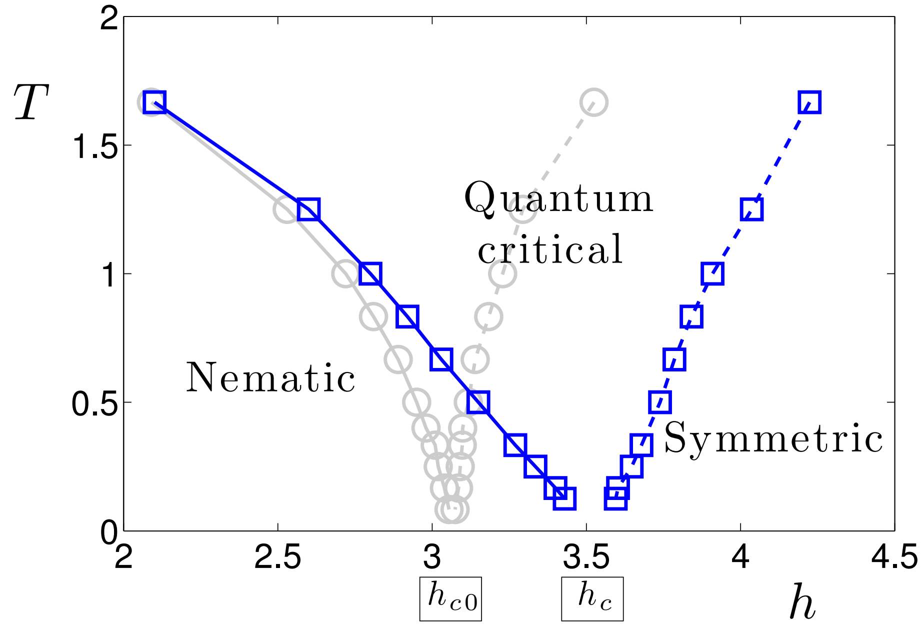
Yoni Schattner,[1,*] Samuel Lederer,[2,*] Steven A. Kivelson,[2] and Erez Berg[1]

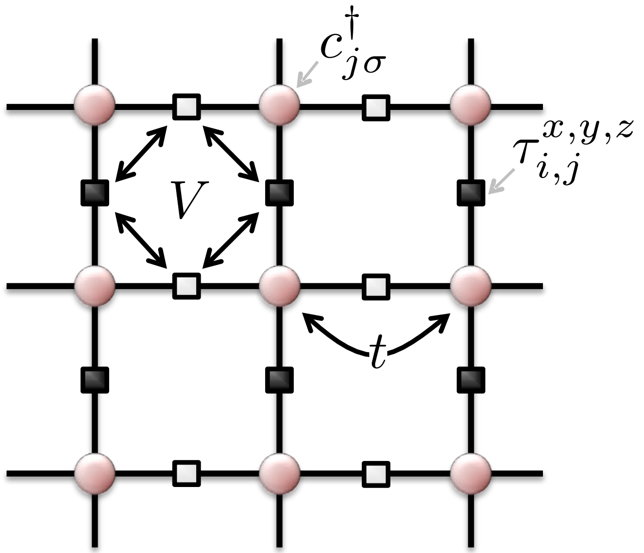
Phys. Rev. X 6, 031028 (2016)

$$H = H_f + H_b + H_{\rm int},$$

$$\begin{aligned}
H_f &= -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma}, \\
H_b &= V \sum_{\langle\langle i,j\rangle;\langle k,l\rangle\rangle} \tau^z_{i,j}\tau^z_{k,l} - h \sum_{\langle i,j\rangle} \tau^x_{i,j}, \\
H_{\rm int} &= \alpha t \sum_{\langle i,j\rangle,\sigma} \tau^z_{i,j} c^\dagger_{i\sigma} c_{j\sigma}.
\end{aligned}$$







At $\mu = 0$, the model has the same symmetries as the SSH model

At $\mu \neq 0$, the the O(2N) symmetry is broken down to U(N)

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Quantum Monte Carlo: Formulation

$$\boxed{Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int D\left\{\Phi(\boldsymbol{x},\tau)\right\} e^{-S\left\{\Phi(\boldsymbol{x},\tau)\right\}}}$$

$\Phi(\boldsymbol{x},\tau)$: Hubbard-Stratonovich (or arbitrary field with predefined dynamics)

Multidimensional integral → Monte Carlo

One body problem in external field → Polynomial complexity

Quantum Monte Carlo: Sign problem

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int D\{\Phi(\boldsymbol{x}, \tau)\} e^{-S\{\Phi(\boldsymbol{x},\tau)\}}$$

Multidimensional integral
→ Monte Carlo

One body problem in external field → Polynomial complexity

Sign problem. S is complex

$$\langle O \rangle_P = \frac{\int d\{\Phi\} e^{-S(\{\Phi\})} O(\{\Phi\})}{\int d\{\Phi\} e^{-S(\{\Phi\})}} = \frac{\dfrac{\int d\{\Phi\} \left| e^{-S(\{\Phi\})} \right| e^{i\varphi(\{\Phi\})} O(\{\Phi\})}{\int d\{\Phi\} \left| e^{-S(\{\Phi\})} \right|}}{\dfrac{\int d\{\Phi\} \left| e^{-S(\{\Phi\})} \right| e^{i\varphi(\{\Phi\})}}{\int d\{\Phi\} \left| e^{-S(\{\Phi\})} \right|}} \equiv \frac{\left\langle e^{i\varphi(\{\Phi\})} O \right\rangle_{\bar{P}}}{\left\langle e^{i\varphi(\{\Phi\})} \right\rangle_{\bar{P}}}$$

But in the low temperature limit: $\left\langle e^{i\varphi(\{\Phi\})} \right\rangle_{\bar{P}} = Z / \bar{Z} \propto e^{-\beta N(e_0 - \bar{e}_0)} = e^{-\beta V \Delta}$

$$\delta(Z/\bar{Z}) \Big/ Z/\bar{Z} \ll 1 \quad \text{but} \quad \delta(Z/\bar{Z}) \approx 1 \Big/ \sqrt{\text{CPU}} \quad \text{so that CPU} \gg \mathrm{e}^{2\beta V \Delta}$$

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Quantum Monte Carlo: Sign problem

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int D\left\{\Phi(\boldsymbol{x},\tau)\right\} e^{-S\{\Phi(\boldsymbol{x},\tau)\}}$$

Multidimensional integral
→ Monte Carlo

One body problem in external field → Polynomial complexity

Sign problem. S is complex → Computational effort $e^{\Delta \beta V}, \Delta > 0$, formulation dependent

Ever growing class of *interesting* negative sign free models → Polynomial complexity

C. Wu and S.-C. Zhang. Phys. Rev. B, 71, 155115, (2005).
E. Huffman and S. Chandrasekharan, Phys. Rev. B 89 (2014), 111101.
Zi-Xiang Li, Yi-Fan Jiang, and H. Yao Phys. Rev. Lett. 117 (2016), 267002.
Z. C. Wei, C. Wu, Yi Li, Shiwei Zhang, and T. Xiang. Phys. Rev. Lett. 116 (2016), 250601.
Z. C. Wei, arXiv:1712.09412

Conditions on $A_1 \cdots A_n, \; A_i^T = -A_i \; | \; \mathrm{Tr}\left(e^{\gamma^T A_1 \gamma} \cdots e^{\gamma^T A_n \gamma}\right) \geq 0$?

Recent application

PHYSICAL REVIEW LETTERS **120,** 107201 (2018)

Quantum Monte Carlo Simulation of Frustrated Kondo Lattice Models

Toshihiro Sato,[1] Fakher F. Assaad,[1] and Tarun Grover[2]

Quantum Monte Carlo: Sampling

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int D\left\{\Phi(\boldsymbol{x},\tau)\right\} e^{-S\{\Phi(\boldsymbol{x},\tau)\}}$$

Multidimensional integral
→ Monte Carlo

One body problem in external
field → Polynomial complexity

Sampling (critical slowing down) → Global updates

Directed loops for bosonic models with retarded interactions

PRL **119,** 097401 (2017) PHYSICAL REVIEW LETTERS week ending 1 SEPTEMBER 2017

Directed-Loop Quantum Monte Carlo Method for Retarded Interactions

Manuel Weber, Fakher F. Assaad, and Martin Hohenadler

Hybrid QMC → Global updates for fermion-boson systems

PHYSICAL REVIEW B **97**, 085144 (2018)

Revisiting the hybrid quantum Monte Carlo method for Hubbard and electron-phonon models

Stefan Beyl, Florian Goth, and Fakher F. Assaad

Machine learning ...

Quantum Monte Carlo: ALF@ http://alf.physik.uni-wuerzburg.de

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int D\left\{\Phi(\boldsymbol{x}, \tau)\right\} e^{-S\{\Phi(\boldsymbol{x},\tau)\}}$$

Multidimensional integral
→ Monte Carlo

One body problem in external field → Polynomial complexity

Efficient, general and documented (!) implementations

SciPost
SciPost Phys. 3, 013 (2017)

The *ALF* (*A*lgorithms for *L*attice *F*ermions) project release 1.0
Documentation for the auxiliary field quantum Monte Carlo code

Martin Bercx, Florian Goth, Johannes S. Hofmann and Fakher F. Assaad

Institut für Theoretische Physik und Astrophysik, Universität Würzburg,
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https://alf.physik.uni-wuerzburg.de

Quantum Monte Carlo: ALF@ http://alf.physik.uni-wuerzburg.de

Kinetic

Potential (sum of perfect squares)

$$\hat{H} = \sum_{k=1}^{M_T} \sum_{\sigma=1}^{N_{\mathrm{col}}} \sum_{s=1}^{N_{\mathrm{fl}}} \sum_{x,y}^{N_{\mathrm{dim}}} \hat{c}^{\dagger}_{x\sigma s} T^{(ks)}_{xy} \hat{c}_{y\sigma s} + \sum_{k=1}^{M_V} U_k \left\{ \sum_{\sigma=1}^{N_{\mathrm{col}}} \sum_{s=1}^{N_{\mathrm{fl}}} \left[\left(\sum_{x,y}^{N_{\mathrm{dim}}} \hat{c}^{\dagger}_{x\sigma s} V^{(ks)}_{xy} \hat{c}_{y\sigma s} \right) + \alpha_{ks} \right] \right\}^2$$

Coupling of fermions to Ising field with predefined dynamics

$$+ \sum_{k=1}^{M_I} \hat{Z}_k \left(\sum_{\sigma=1}^{N_{\mathrm{col}}} \sum_{s=1}^{N_{\mathrm{fl}}} \sum_{x,y}^{N_{\mathrm{dim}}} \hat{c}^{\dagger}_{x\sigma s} I^{(ks)}_{xy} \hat{c}_{y\sigma s} \right) + \hat{H}_{\mathrm{Ising}}$$

- Block diagonal in flavors, N_{fl}
- SU(N_{col}) symmetric in colors N_{col}
- Arbitrary Bravais lattice for d=1,2
- Model can be specified at minimal programming cost
- Fortran 2003 standard
- MPI implementation
- Parallel tempering, projective and finite T approaches
- Long range Coulomb


F. Goth


M. Bercx


J. Hoffmann


M. Ulybyshev

KONWIHR

DFG Wissenschaftliche
Literaturversorgungs
und Informationssysteme (LIS)

M. Bercx, F. Goth, J. S. Hofmann and F. F. Assaad, SciPost Phys. 3 (2017), 013

Fakher F. Assaad (Autumn School on Correlated Electrons, Jülich 20th September 2018)

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GCS Gauss Centre for Supercomputing

SSH: Integrating out bosons

$$\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \right) + g \sum_{\langle i,j\rangle,\sigma} \hat{X}_{\langle i,j\rangle} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \right) + \sum_{\langle i,j\rangle} \left[\frac{\hat{P}^2_{\langle i,j\rangle}}{2m} + \frac{k}{2}\hat{X}^2_{\langle i,j\rangle} \right]$$

<u>Integrate out the phonons in favor of a retarded interaction</u>

$$Z = \int \left[dc^{+} dc \right] \exp\left[-S_0 + \int_0^{\beta} d\tau \int_0^{\beta} d\tau' \sum_{b,b'} K_b(\tau) D^0(b-b',\tau-\tau') K_{b'}(\tau') \right]$$

$$\hat{K}_b = \sum_{\sigma} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma} \right)$$

Phonon propagator
$$\begin{cases} D^0(b-b',\tau-\tau') = \delta_{b,b'} \dfrac{g^2}{2k} P(\tau-\tau') \\ P(\tau) = \dfrac{\omega_0}{2(1-e^{-\beta\omega_0})}\left[e^{-|\tau|\omega_0} + e^{-(\beta-|\tau|)\omega_0} \right], \quad \omega_0 = \sqrt{k/M} \end{cases}$$

<u>Simulation:</u> Expand in the interaction and use MC to sum up all connected and disconnected Feynman diagrams.

CT-INT: A. N. Rubtsov, V. V. Savkin, and A. I. Lichtenstein, Phys. Rev. B 72 (2005), 035122.

Computational effort $(V\beta)^3$. No sign problem in 1+1 Dimension. Sign problem in higher dimensions.

F. F. Assaad and T. C. Lang Phys. Rev. B76, 035116 (2007).
http://www.cond-mat.de/events/correl14/manuscripts/assaad.pdf
Continuous-time QMC Solvers for Electronic Systems in Fermionic and Bosonic Baths

SSH: Real space path integral

$$\hat{H} = \underbrace{\sum_{\langle i,j\rangle,\sigma} \left(-t + g\hat{X}_{\langle i,j\rangle}\right)\left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma}\right)}_{\hat{H}_0\left(\{\hat{X}_b\}\right)} + \underbrace{\sum_{\langle i,j\rangle}\left[\frac{\hat{P}^2_{\langle i,j\rangle}}{2m} + \frac{k}{2}\hat{X}^2_{\langle i,j\rangle}\right]}_{\hat{H}_1}$$

Aim: $Z = \mathrm{Tr}_{\{\hat{X}_b\},\{\hat{c}_{i,\sigma}\}}\left[e^{-\beta\hat{H}}\right] = \mathrm{Tr}_{\{\hat{X}_b\},\{\hat{c}_{i,\sigma}\}}\left[\prod_{\tau=1}^{L_\tau} e^{-\Delta\tau\hat{H}_1}e^{-\Delta\tau\hat{H}_0\left(\{\hat{X}_b\}\right)}\right] + \mathcal{O}(\Delta\tau^2)$

$L_\tau\Delta\tau = \beta$

Real space path integral $\quad \hat{X}_b|x_b\rangle = x_b|x_b\rangle$

Insert the resolution of unity at each time step:

$$\hat{1}_B = \int\prod_b dx_b|x_b\rangle\langle x_b| = \int\prod_b \frac{dp_b}{2\pi}|p_b\rangle\langle p_b|, \quad \langle x_b|p_b\rangle = e^{-ipx}$$

to obtain

$$Z = \int\prod_{\tau,b} dx_b(\tau)\mathrm{Tr}_{\{\hat{c}_{i,\sigma}\}}\left[\prod_{\tau=1}^{L_\tau}\langle\{x_b(\tau+1)\}|e^{-\Delta\tau\hat{H}_1}|\{x_b(\tau)\}\rangle e^{-\Delta\tau\hat{H}_0(\{x_b(\tau)\})}\right] + \mathcal{O}(\Delta\tau^2)$$

with boundary condition

$$|\{x_b(L_\tau+1)\}\rangle = |\{x_b(1)\}\rangle$$

SSH: Real space path integral

$$\hat{H} = \underbrace{\sum_{\langle i,j\rangle,\sigma} \left(-t + g\hat{X}_{\langle i,j\rangle}\right)\left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma}\right)}_{\hat{H}_0\left(\left\{\hat{X}_b\right\}\right)} + \underbrace{\sum_{\langle i,j\rangle}\left[\frac{\hat{P}^2_{\langle i,j\rangle}}{2m} + \frac{k}{2}\hat{X}^2_{\langle i,j\rangle}\right]}_{\hat{H}_1}$$

$$\begin{aligned}
\langle\{x_b(\tau+1)\}\,|e^{-\Delta\tau \hat{H}_1}\,\{x_b(\tau)\}\rangle &\simeq \int \prod_b \frac{dp_b}{2\pi} \langle x_b(\tau+1)|e^{-\Delta\tau \frac{\hat{P}^2}{2m}}|p_b\rangle\langle p_b|e^{-\Delta\tau\frac{k}{2}\hat{X}^2_b}|x_b(\tau)\rangle \\
&= \int \prod_b \frac{dp_b}{2\pi} e^{ip_b[x_b(\tau+1)-x_b(\tau)]} e^{-\Delta\tau\left[\frac{p_b^2}{2m}+\frac{k}{2}x_b^2(\tau)\right]} \\
&= e^{-\Delta\tau\sum_b\left(\frac{m}{2}\left[\frac{\boldsymbol{x}_b(\tau+1)-\boldsymbol{x}_b(\tau)}{\Delta\tau}\right]^2+\frac{k}{2}\boldsymbol{x}_b(\tau)^2\right)}
\end{aligned}$$

SSH: Real space path integral

$$\boxed{\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + g \sum_{\langle i,j \rangle,\sigma} \hat{X}_{\langle i,j \rangle} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right]}$$

Real space path integral $\hat{X}_b | x_b \rangle = x_b | x_b \rangle$

$$Z = \int D\left\{ \boldsymbol{x} \right\} e^{-S_0(\boldsymbol{x})} \left[\mathrm{Tr} \prod_{\tau,b} e^{-\Delta\tau(-t + g\boldsymbol{x}_{b,\tau})\left(\hat{c}^{\dagger}_i \hat{c}_j + \hat{c}^{\dagger}_j \hat{c}_i\right)} \right]^{N_{col}}$$

$$S_0(\boldsymbol{x}) = \Delta\tau \sum_{b,\tau} \left(\frac{m}{2} \left[\frac{\boldsymbol{x}_b(\tau+1) - \boldsymbol{x}_b(\tau)}{\Delta\tau} \right]^2 + \frac{k}{2} \boldsymbol{x}_b(\tau)^2 \right)$$

Integrating out the fermions. Use determinant formula (see lecture notes)

$$\mathrm{Tr} \left[e^{\hat{\boldsymbol{c}}^{\dagger} A(\boldsymbol{x}_{N_b L_\tau}) \hat{\boldsymbol{c}}} \cdots e^{\hat{\boldsymbol{c}}^{\dagger} A(\boldsymbol{x}_2) \hat{\boldsymbol{c}}} e^{\hat{\boldsymbol{c}}^{\dagger} A(\boldsymbol{x}_1) \hat{\boldsymbol{c}}} \right] = \det \left(1 + e^{A(\boldsymbol{x}_{N_b L_\tau})} \cdots e^{A(\boldsymbol{x}_2)} e^{A(\boldsymbol{x}_1)} \right)$$

with $\hat{\boldsymbol{c}}^{\dagger} A(\boldsymbol{x}_{b,\tau}) \hat{\boldsymbol{c}} = -\Delta\tau \left(-t + g\boldsymbol{x}_{b,\tau} \right) \left(\hat{c}^{\dagger}_i \hat{c}_j + \hat{c}^{\dagger}_j \hat{c}_i \right)$

SSH: Real space path integral

$$\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + g \sum_{\langle i,j \rangle,\sigma} \hat{X}_{\langle i,j \rangle} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right]$$

Real space path integral $\hat{X}_b | x_b \rangle = x_b | x_b \rangle$

$$Z = \int D\{\boldsymbol{x}\}\, e^{-(S_0(\boldsymbol{x}) - N_{\mathrm{col}} \log \det(M(\boldsymbol{x})))} \equiv \int D\{\boldsymbol{x}\}\, e^{-S(\boldsymbol{x})}$$

$$M(\boldsymbol{x}) = 1 + e^{A(\boldsymbol{x}_{N_b L_\tau})} \cdots e^{A(\boldsymbol{x}_2)} e^{A(\boldsymbol{x}_1)}$$

$$S_0(\boldsymbol{x}) = \Delta\tau \sum_{b,\tau} \left(\frac{m}{2} \left[\frac{\boldsymbol{x}_b(\tau+1) - \boldsymbol{x}_b(\tau)}{\Delta\tau} \right]^2 + \frac{k}{2} \boldsymbol{x}_b(\tau)^2 \right)$$

SSH: Real space path integral

$$\boxed{\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + g \sum_{\langle i,j \rangle,\sigma} \hat{X}_{\langle i,j \rangle} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + \sum_{\langle i,j \rangle} \left[\frac{\hat{P}^2_{\langle i,j \rangle}}{2m} + \frac{k}{2} \hat{X}^2_{\langle i,j \rangle} \right]}$$

Real space path integral $\hat{X}_b | x_b \rangle = x_b | x_b \rangle$

$$Z = \int D\{\boldsymbol{x}\} \, e^{-S_0(\boldsymbol{x})} \left[\mathrm{Tr} \prod_{\tau,b} e^{-\Delta\tau(-t+g\boldsymbol{x}_{b,\tau})(\hat{c}^{\dagger}_i \hat{c}_j + \hat{c}^{\dagger}_j \hat{c}_i)} \right]^{N_{col}}$$

$$S_0(\boldsymbol{x}) = \Delta\tau \sum_{b,\tau} \left(\frac{m}{2} \left[\frac{\boldsymbol{x}_b(\tau+1) - \boldsymbol{x}_b(\tau)}{\Delta\tau} \right]^2 + \frac{k}{2} \boldsymbol{x}_b(\tau)^2 \right)$$

The trace is positive. Consider the Majorana representation:

$$\left.\begin{array}{l} \boldsymbol{i} \in A : \gamma_{\boldsymbol{i},1} = \hat{c}_{\boldsymbol{i}} + \hat{c}^{\dagger}_{\boldsymbol{i}}, \quad \gamma_{\boldsymbol{i},2} = -i \left(\hat{c}_{\boldsymbol{i}} - \hat{c}^{\dagger}_{\boldsymbol{i}} \right) \\ \boldsymbol{i} \in B : \gamma_{\boldsymbol{i},2} = -\left(\hat{c}_{\boldsymbol{i}} + \hat{c}^{\dagger}_{\boldsymbol{i}} \right), \quad \gamma_{\boldsymbol{i},1} = -i \left(\hat{c}_{\boldsymbol{i}} - \hat{c}^{\dagger}_{\boldsymbol{i}} \right) \end{array}\right\} \quad \sum_{\sigma=1}^{N_{col}} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} = \sum_{\sigma=1}^{N_{col}} \sum_{n=1}^{2} \frac{i}{2} \hat{\gamma}_{i,\sigma,n} \hat{\gamma}_{j,\sigma,n}$$

$$\mathrm{Tr} \prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \sum_b (-t+g\boldsymbol{x}_{b,\tau})(\hat{c}^{\dagger}_i \hat{c}_j + \hat{c}^{\dagger}_j \hat{c}_i)} = \left[\mathrm{Tr} \prod_{\tau=1}^{L_\tau} e^{-i\frac{\Delta\tau}{4} \sum_b (-t+g\boldsymbol{x}_{b,\tau}) \gamma_i \gamma_j} \right]^2 \geq 0$$

Z. C. Wei, Congjun Wu, Yi Li, Shiwei Zhang, and T. Xiang, Phys. Rev. Lett. 116, 250601, (2016).
Z.-X. Li, Y.-F. Jiang, and H. Yao. Phys. Rev. B, 91, 241117, (2015).
E. F. Huffman and S. Chandrasekharan. Phys. Rev. B, 89, 111101, (2014).

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Real space path integral $\hat{X}_b|x_b\rangle = x_b|x_b\rangle$

$$Z = \int D\{\boldsymbol{x}\}\, e^{-(S_0(\boldsymbol{x}) - N_{\mathrm{col}} \log\det(M(\boldsymbol{x})))} \equiv \int D\{\boldsymbol{x}\}\, e^{-S(\boldsymbol{x})}$$

$$M(\boldsymbol{x}) = 1 + e^{A(\boldsymbol{x}_{N_b L_\tau})} \cdots e^{A(\boldsymbol{x}_2)} e^{A(\boldsymbol{x}_1)}$$

$$S_0(\boldsymbol{x}) = \Delta\tau \sum_{b,\tau} \left(\frac{m}{2} \left[\frac{\boldsymbol{x}_b(\tau+1) - \boldsymbol{x}_b(\tau)}{\Delta\tau} \right]^2 + \frac{k}{2} \boldsymbol{x}_b(\tau)^2 \right)$$

The action is real for any number of fermion flavors !

(At finite chemical potential there is no sign problem for even number of flavors!)

SSH: Observables

Def $\underline{t} = (\tau, b)$ $\qquad \hat{U}_x(\underline{t}_2, \underline{t}_1) = \prod_{\underline{t}=\underline{t}_1+1}^{\underline{t}_2} e^{-\Delta\tau(-t+gx_{\underline{t}}))\hat{K}_{b_{\underline{t}}}}$ for $\underline{t}_2 \geq \underline{t}_1$.

Let O be an observable that involves only fermion degrees of freedom

$$\boxed{\langle \hat{O} \rangle = \frac{1}{\int D\boldsymbol{x} e^{-S(\boldsymbol{x})}} \int D\boldsymbol{x} e^{-S(\boldsymbol{x})} \frac{\mathrm{Tr}_F \left[\hat{U}_x(L_\tau N_b, 0) \hat{O} \right]}{\mathrm{Tr}_F \left[\hat{U}_x(L_\tau N_b, 0) \right]}}$$

For $\hat{O} = T \hat{c}_{i_1}(\underline{t}_1) \hat{c}^\dagger_{i'_1}(\underline{t}'_1) \cdots \hat{c}_{i_n}(\underline{t}_n) \hat{c}^\dagger_{i'_n}(\underline{t}'_n)$ with $\hat{c}_i(\underline{t}) = \hat{U}_x^{-1}(\underline{t}, 0) \hat{c}_i \hat{U}_x(\underline{t}, 0)$.

Wick's theorem $\dfrac{\mathrm{Tr}_F \left[\hat{U}_x(L_\tau N_b, 0) \hat{O} \right]}{\mathrm{Tr}_F \left[\hat{U}_x(L_\tau N_b, 0) \right]} = \det \begin{pmatrix} G_{i_1, i'_1}(\underline{t}_1, \underline{t}'_1) & \cdots & G_{i_1, i'_n}(\underline{t}_1, \underline{t}'_n) \\ \vdots & \ddots & \vdots \\ G_{i_n, i'_1}(\underline{t}_n, \underline{t}'_1) & \cdots & G_{i_n, i'_n}(\underline{t}_n, \underline{t}'_n) \end{pmatrix}.$ holds.

Equal time Green functions

$$G(\underline{t}', \underline{t}') = \left[1 + B_x(\underline{t}', 0) B_x(L_\tau N_b, \underline{t}') \right]^{-1}, \text{ with } B_x(\underline{t}_2, \underline{t}_1) = \prod_{\underline{t}=\underline{t}_1+1}^{\underline{t}_2} e^{-\Delta\tau(-t+gx_{\underline{t}}))K_{b_{\underline{t}}}} \text{ for } \underline{t}_2 \geq \underline{t}_1$$

SSH: Sampling

$$Z = \int D\left\{\boldsymbol{x}\right\} e^{-(S_0(\boldsymbol{x}) - N_{\mathrm{col}} \log\det(M(\boldsymbol{x})))} \equiv \int D\left\{\boldsymbol{x}\right\} e^{-S(\boldsymbol{x})}$$

$$S_0(\boldsymbol{x}) = \Delta\tau \sum_{b,\tau} \left(\frac{m}{2} \left[\frac{\boldsymbol{x}_b(\tau+\Delta\tau) - \boldsymbol{x}_b(\tau)}{\Delta\tau} \right]^2 + \frac{k}{2} \boldsymbol{x}_b(\tau)^2 \right)$$

$$\det M(\boldsymbol{x}) = \mathrm{Tr} \prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \sum_b (-t + g\boldsymbol{x}_{b,\tau})(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i)}$$

Metropolis-Hastings (C is a configuration in Monte Carlo space)

$$P(C \to C') = \max\left(\frac{T_0(C' \to C) P(C')}{T_0(C \to C') P(C)}, 1 \right)$$

Aim: Find T_0 such that acceptance is high and moves allow efficient sampling of configuration space.

Possible solutions:

- Single spin-flip → Very long autocorrelations
- Machine learning
- Hybrid molecular dynamics

SSH: Sampling

$$Z = \int D\left\{\boldsymbol{x}\right\} e^{-(S_0(\boldsymbol{x}) - N_{\mathrm{col}} \log \det(M(\boldsymbol{x}))} \equiv \int D\left\{\boldsymbol{x}\right\} e^{-S(\boldsymbol{x})}$$

$$S_0(\boldsymbol{x}) = \Delta\tau \sum_{b,\tau} \left(\frac{m}{2} \left[\frac{\boldsymbol{x}_b(\tau+\Delta\tau) - \boldsymbol{x}_b(\tau)}{\Delta\tau} \right]^2 + \frac{k}{2} \boldsymbol{x}_b(\tau)^2 \right) \qquad \det M(\boldsymbol{x}) = \mathrm{Tr} \prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \sum_b (-t + g\boldsymbol{x}_{b,\tau})(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i)}$$

Hybrid Molecular dynamics. Basics.

Introduce conjugate momentum $H(\boldsymbol{p}, \boldsymbol{x}) = \frac{\boldsymbol{p}^2}{2} + S(\boldsymbol{x})$ and sample $e^{-H(\boldsymbol{p},\boldsymbol{x})}$

Start with random **x**

<u>Step 1.</u> Sample **p** from Gauss distribution

<u>Step 2.</u> Hamiltonian dynamics with H over time T_m $(\boldsymbol{p}, \boldsymbol{x})(t) \rightarrow (\boldsymbol{p}, \boldsymbol{x})(t + T_m)$

$$\max\left(\frac{T_0\left(\{\boldsymbol{p},\boldsymbol{x}\}(t_m + T_m) \rightarrow \{\boldsymbol{p},\boldsymbol{x}\}(t_m)\right) e^{-H(\{\boldsymbol{p},\boldsymbol{x}\}(t_m+T_m))}}{T_0\left(\{\boldsymbol{p},\boldsymbol{x}\}(t_m) \rightarrow \{\boldsymbol{p},\boldsymbol{x}\}(t_m + T_m)\right) e^{-H(\{\boldsymbol{p},\boldsymbol{x}\}(t_m))}}, 1 \right) = \max\left(\frac{e^{-H(\{\boldsymbol{p},\boldsymbol{x}\}(t_m+T_m))}}{e^{-H(\{\boldsymbol{p},\boldsymbol{x}\}(t_m))}}, 1 \right) \simeq 1$$

Time reversal (Leapfrog)
Liouville

Finite time step

<u>Step 3</u>. → Step1.

SSH: Sampling

$$Z = \int D\{\boldsymbol{x}\}\, e^{-(S_0(\boldsymbol{x}) - N_{\text{col}} \log \det(M(\boldsymbol{x})))} \equiv \int D\{\boldsymbol{x}\}\, e^{-S(\boldsymbol{x})}$$

$$S_0(\boldsymbol{x}) = \Delta\tau \sum_{b,\tau} \left(\frac{m}{2} \left[\frac{\boldsymbol{x}_b(\tau+\Delta\tau) - \boldsymbol{x}_b(\tau)}{\Delta\tau} \right]^2 + \frac{k}{2} \boldsymbol{x}_b(\tau)^2 \right) \qquad \det M(\boldsymbol{x}) = \mathrm{Tr} \prod_{\tau=1}^{L_\tau} e^{-\Delta\tau \sum_b (-t + g\boldsymbol{x}_{b,\tau})(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i)}$$

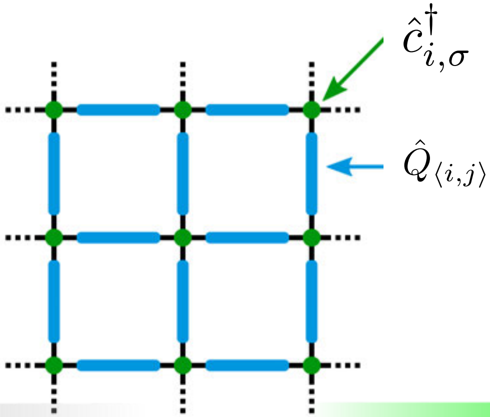
Hybrid Molecular dynamics. Key questions

	Hubbard (2D, fields couple to z-component of magnetization)	**O**($2N_{col}$) symmetric models such as SSH.
Are the forces $\frac{\partial S(\boldsymbol{x})}{\partial \boldsymbol{x}}$ bounded ?	No	Most of the time. Each determinant is positive semidefinite
Does the configuration space split into regions split by potential barriers	Yes	No

See: Stefan Beyl, Florian Goth, and Fakher F. Assaad,
Revisiting the hybrid quantum Monte Carlo method for Hubbard and electron-phonon models,
Phys. Rev. B 97 (2018), 085144.

Deconfined quantum critical points in the SSH model

$$\boxed{H=-t\sum_{\langle i,j\rangle,\sigma}\left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma}+\hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma}\right)+\sum_{\langle i,j\rangle}\left[\frac{\hat{P}^2_{\langle i,j\rangle}}{2m}+\frac{k}{2}\hat{Q}^2_{\langle i,j\rangle}\right]+g\sum_{\langle i,j\rangle,\sigma}\hat{Q}_{\langle i,j\rangle}\left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma}+\hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma}\right)}$$

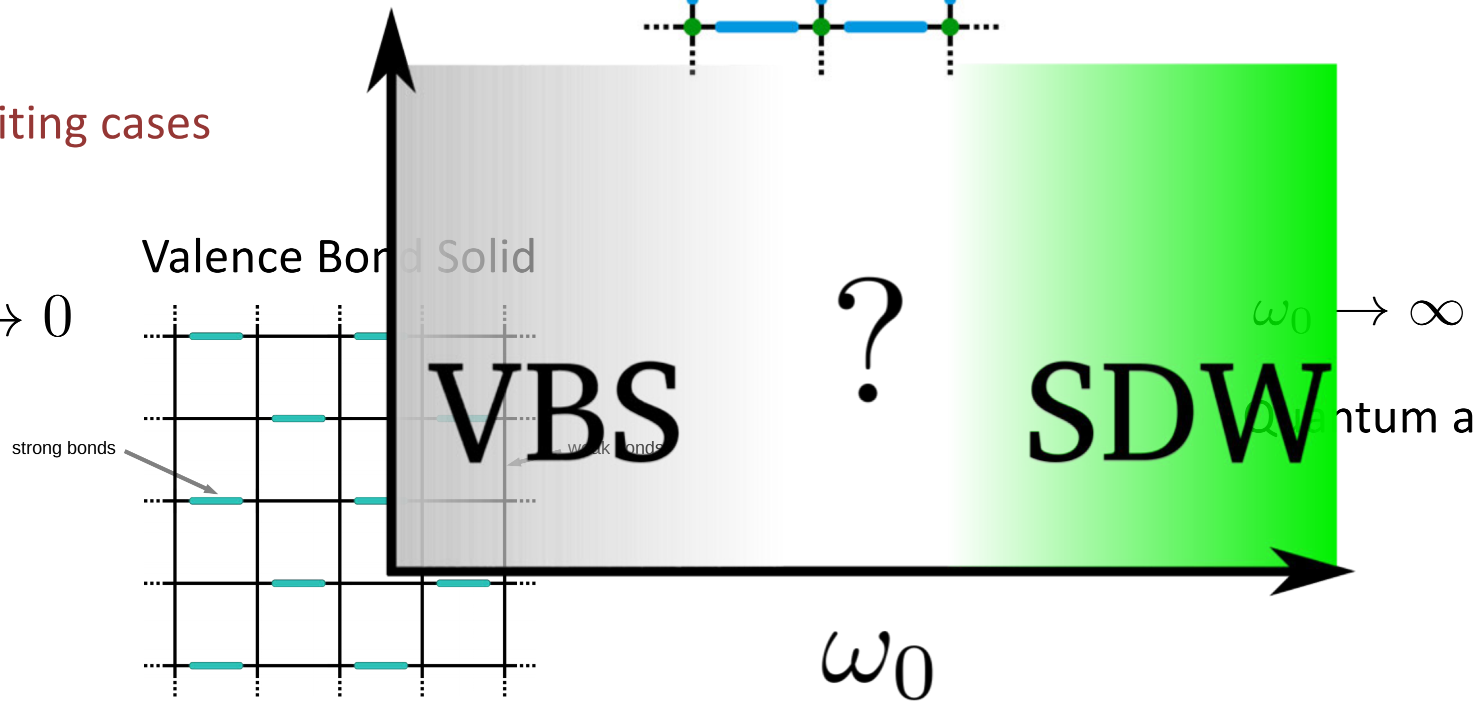


$$\boxed{\omega_0=\sqrt{\frac{k}{m}}}$$

Limiting cases

Valence Bond Solid

$\omega_0 \to 0$



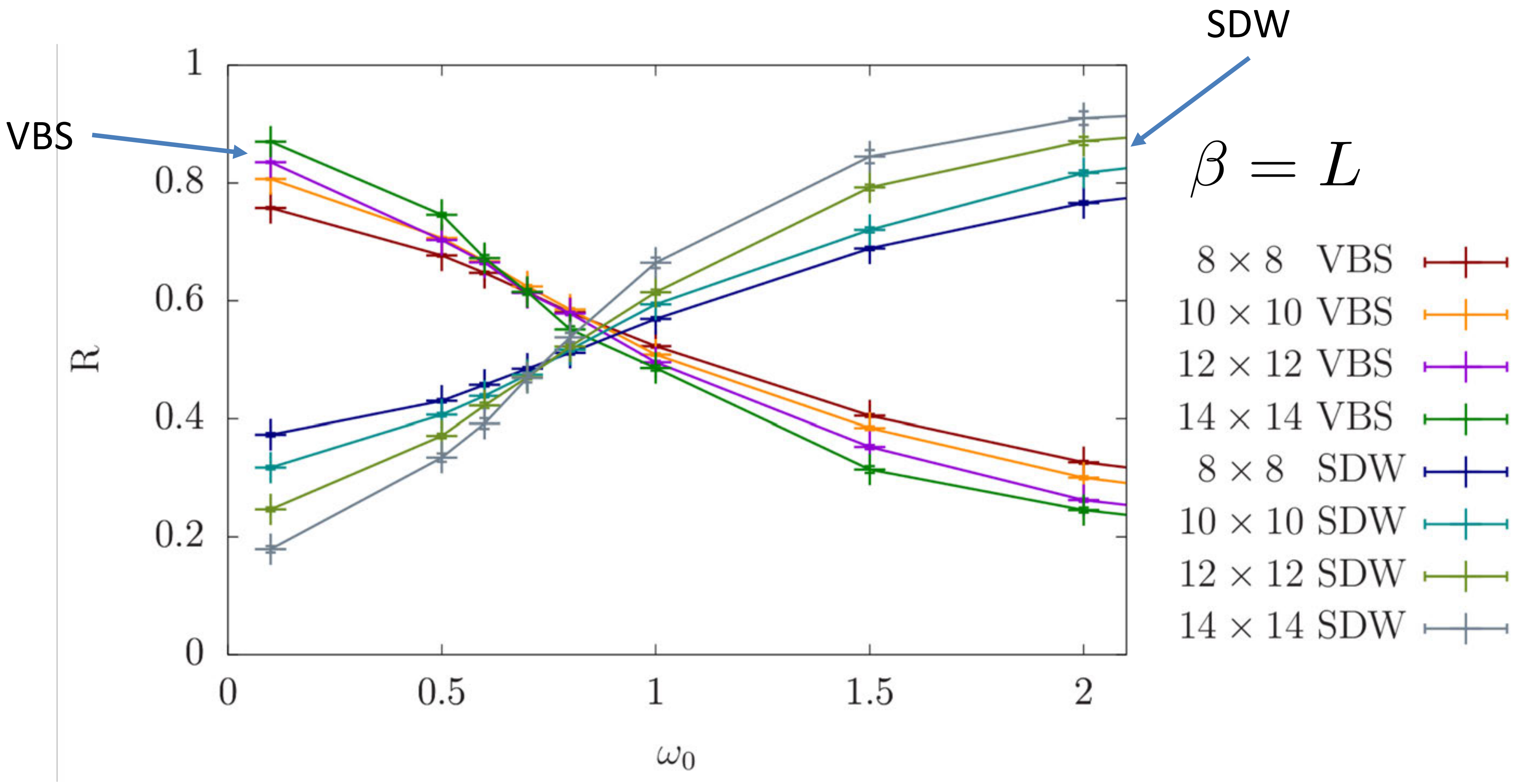
$\omega_0 \to \infty$

Quantum antiferromagnet

Deconfined quantum critical points in the SSH model

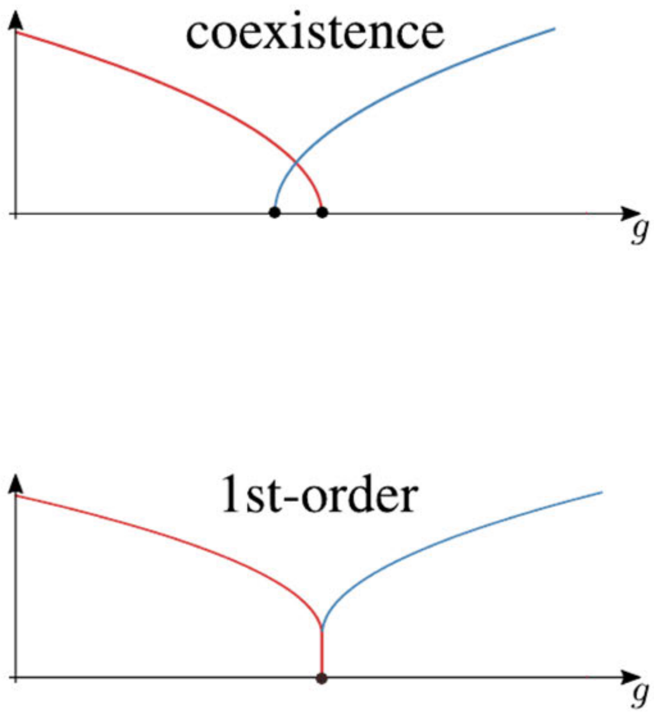
S. Beyl, F. Goth, M. Hohenadler and FFA, (Unpublished)

$$R = 1 - \frac{\chi(Q + \delta Q)}{\chi(Q)} = F\left((\omega_0 - \omega_0^c)L^{1/\nu}, L^z/\beta, L^{-\omega}\right)$$



Direct and continuous transition between VBS and SDW !

Order parameter theory, Ginzburg-Landau



Fine tuning → not generic

Deconfined quantum critical points in the SSH model

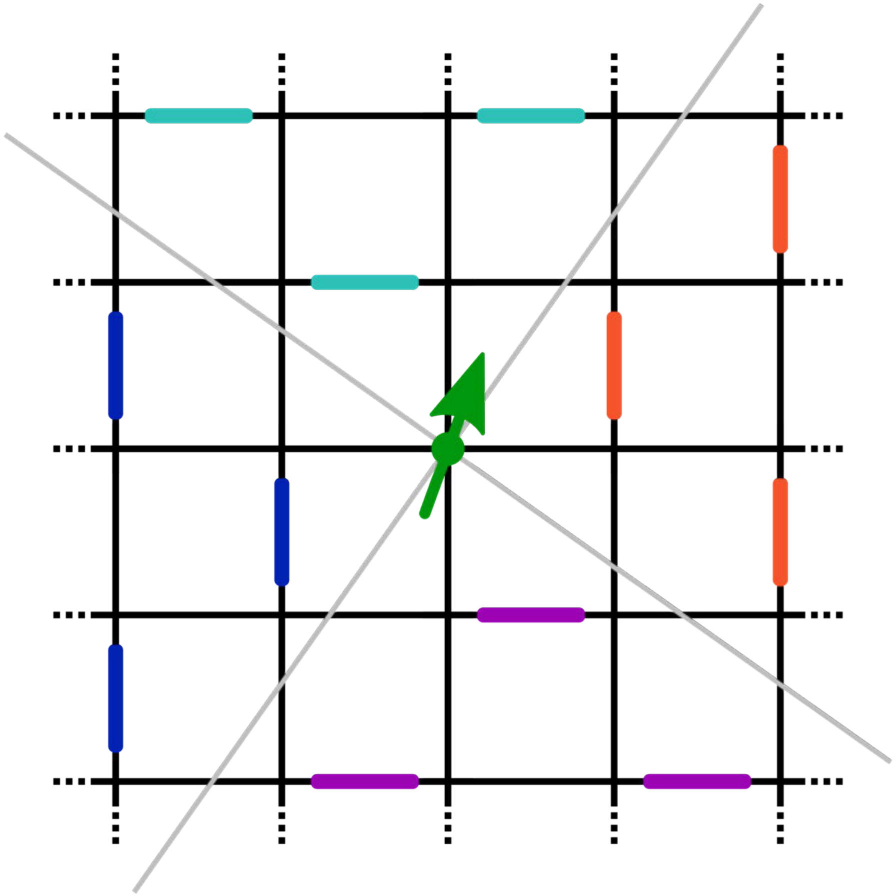
Deconfined quantum criticality T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M. P. A. Fisher, Deconfined quantum critical points, Science 303 (2004), 1490–1494.

Topological defects of one phase carry the charge of the other phase.

Possible realization:

$SrCu_2(BO_3)_2$

M. Zayed et al.
Nat. Phys. 13, 962 (2017).



C_4 VBS vortex carries a spinon. Proliferation of vortices destroys the VBS and generates SDW order.

Fakher F. Assaad (Autumn School on Correlated Electrons, Jülich 20th September 2018)

Conclusion:

- Fermion-Boson problems cover an extremely rich class of phenomena
- Quantum Monte Carlo simulations are challenging
- Ever growing class of negative sign free problems
- Progress in sampling methods.

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Quantum Monte Carlo Methods for Fermion-Boson problems

Fakher F. Assaad (Autumn School on Correlated Electrons, Jülich 20th September 2018)

Review:

World-line and determinantal quantum monte carlo methods for spins, phonons and electrons,
F.F.A and H.G. Evertz. Lecture Notes in Physics, vol. 739, Springer, Berlin Heidelberg, 2008, pp. 277–356

Continuous-time QMC Solvers for Electronic Systems in Fermionic and Bosonic Baths,
F. F. Assaad, DMFT at 25: Infinite dimensions: Lecture notes of the autumn school on correlated electrons, vol. 4, ch. 7. Verlag des Forschungszentrum Jülich, Jülich, 2014, ISBN 978-3-89336-953-9

Lecture notes of this school.

ALF: General Implementation:

Martin Bercx, Florian Goth, Johannes S. Hofmann, and Fakher F. Assaad
The ALF (Algorithms for Lattice Fermions) project release 1.0. Documentation for the auxiliary field quantum Monte Carlo code, SciPost Phys. 3 (2017), 013.