Auxiliary field quantum Monte Carlo at work.

F. F. Assaad.

School on Quantum Monte methods at work for novel phases of matter
ICTP Trieste January 23, 2012 to January 27, 2012

Outline:

- Class of problems which one can solve.
- The method with details of the projective method.
  (All the relevant calculations can be done on the blackboard)
- Selected applications (novel phases of matter)

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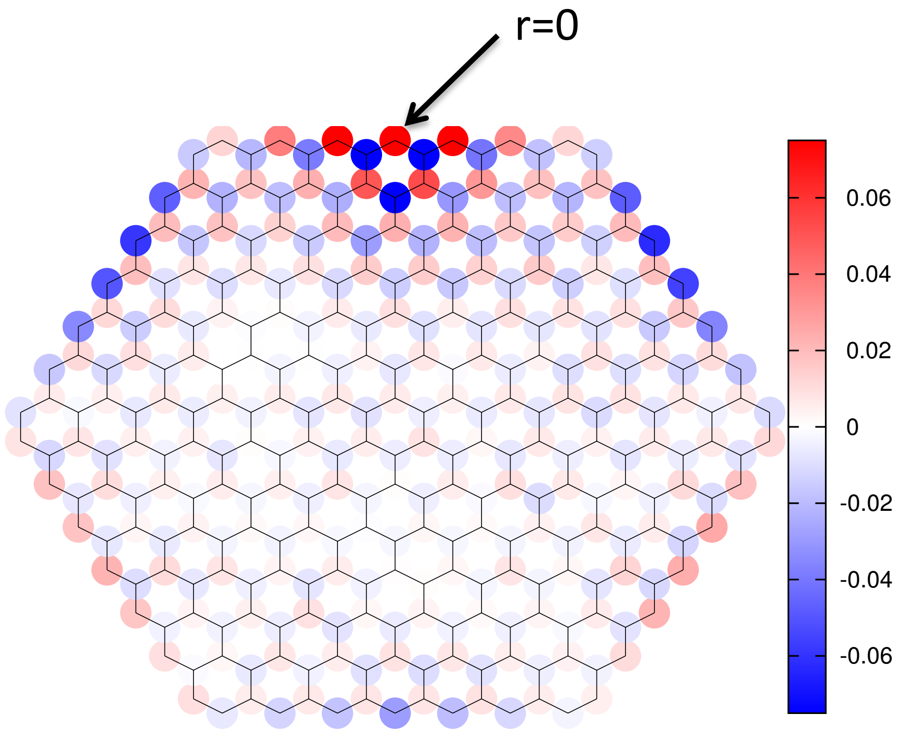
<u>Lab:</u>

Edge magnetism in graphene nano-flakes.

$$\langle S(r=0)S(r)\rangle$$

U/t=3



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- Class of problems which one can solve.
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- Selected application

Class of problems (Polynomial time)

Particle hole + time reversal symmetry
Half-filled repulsive Hubbard model.
Periodic Anderson and Kondo Lattice models.
Kane-Mele Hubbard.

Attractive even flavored models SU(2n)
Attractive Hubbard model.

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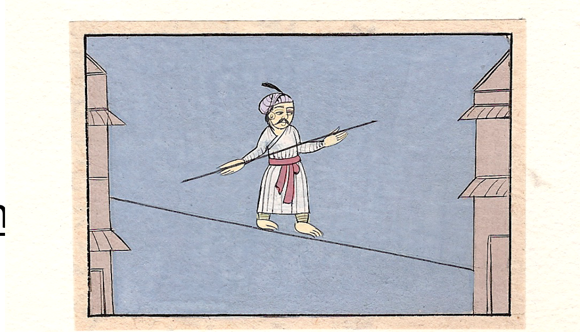

Outlin

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Class of problems (Polynomial time)

Particle hole + time reversal symmetry
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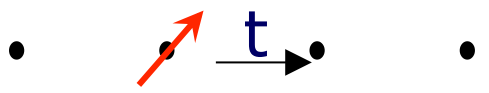
Attractive even flavored models SU(2n)
Attractive Hubbard model.

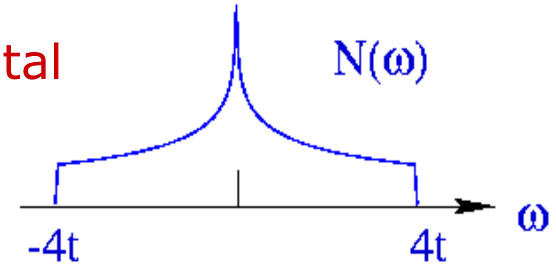
- The method with de
- Selected application

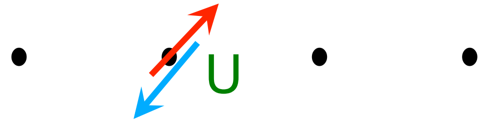
Hubbard and Heisenberg models.

$$\hat{H} = -t \sum_{<i,j>,\sigma} \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} \quad + \quad U\,(\hat{c}^{+}_{i,\uparrow}\hat{c}_{i,\uparrow} - 1/2)(\hat{c}^{+}_{i,\downarrow}\hat{c}_{i,\downarrow} - 1/2)$$

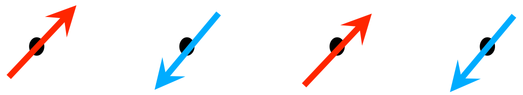


Metal



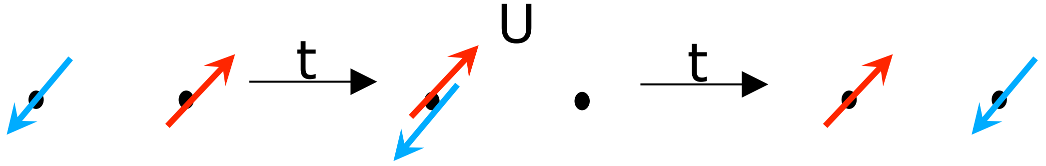


Half-filling: Insulator. Charge scale **U**



Charge is localized spin is still active.

Strong coupling: U/t >>1, Half-filling.



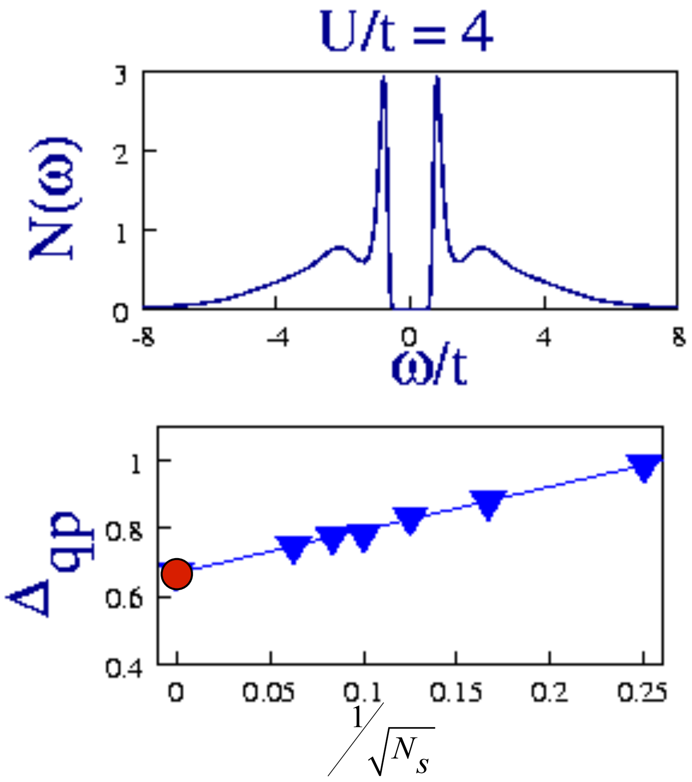
Magnetic scale: $J \sim t^2/U$

$$H = J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j$$

Heisenberg model.

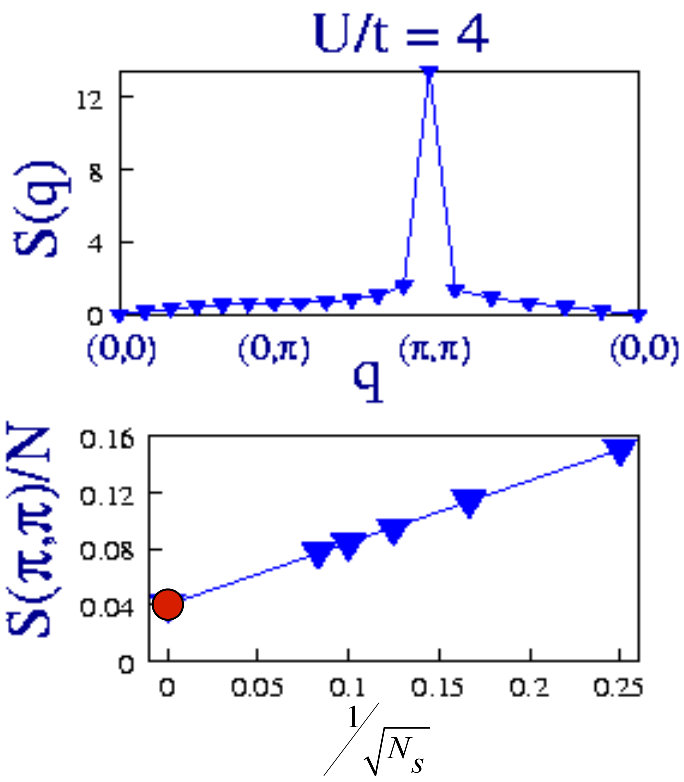
The Mott Insulator. Half-band filling (2D square lattice)

Charge.



Quasiparticle gap > 0

Spin.



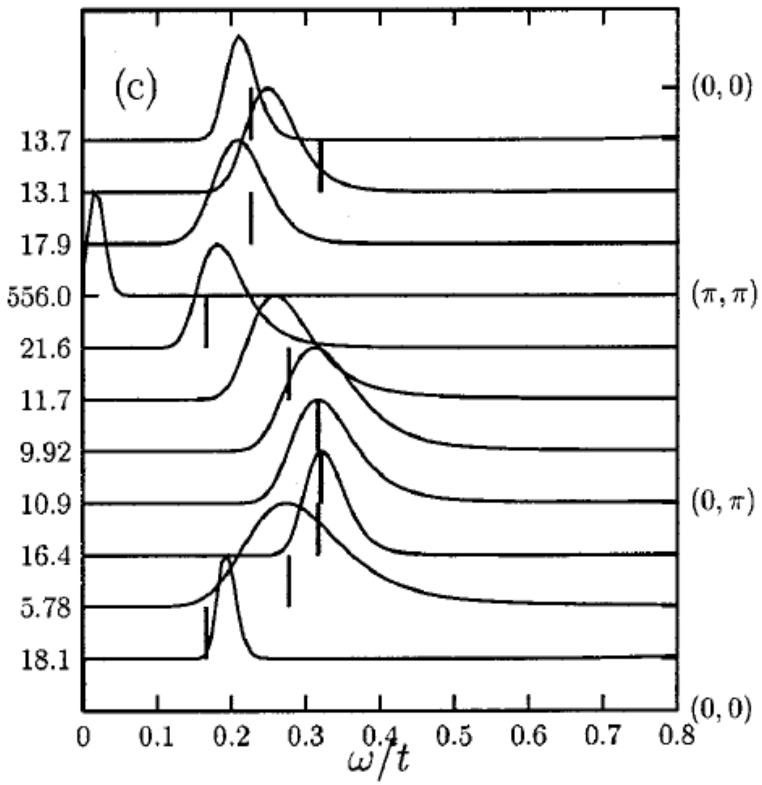
Long-range antiferromagnetic order.
Gapless spin excitations: Spin waves.

F.F. Assaad M. Imada JPSJ 95. (Auxiliary field QMC)

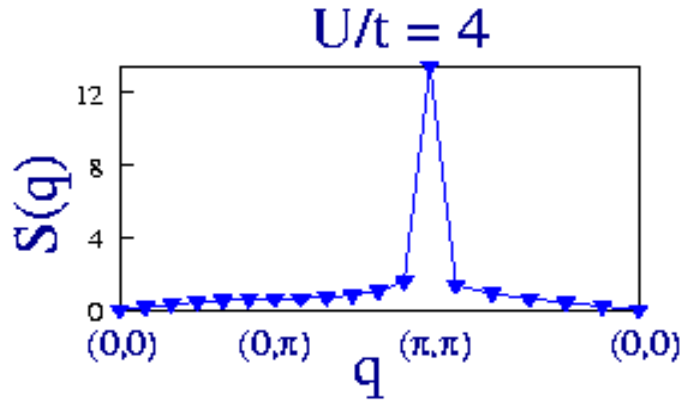
The Mott Insulator. Half-band filling (2D square lattice)

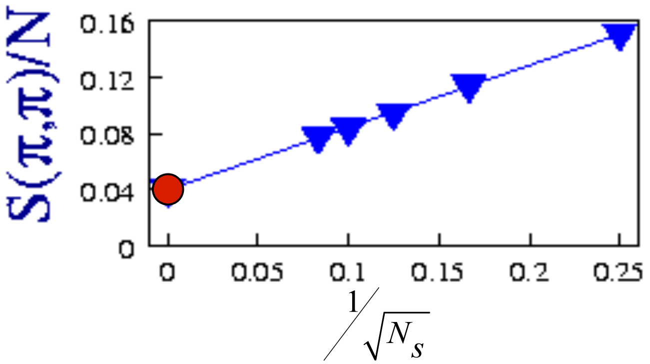
Spin excitations are present below the charge gap (1.3t)

Spin.



$$S(\vec{q},\omega) = \sum_n |\langle n|\hat{S}^+(\vec{q})|0\rangle|^2 \delta(\omega - (E_n - E_0))$$

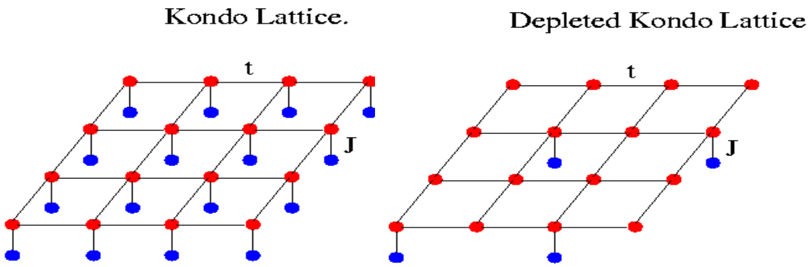




Long-range antiferromagnetic order.
Gapless spin excitations: Spin waves.

F.F. Assaad M. Imada JPSJ 95. (Auxiliary field QMC)

Models of heavy fermions.


Kondo Lattice.

Depleted Kondo Lattice

Conduction orbitals $c^{+}_{\mathbf{i},\sigma}$
(half-filled particle hole symmetric band)

Impurity orbitals: $f^{+}_{\mathbf{R},\sigma}$

Periodic Anderson model (PAM).

Charge fluctuations on f-sites.

$$H = -t \sum_{(\mathbf{i},\mathbf{j}),\sigma} c^{+}_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + V \sum_{\mathbf{i},\sigma} c^{+}_{\mathbf{i},\sigma} f_{\mathbf{i},\sigma} + f^{+}_{\mathbf{i},\sigma} c_{\mathbf{i},\sigma} + U_f \sum_{\mathbf{R}} (n^{f}_{\mathbf{R},\downarrow} - \tfrac{1}{2})(n^{f}_{\mathbf{R},\uparrow} - \tfrac{1}{2})$$

Kondo lattice model (KLM).

Charge fluctuations on f-sites are frozen.

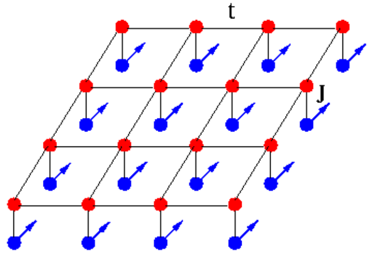
$$\boxed{J \propto V^{2}/U_{f}}$$

$$H = -t \sum_{(\mathbf{i},\mathbf{j}),\sigma} c^{+}_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + J \sum_{\mathbf{R}} \mathbf{S}^{c}_{\mathbf{R}} \cdot \mathbf{S}^{f}_{\mathbf{R}}$$

Half-filled Kondo lattice.

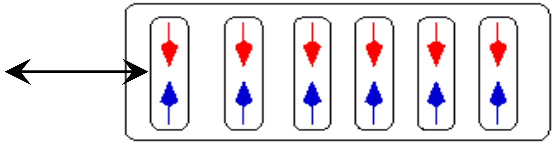
Model

One conduction electron per impurity spin.

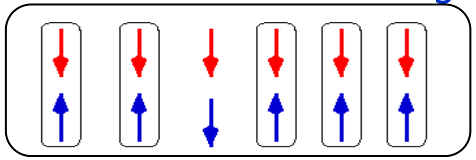


Strong coupling limit. J/t >> 1

Spin Singlet

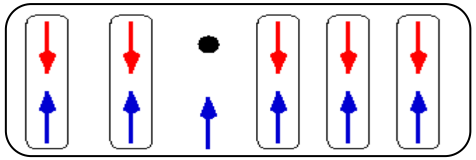


1) Spin gap Δ_s



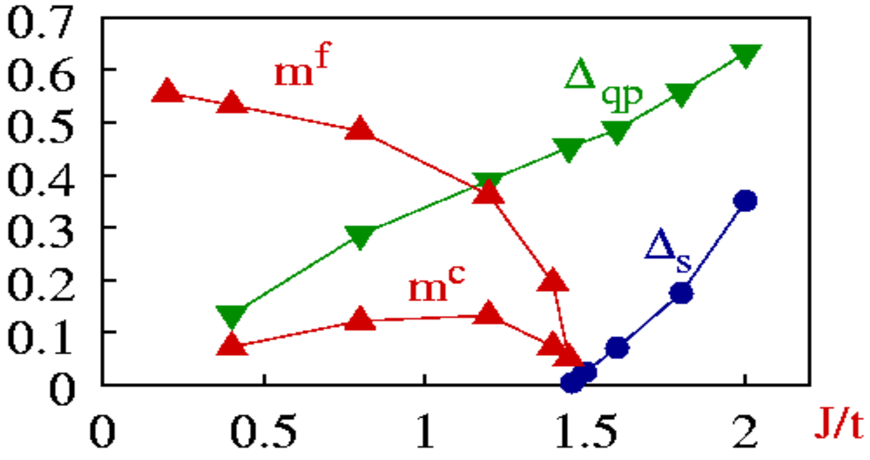
Energy J

2) Quasiparticle gap. Δ_{qp}



Energy 3J/4

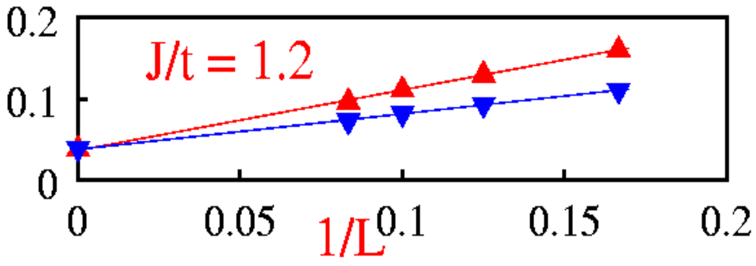
QMC, T=0, L $\longrightarrow \infty$



3) *Magnetism.*

$$(m^f)^2 = \lim_{N\to\infty} \frac{4}{3N} \sum_{\mathbf{R}} e^{iQR} \langle \mathbf{S}_0^f \mathbf{S}_{\mathbf{R}}^f \rangle$$

m > 0, Q=(π,π): long range antiferromagnetic order.



School on Quantum Monte methods at work for **novel** phases of matter

Because the (honeycomb) lattice is bipartite, quantum Monte-Carlo calculations are not vexed by fermion minus sign problems so long as the band is half filled (one electron per site). According to Murphy's Law, this should guarantee that nothing interesting occurs (in this model).

S. Kivelson in Commentary on "Spin Liquid Ground states"
(Journal Club for Condensed Matter Physics January 2011)

Exceptions to Murphy's law.

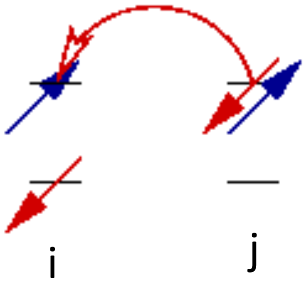
SU(4) Hubbard-Heisenberg model on the square lattice

(self-adjoint antisymmetric representation)

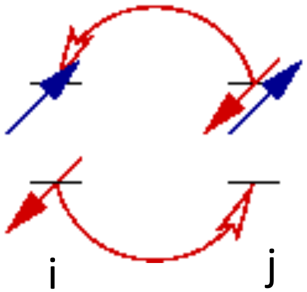
$$\hat{H}_N = \underbrace{-t\sum_b \hat{D}_b^+ + \hat{D}_b}_{\hat{H}_t} \underbrace{-{}^{J}\!/_{4N}\sum_b (\hat{D}_b^+ + \hat{D}_b)^2 - (\hat{D}_b^+ - \hat{D}_b)^2}_{\hat{H}_J} + \underbrace{{}^{U}\!/_{N}\sum_i (\hat{\mathbf{c}}_i^+ \hat{\mathbf{c}}_i - N/2)^2}_{\hat{H}_U}$$

$$b = \text{Bond} = < i, j >, \qquad \hat{D}_b^+ = \mathbf{c}_i^+ \mathbf{c}_j$$

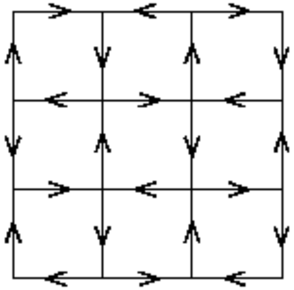
N=4 Two orbitals per unit cell.



t: Diagonal hopping

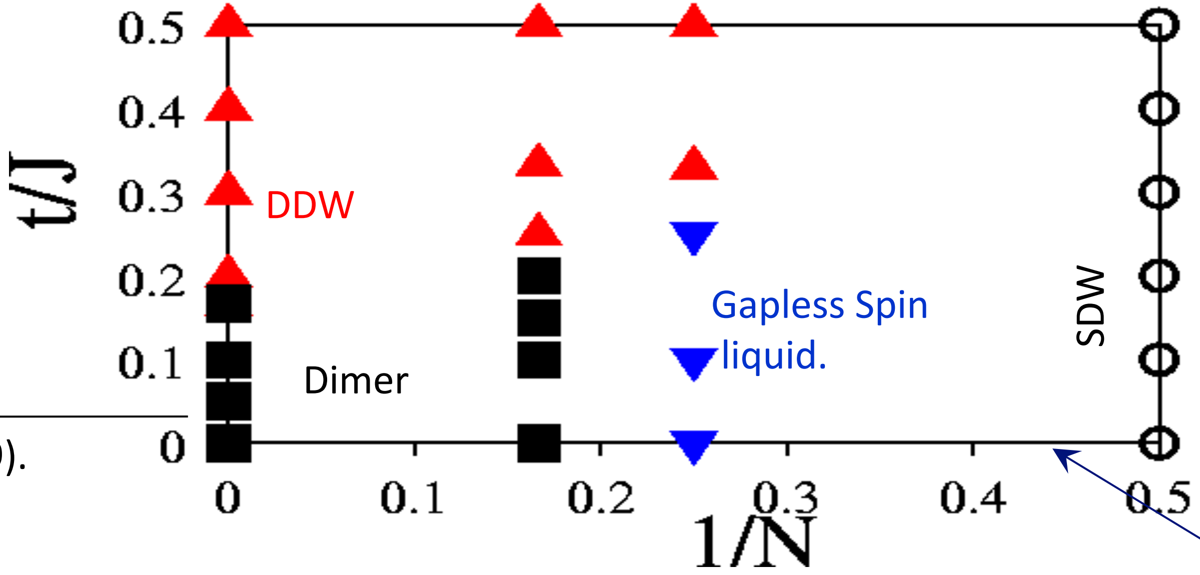


J: Exchange

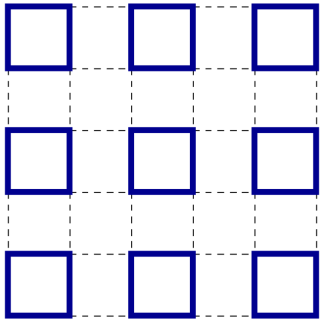


DDW.
Broken time
and lattice symmetries.
Semimetal. Nodes at k=(π/2,π/2)

T=0, (U/J=0)



Affleck-Marston (89).



Dimer: Broken
lattice symmetries.
Insulator.
Spin gap.

Heisenberg

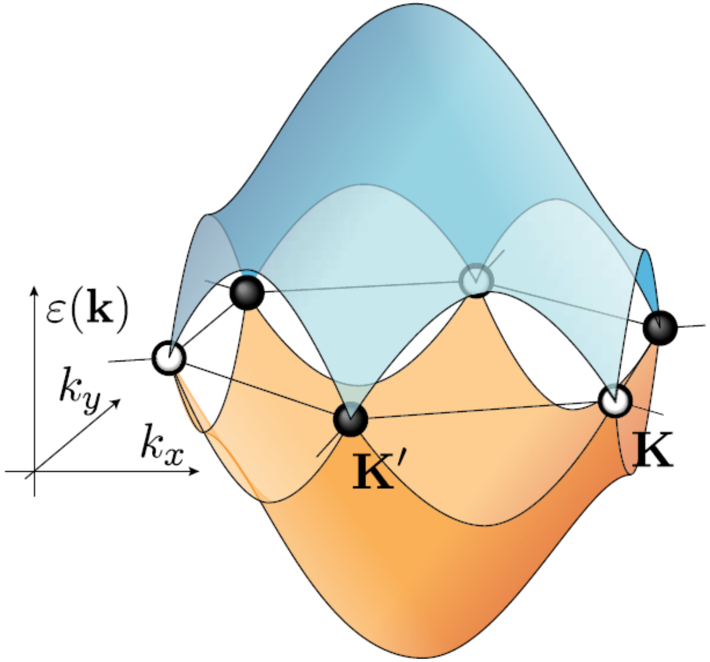
$$H = \frac{J}{N}\sum_{\substack{\langle \mathbf{i},\mathbf{j}\rangle \\ \alpha,\beta}} S_{\mathbf{i}}^{\alpha,\beta}\, S_{\mathbf{j}}^{\beta,\alpha}$$

$$S_{\mathbf{i}}^{\alpha,\beta} = c^{+}_{\mathbf{i},\alpha}\, c_{\mathbf{i},\beta} - \delta_{\alpha,\beta} N/2$$

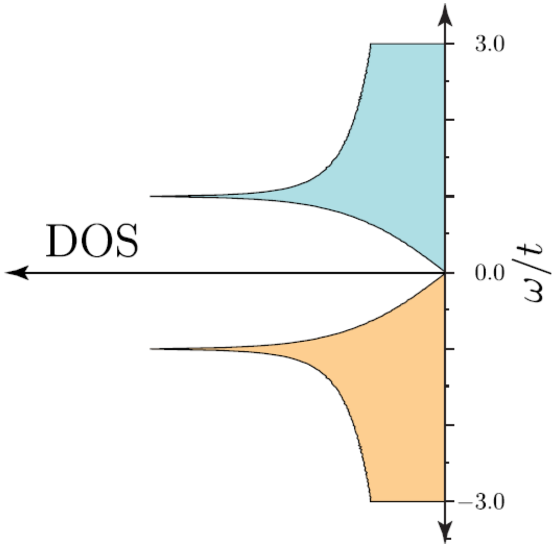
$$\mathbf{c}_i^{+}\mathbf{c}_i = N/2$$

FFA PRB (2005)

Exceptions to Murphy's Law: Hubbard model on the Honeycomb lattice.



Semi-metal
of massless
Dirac Fermions



Direct transition
or intermediate
phase ?

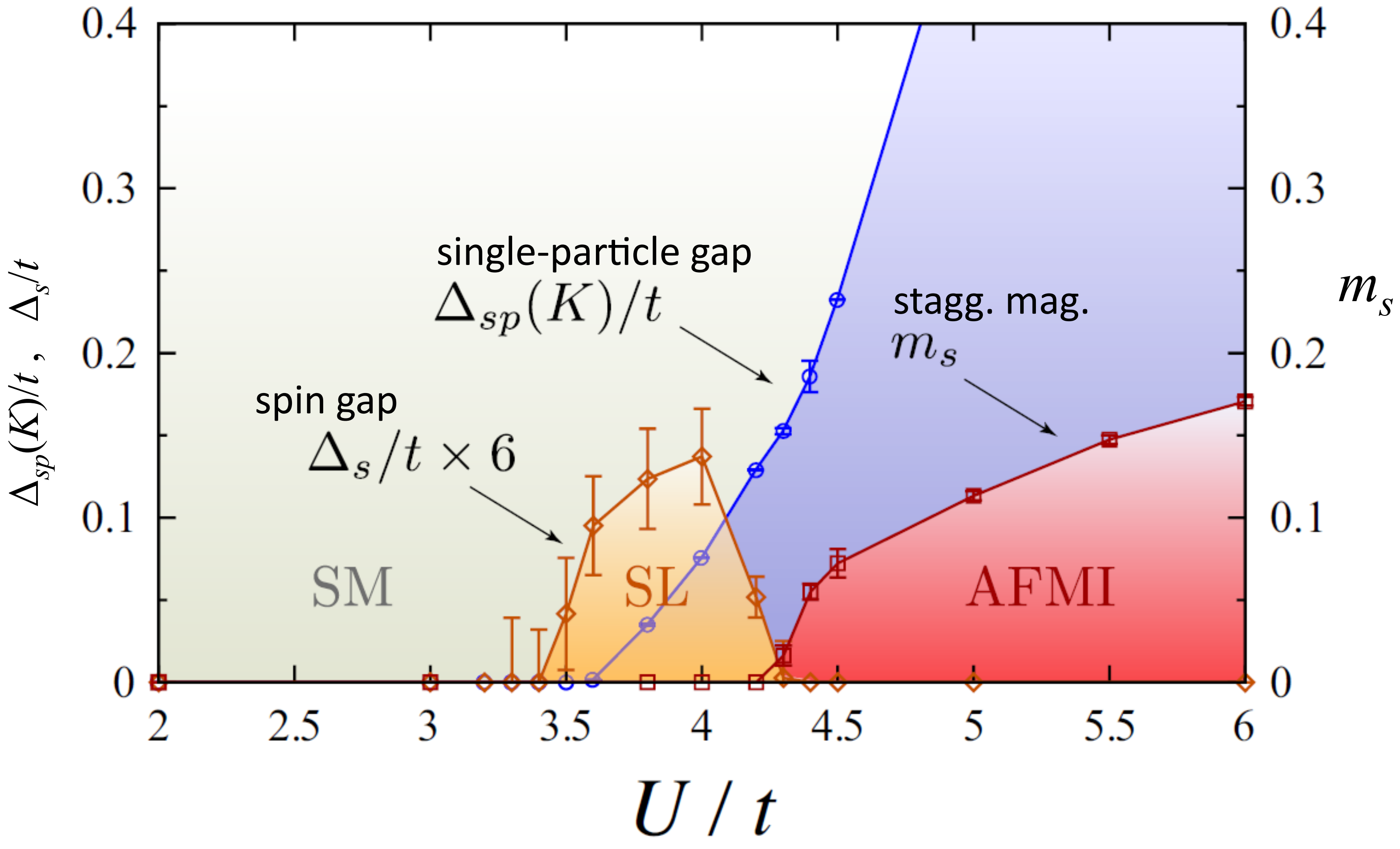
U/t

Semi-metal.
Is stable, due to the
vanishing of the density of states.

Antiferromagnetic
Mott insulator.

Exceptions to Murphy's Law: Hubbard model on the Honeycomb lattice.

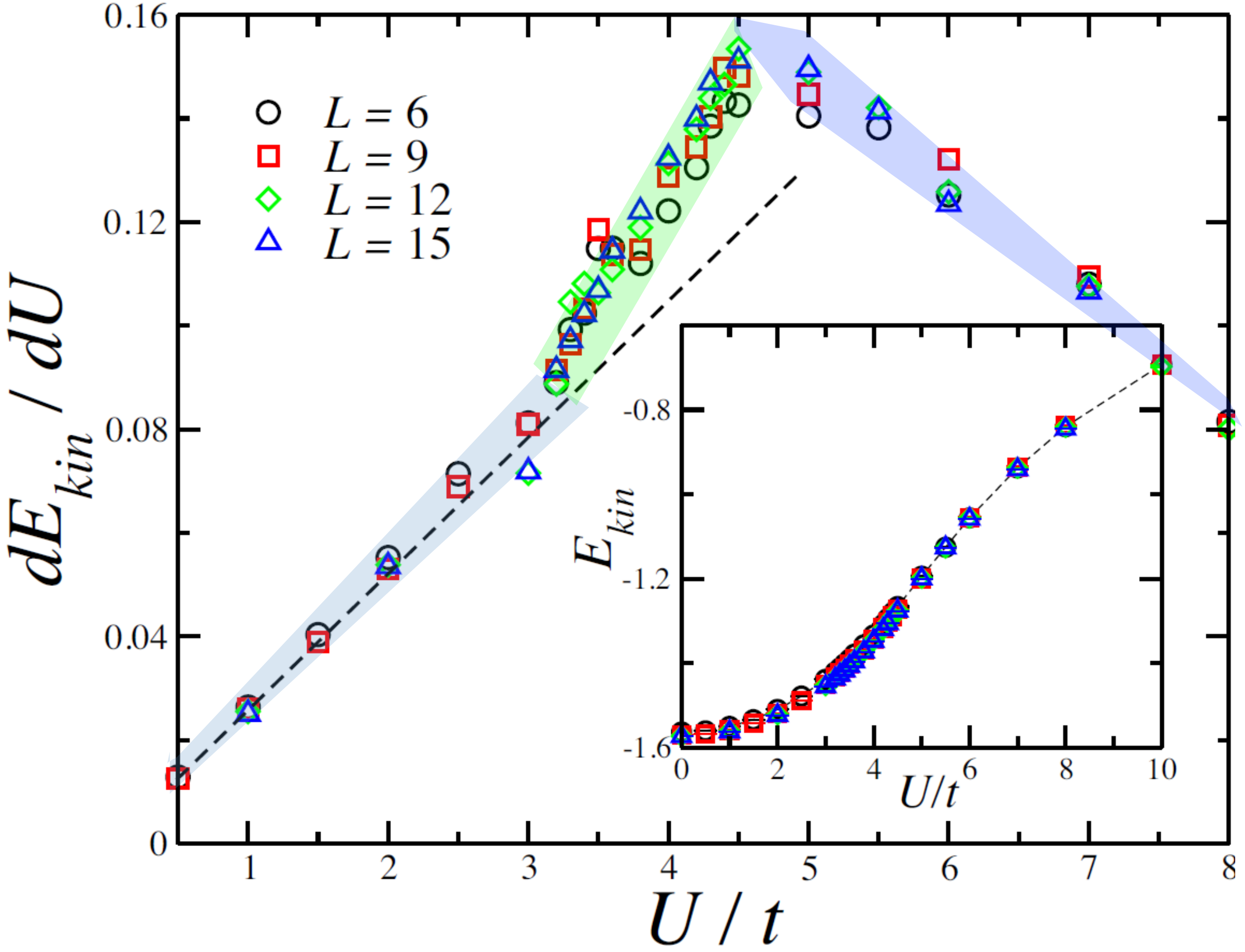
- Intermediate spin liquid phase



tU

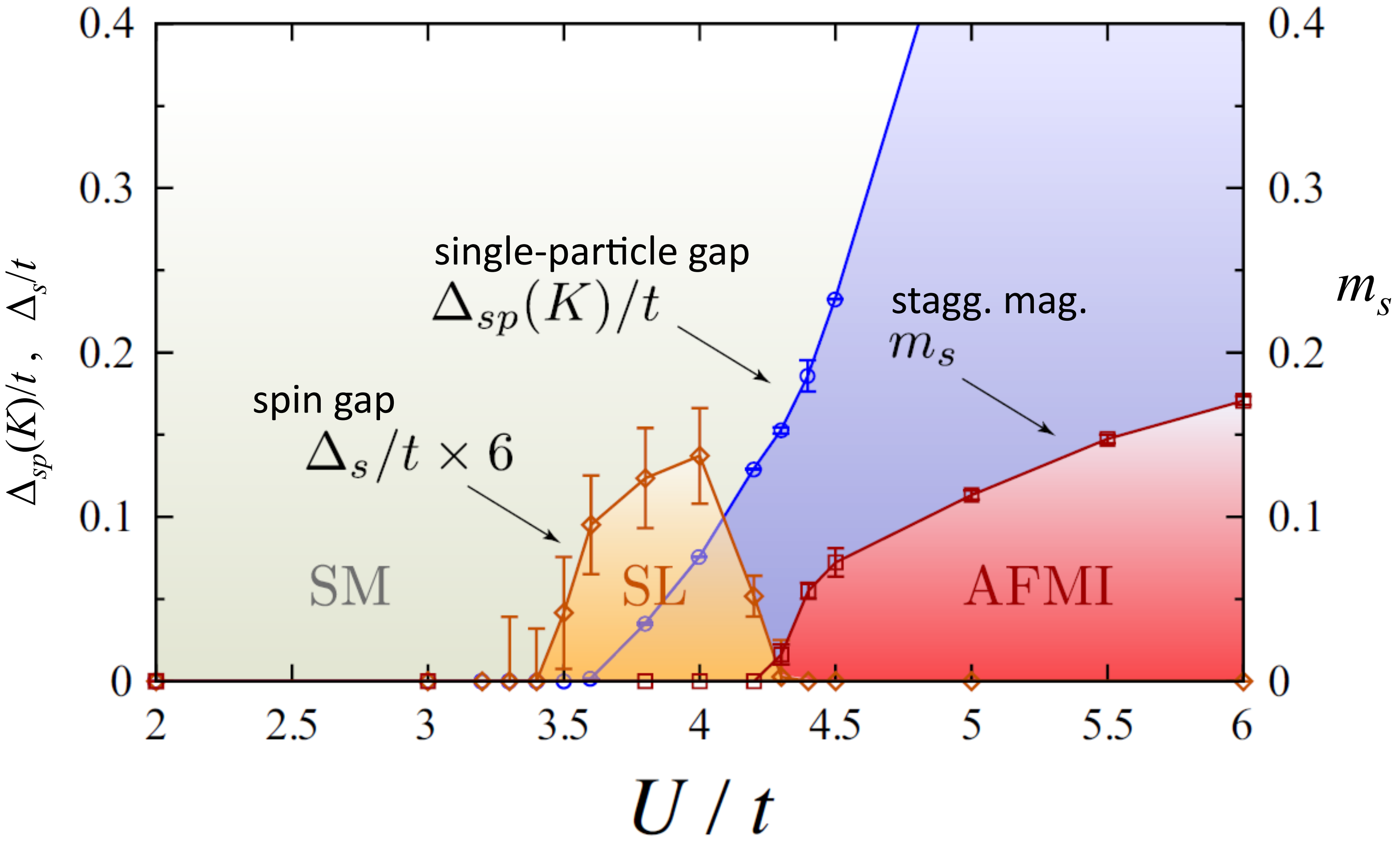
The Mott transition

Kinetic energy.



Exceptions to Murphy's Law: Hubbard model on the Honeycomb lattice.

- Intermediate spin liquid phase



→ Correlation effects in topological insulators.

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- The method with details of the projective method.
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General idea.

Path integral.
Hubbard Stratonovitch.

Single particle problem in an external field.
Solvable Φ

Many body problem.

$$\mathrm{Tr}\, e^{-\beta H} = \int d\phi \, e^{-S(\phi)}$$

High dimensional integral. [Φ=Φ (x,t)]

Sampling.

$$\phi(t+\delta t) = \phi(t) - \frac{\partial S(\phi)}{\partial \phi(t)} + \sqrt{2\delta t}\,\eta(t) \quad \text{so that} \quad P(\phi, t \to \infty) = e^{-S(\phi)}$$

- S(Φ) real. CPU time: $N^3\beta$
- S(Φ) complex. CPU time: $e^{\Delta\beta N}$ Sign problem

Hubbard.

$$\hat{H} = -t\sum_{\langle i,j\rangle,\sigma} e^{\frac{2\pi i}{\Phi_0}\int_i^j \mathbf{A}\,d\mathbf{l}}\, \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} + U\sum_{i} (\hat{n}_{i,\uparrow}-1/2)(\hat{n}_{i,\downarrow}-1/2),\quad \hat{n}_{i,\sigma} = \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma}$$

$$\mathbf{B} = \nabla \wedge \mathbf{A} = (0,0,B)$$

Ground state method:CPU $V^3\beta$

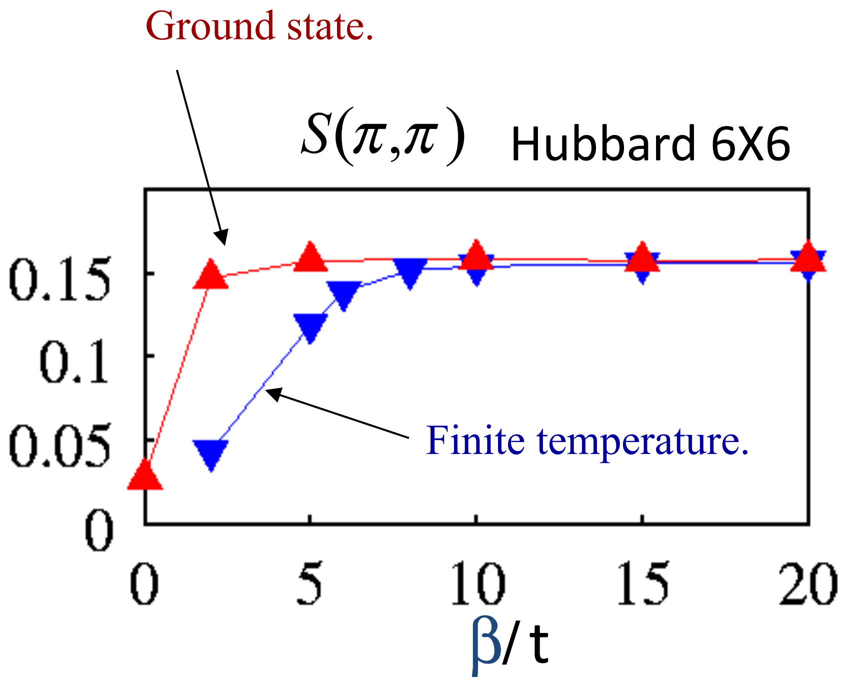
$$\langle \hat{O} \rangle_0 = \lim_{\beta\to\infty} \frac{\langle \Psi_T | e^{-\beta\hat{H}/2}\hat{O}e^{-\beta\hat{H}/2} | \Psi_T \rangle}{\langle \Psi_T | e^{-\beta\hat{H}} | \Psi_T \rangle}$$

$$\langle \Psi_0 | \Psi_T \rangle \neq 0$$

Ground state should be unique.

Finite temperature: CPU $V^3\beta$

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{O} \right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}} \right]}$$



Basic formalism for the case of the Hubbard model.

$$\hat{H} = -t \underbrace{\sum_{<\mathrm{i,j}>,\sigma} e^{\frac{2\pi i}{\Phi_0}\int_i^j \mathbf{A}\, d\mathbf{l}}\, \hat{c}^{+}_{\mathrm{i},\sigma}\hat{c}_{\mathrm{j},\sigma}}_{\hat{H}_t = \sum_{\sigma} \hat{\mathbf{c}}^{\dagger}_{\sigma} T_{\sigma}\, \hat{\mathbf{c}}_{\sigma}} + \underbrace{U\sum_{\mathrm{i}} (\hat{n}_{i,\uparrow}-1/2)(\hat{n}_{i,\downarrow}-1/2)}_{\hat{H}_U}, \quad \hat{n}_{i,\sigma} = \hat{c}^{+}_{\mathrm{i},\sigma}\hat{c}_{\mathrm{i},\sigma}$$

Magnetic field in z-direction: $\mathbf{B} = \nabla \wedge \mathbf{A} = (0,0,B)$

Organization.

- Trotter decomposition.
- The choice of the Hubbard Stratonovitch transformation.
- Properties of Slater determinants → Integrating out the Fermions.
- Equal time observables. (Green functions and Wicks theorem)
- Sequential sampling.

Trotter.

Ground state.

$$Z_0 = \langle \Psi_T | e^{-\beta \hat{H}} | \Psi_T \rangle = \langle \Psi_T | \left(e^{-\Delta\tau \hat{\mathrm{H}}_{\mathrm{U}}} e^{-\Delta\tau \hat{\mathrm{H}}_{\mathrm{t}}} \right)^L | \Psi_T \rangle + O\left(\left(\Delta \tau U \right)^2 \right)$$

Finite temperature.

R. M. Fye Phys. Rev. B **33, 6271 (1986)**

$$Z = \mathrm{Tr}\left[e^{-\beta \hat{H}} \right] = \mathrm{Tr}\left[\left(e^{-\Delta\tau \hat{\mathrm{H}}_{\mathrm{U}}} e^{-\Delta\tau \hat{\mathrm{H}}_{\mathrm{t}}} \right)^L \right] + O\left(\left(\Delta \tau U \right)^2 \right)$$

$$L \Delta \tau = \beta$$

Notation: Unification of finite temperature and projective formalism.

Let the trial wave function be the non-degenerate ground state of H_T with energy E_T .

→ $$|\psi_T\rangle\langle\psi_T| = \lim_{\theta_T \to \infty} e^{-\theta_T (\hat{H}_T - E_T)}$$

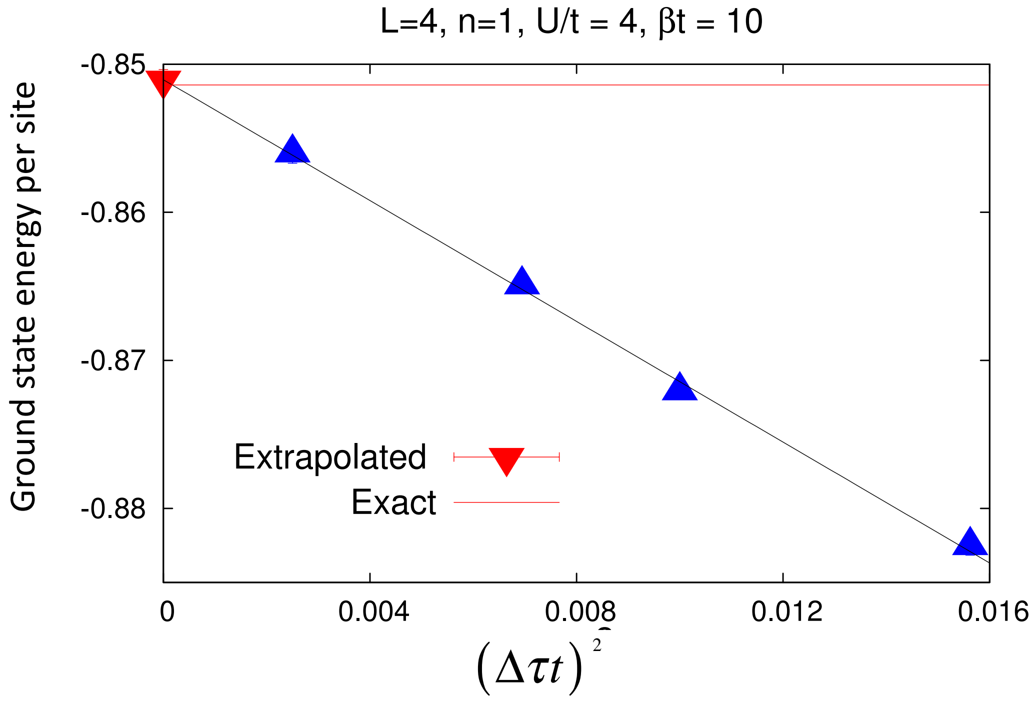
$$Z_0 = \lim_{\theta_T \to \infty} \mathrm{Tr}\left[e^{-\theta_T (\hat{H}_T - E_T)} e^{-\beta \hat{H}} \right]$$

Note. Trotter violates Hermiticity.
Energy is not variational.

→ Way out,

$$Z = \mathrm{Tr}\left[e^{-\beta\hat{H}}\right] = \mathrm{Tr}\left[\left(e^{-\Delta\tau\hat{H}_t/2}e^{-\Delta\tau\hat{H}_U}e^{-\Delta\tau\hat{H}_t/2}\right)^L\right] + O\left(\left(\Delta\tau U\right)^2\right)$$

but is more expensive.



Exact result:

Alberto Parola, Sandro Sorella,
Michele Parrinello, and Erio Tosatti
Phys. Rev. B **43, 6190 (1991)**

Basic formalism for the case of the Hubbard model.

$$\hat{H} = -t \underbrace{\sum_{<i,j>,\sigma} e^{\frac{2\pi i}{\Phi_0}\int_i^j \mathbf{A}\,d\mathbf{l}} \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma}}_{\hat{H}_t = \sum_\sigma \hat{\mathbf{c}}^\dagger_\sigma T_\sigma \hat{\mathbf{c}}_\sigma} + \underbrace{U\sum_i (\hat{n}_{i,\uparrow}-1/2)(\hat{n}_{i,\downarrow}-1/2)}_{\hat{H}_U}, \quad \hat{n}_{i,\sigma} = \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma}$$

Magnetic field in z-direction: $\mathbf{B} = \nabla \wedge \mathbf{A} = (0,0,B)$

Organization.

- Trotter decomposition. ✓
- The choice of the Hubbard Stratonovitch transformation.
- Properties of Slater determinants → Integrating out the Fermions.
- Equal time observables. (Green functions and Wicks theorem)
- Sequential sampling.

The choice of Hubbard Stratonovich transformation.

(Decouples many body propagator into sum of single particle propagator interacting with external field.)

Generic.

$$e^{\Delta\tau \hat{A}^2} = \frac{1}{\sqrt{2\pi}}\int d\varphi \; e^{-\varphi^2/2 \,+\, \sqrt{2\Delta\tau}\,\varphi \hat{A}} \longrightarrow \boxed{e^{\Delta\tau \hat{A}^2} = \sum_{l=\pm1,\pm2} \gamma(l)\, e^{\sqrt{\Delta\tau}\,\eta(l)\,\hat{A}} + O(\Delta\tau^4)}$$

$$\gamma(\pm1) = 1 + \sqrt{6}/3, \quad \gamma(\pm2) = 1 - \sqrt{6}/3$$

$$\eta(\pm1) = \pm\sqrt{2(3-\sqrt{6})}, \quad \eta(\pm2) = \pm\sqrt{2(3+\sqrt{6})}$$

Hubbard.

$$H_U = U(\hat{n}_\uparrow - 1/2)(\hat{n}_\downarrow - 1/2), \quad U > 0$$

$$e^{-\Delta\tau \hat{H}_U} = \underbrace{\frac{1}{2} e^{-\Delta\tau U/4} \sum_{s=\pm1} e^{-\alpha s(\hat{n}_\uparrow - \hat{n}_\downarrow)}}_{\text{Breaks SU(2) spin symmetry. Symmetry is restored after summation over HS. Fields.}} = \underbrace{\frac{1}{2} e^{-\Delta\tau U/4} \sum_{s=\pm1} e^{-i\alpha' s(\hat{n}_\uparrow + \hat{n}_\downarrow - 1)}}_{\text{Complex but conserves SU(2) spin symmetry.}} \quad \left\{ \begin{array}{c} \cosh(a) = e^{\Delta\tau U/2} \\ \cos(a') = e^{-\Delta\tau U/2} \end{array} \right\}$$

$$\boxed{e^{-\Delta\tau \hat{H}_U} e^{-\Delta\tau \hat{H}_t} = \sum_{\mathbf{s}} a(\mathbf{s}) \hat{\mathbf{B}}(\mathbf{s}) \quad \text{with:} \quad \hat{\mathbf{B}}(\mathbf{s}) = e^{\hat{\mathbf{c}}^{+} A(\mathbf{s}) \hat{\mathbf{c}}} e^{\hat{\mathbf{c}}^{+} T \hat{\mathbf{c}}}, \quad \mathbf{s} = (s_1 \cdots s_N)}$$

Basic formalism for the case of the Hubbard model.

$$\hat{H} = -t\underbrace{\sum_{<\mathrm{i,j}>,\sigma} e^{\frac{2\pi i}{\Phi_0}\int_i^j \mathbf{A}\,d\mathbf{l}}\, \hat{c}^{+}_{\mathrm{i},\sigma}\hat{c}_{\mathrm{j},\sigma}}_{\hat{H}_t = \sum_\sigma \hat{\mathbf{c}}^\dagger_\sigma T_\sigma \hat{\mathbf{c}}_\sigma} + \underbrace{U\sum_{\mathrm{i}} (\hat{n}_{i,\uparrow}-1/2)(\hat{n}_{i,\downarrow}-1/2)}_{\hat{H}_U}, \quad \hat{n}_{i,\sigma} = \hat{c}^{+}_{\mathrm{i},\sigma}\hat{c}_{\mathrm{i},\sigma}$$

Magnetic field in z-direction: $\mathbf{B} = \nabla \wedge \mathbf{A} = (0,0,B)$

Organization.

- Trotter decomposition. ✓
- The choice of the Hubbard Stratonovitch transformation. ✓
- Properties of Slater determinants → Integrating out the Fermions.
- Equal time observables. (Green functions and Wicks theorem)
- Sequential sampling.

Integrating out the Fermions. Properties of Slater Determinants.

$$|\Psi_T\rangle = \prod_{y=1}^{N_p}\left(\sum_{x=1}^{N}\hat{c}_x^{+}P_{x,y}\right)|0\rangle$$

(1) Propagation of a Slater determinant with single body operator remains a Slater determinant.

$$e^{\sum_{x,y}\hat{c}_x^\dagger A_{x,y}\hat{c}_y}|\Psi_T\rangle = \prod_{y=1}^{N_p}\left(\sum_{x=1}^{N}\hat{c}_x^\dagger\left(e^A P\right)_{x,y}\right)|0\rangle$$

(2) Overlap.

$$\left\langle \Psi_T \middle| \Psi_T^{'} \right\rangle = \det(P^\dagger P^{'})$$

(3) Trace over the Fock space.

$$\mathrm{Tr}\left(e^{\hat{c}^\dagger A\hat{c}}\ e^{\hat{c}^\dagger B\hat{c}}\right) = \det\left(1+e^{A}\ e^{B}\right)$$

See Notes.

Ground state.

Trial wave function is slater determinant:

$$|\Psi_T\rangle = \prod_{y=1}^{N_p}\left(\sum_{x=1}^{N}\hat{c}_x^{+}P_{x,y}\right)|0\rangle$$

P is N x N_p matrix.

$$\boxed{Z = \sum_{\mathbf{s}_1\cdots\mathbf{s}_L}\prod_{\tau=1}^{L}a(\mathbf{s}_\tau)\langle\Psi_T|\hat{\mathbf{B}}(\mathbf{s}_L)\cdots\hat{\mathbf{B}}(\mathbf{s}_1)|\Psi_T\rangle = \sum_{\mathbf{s}_1\cdots\mathbf{s}_L}\prod_{\tau=1}^{L}a(\mathbf{s}_\tau)\det\left[P^\dagger B(\mathbf{s}_L)\cdots B(\mathbf{s}_1)P\right]}$$

$$\hat{\mathbf{B}}(\mathbf{s}) = e^{\hat{\mathbf{c}}^{+}A(\mathbf{s})\hat{\mathbf{c}}}e^{\hat{\mathbf{c}}^{+}T\hat{\mathbf{c}}}, \quad B(\mathbf{s}) = e^{A(\mathbf{s})}e^{T}$$

Finite temperature.

$$\boxed{Z = \sum_{\mathbf{s}_1\cdots\mathbf{s}_L}\prod_{\tau=1}^{L}\alpha(\mathbf{s}_\tau)\det\left[1 + B(\mathbf{s}_L)\cdots B(\mathbf{s}_1)\right]}$$

Basic formalism for the case of the Hubbard model.

$$\hat{H} = -t \underbrace{\sum_{<i,j>,\sigma} e^{\frac{2\pi i}{\Phi_0}\int_i^j \mathbf{A}\, d\mathbf{l}} \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma}}_{\hat{H}_t = \sum_{\sigma} \hat{\mathbf{c}}^{\dagger}_{\sigma} T_{\sigma} \hat{\mathbf{c}}_{\sigma}} + \underbrace{U \sum_{i} (\hat{n}_{i,\uparrow} - 1/2)(\hat{n}_{i,\downarrow} - 1/2)}_{\hat{H}_U}, \quad \hat{n}_{i,\sigma} = \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma}$$

Magnetic field in z-direction: $\mathbf{B} = \nabla \wedge \mathbf{A} = (0,0,B)$

Organization.

- Trotter decomposition. ✓
- The choice of the Hubbard Stratonovitch transformation. ✓
- Properties of Slater determinants → Integrating out the Fermions. ✓
- Equal time observables. (Green functions and Wicks theorem)
- Sequential sampling.

Observables ground state.

$$\left\langle \hat{O} \right\rangle = \frac{1}{Z} \sum_{\mathbf{s}_1 \cdots \mathbf{s}_L} \prod_{\tau=1}^{L} a(\mathbf{s}_\tau) \;\; \det\left(P^\dagger B(\mathbf{s}_L)\cdots B(\mathbf{s}_1) P\right) \left\langle \hat{O} \right\rangle(\mathbf{s})$$

$$\left\langle \hat{O} \right\rangle(\mathbf{s},\tau) = \frac{\left\langle \boldsymbol{\Psi}_T \middle| \hat{\mathbf{B}}(\mathbf{s}_L)\cdot\cdot\hat{\mathbf{B}}(\mathbf{s}_{\tau+1})\hat{O}\hat{\mathbf{B}}(\mathbf{s}_\tau)\cdot\cdot\hat{\mathbf{B}}(\mathbf{s}_1)\middle|\boldsymbol{\Psi}_T\right\rangle}{\left\langle \boldsymbol{\Psi}_T \middle| \hat{\mathbf{B}}(\mathbf{s}_L)\cdots\hat{\mathbf{B}}(\mathbf{s}_1)\middle|\boldsymbol{\Psi}_T\right\rangle}$$

For a given HS configuration Wick‘s theorem holds. Thus is suffices to compute Green functions.

$$\boxed{G_{x,y,\mathbf{s}}(\tau) = \left\langle \hat{c}_x \hat{c}^\dagger_y \right\rangle(\mathbf{s},\tau)}$$

$$\boxed{G_{\mathbf{s}}(\tau) = 1 - U^>_\tau \left(U^<_\tau U^>_\tau\right)^{-1} U^<_\tau}$$

$$\boxed{U^>_\tau = B\left(\mathbf{s}_\tau\right)\cdots B\left(\mathbf{s}_1\right)P, \quad U^<_\tau = P^\dagger B\left(\mathbf{s}_L\right)\cdots B\left(\mathbf{s}_{\tau+1}\right)}$$

Observables finite temperature/General formulation.

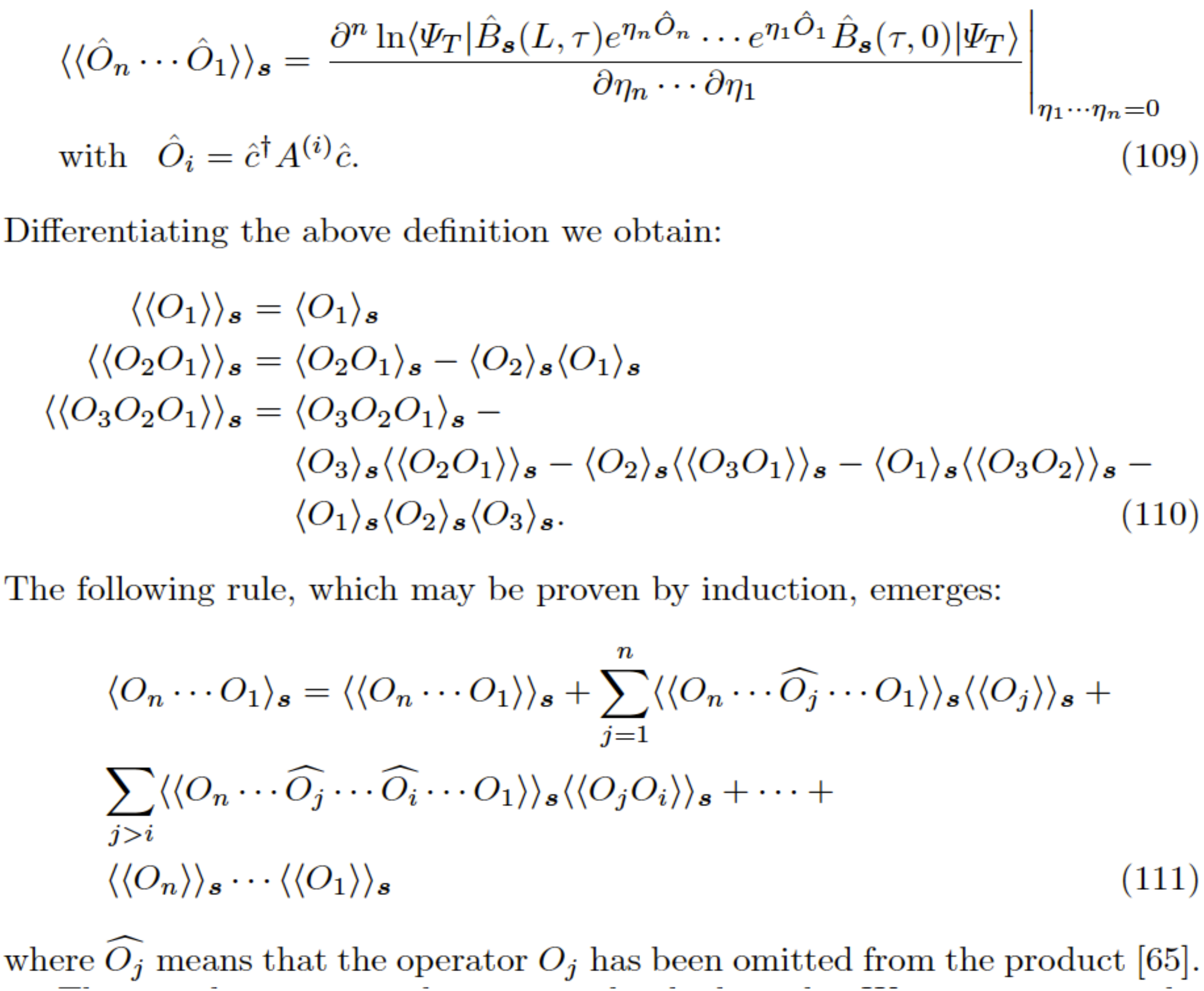
$$\left\langle \hat{O}\right\rangle(s,\tau) = \frac{\mathrm{Tr}\left(e^{-\theta(\hat{H}_T - E_T)}\hat{\mathbf{B}}(\mathbf{s}_L)\cdot\cdot\hat{\mathbf{B}}(\mathbf{s}_{\tau+1}\ )\hat{O}\hat{\mathbf{B}}(\mathbf{s}_\tau)\cdot\cdot\hat{\mathbf{B}}(\mathbf{s}_1)\right)}{\mathrm{Tr}\left(e^{-\theta(\hat{H}_T-E_T)}\hat{\mathbf{B}}(\mathbf{s}_L)\cdot\cdot\hat{\mathbf{B}}(\mathbf{s}_1)\right)}, \qquad \hat{H}_T = \mathbf{c}^\dagger h_T \mathbf{c}$$

$$\boxed{G_{\mathbf{s}}(\tau) = \left(1 + B_{\mathbf{s}}(\tau,0)\, e^{-\theta(h_T - E_T)} B_{\mathbf{s}}(L,\tau)\right)^{-1}}$$

$$\boxed{B_{\mathbf{s}}(\tau,0) = B\left(\mathbf{s}_\tau\right)\cdots B\left(\mathbf{s}_1\right), \;\; B_{\mathbf{s}}(L,\tau) = B\left(\mathbf{s}_L\right)\cdots B\left(\mathbf{s}_{\tau+1}\right)}$$

Wick´s Theorm

Cumulants.



$$\langle\langle \hat{O}_n \cdots \hat{O}_1 \rangle\rangle_{\boldsymbol{s}} = \left. \frac{\partial^n \ln \langle \Psi_T | \hat{B}_{\boldsymbol{s}}(L,\tau) e^{\eta_n \hat{O}_n} \cdots e^{\eta_1 \hat{O}_1} \hat{B}_{\boldsymbol{s}}(\tau,0) | \Psi_T \rangle}{\partial \eta_n \cdots \partial \eta_1} \right|_{\eta_1 \cdots \eta_n = 0}$$

$$\text{with} \quad \hat{O}_i = \hat{c}^\dagger A^{(i)} \hat{c}. \tag{109}$$

Differentiating the above definition we obtain:

$$\begin{aligned}
\langle\langle O_1 \rangle\rangle_{\boldsymbol{s}} &= \langle O_1 \rangle_{\boldsymbol{s}} \\
\langle\langle O_2 O_1 \rangle\rangle_{\boldsymbol{s}} &= \langle O_2 O_1 \rangle_{\boldsymbol{s}} - \langle O_2 \rangle_{\boldsymbol{s}} \langle O_1 \rangle_{\boldsymbol{s}} \\
\langle\langle O_3 O_2 O_1 \rangle\rangle_{\boldsymbol{s}} &= \langle O_3 O_2 O_1 \rangle_{\boldsymbol{s}} - \\
&\quad \langle O_3 \rangle_{\boldsymbol{s}} \langle\langle O_2 O_1 \rangle\rangle_{\boldsymbol{s}} - \langle O_2 \rangle_{\boldsymbol{s}} \langle\langle O_3 O_1 \rangle\rangle_{\boldsymbol{s}} - \langle O_1 \rangle_{\boldsymbol{s}} \langle\langle O_3 O_2 \rangle\rangle_{\boldsymbol{s}} - \\
&\quad \langle O_1 \rangle_{\boldsymbol{s}} \langle O_2 \rangle_{\boldsymbol{s}} \langle O_3 \rangle_{\boldsymbol{s}}.
\end{aligned} \tag{110}$$

The following rule, which may be proven by induction, emerges:

$$\begin{aligned}
&\langle O_n \cdots O_1 \rangle_{\boldsymbol{s}} = \langle\langle O_n \cdots O_1 \rangle\rangle_{\boldsymbol{s}} + \sum_{j=1}^{n} \langle\langle O_n \cdots \widehat{O_j} \cdots O_1 \rangle\rangle_{\boldsymbol{s}} \langle\langle O_j \rangle\rangle_{\boldsymbol{s}} + \\
&\sum_{j>i} \langle\langle O_n \cdots \widehat{O_j} \cdots \widehat{O_i} \cdots O_1 \rangle\rangle_{\boldsymbol{s}} \langle\langle O_j O_i \rangle\rangle_{\boldsymbol{s}} + \cdots + \\
&\langle\langle O_n \rangle\rangle_{\boldsymbol{s}} \cdots \langle\langle O_1 \rangle\rangle_{\boldsymbol{s}}
\end{aligned} \tag{111}$$

where $\widehat{O_j}$ means that the operator O_j has been omitted from the product [65].

Computing cumulants. (n=2)

$$\hat{O}_i = \hat{c}^\dagger A^{(i)} \hat{c}$$

$$A^{(i)}_{x,y} = \delta_{x,x_i}\delta_{y,y_i}$$

$$\begin{aligned}
\langle\langle \hat{O}_2 \hat{O}_1 \rangle\rangle_{\boldsymbol{s}} &= \langle\langle c^\dagger_{x_2} c_{y_2} c^\dagger_{x_1} c_{y_1} \rangle\rangle_{\boldsymbol{s}} \\
&= \left. \frac{\partial^2 \mathrm{Tr} \ln \left(P^\dagger B_{\boldsymbol{s}}(L,\tau) e^{\eta_2 A^{(2)}} e^{\eta_1 A^{(1)}} B_{\boldsymbol{s}}(\tau,0) P \right)}{\partial \eta_2 \partial \eta_1} \right|_{\eta_2,\eta_1=0} \\
&= \frac{\partial}{\partial \eta_2} \mathrm{Tr} \left[\left(U^{\langle} e^{\eta_2 A^{(2)}} U^{\rangle} \right)^{-1} U^{\langle} e^{\eta_2 A^{(2)}} A^{(1)} U^{\rangle} \right] \Big|_{\eta_2=0} \\
&= -\mathrm{Tr} \left[\left(U^{\langle} U^{\rangle} \right)^{-1} U^{\langle} A^{(2)} U^{\rangle} \left(U^{\langle} U^{\rangle} \right)^{-1} U^{\langle} A^{(1)} U^{\rangle} \right] \\
&\quad + \mathrm{Tr} \left[\left(U^{\langle} U^{\rangle} \right)^{-1} U^{\langle} A^{(2)} A^{(1)} U^{\rangle} \right] \\
&= \mathrm{Tr} \left(\overline{G_{\boldsymbol{s}}} A^{(2)} G_{\boldsymbol{s}} A^{(1)} \right) \\
&= \langle c^\dagger_{x_2} c_{y_1} \rangle_{\boldsymbol{s}} \langle c_{y_2} c^\dagger_{x_1} \rangle_{\boldsymbol{s}}, \quad \text{with } \overline{G} = 1 - G
\end{aligned}$$

Note. $\frac{\partial}{\partial \eta} A^{-1}(\eta) = -A^{-1}(\eta) \left(\frac{\partial}{\partial \eta} A(\eta) \right) A^{-1}(\eta).$

Example. (n=2)

$$\langle c^\dagger_{x_2} c_{y_2} c^\dagger_{x_1} c_{y_1} \rangle_{\boldsymbol{s}} = \langle c^\dagger_{x_2} c_{y_1} \rangle_{\boldsymbol{s}} \langle c_{y_2} c^\dagger_{x_1} \rangle_{\boldsymbol{s}} + \langle c^\dagger_{x_2} c_{y_2} \rangle_{\boldsymbol{s}} \langle c^\dagger_{x_1} c_{y_1} \rangle_{\boldsymbol{s}}.$$

Basic formalism for the case of the Hubbard model.

$$\hat{H} = \underbrace{-t \sum_{<i,j>,\sigma} e^{\frac{2\pi i}{\Phi_0}\int_i^j \mathbf{A}\, d\mathbf{l}}\, \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma}}_{\hat{H}_t = \sum_{\sigma} \hat{\mathbf{c}}^{\dagger}_{\sigma} T_{\sigma} \hat{\mathbf{c}}_{\sigma}} + \underbrace{U \sum_{i} (\hat{n}_{i,\uparrow} - 1/2)(\hat{n}_{i,\downarrow} - 1/2)}_{\hat{H}_U}, \quad \hat{n}_{i,\sigma} = \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma}$$

Magnetic field in z-direction: $\mathbf{B} = \nabla \wedge \mathbf{A} = (0,0,B)$

Organization.

- Trotter decomposition. ✓
- The choice of the Hubbard Stratonovitch transformation. ✓
- Properties of Slater determinants → Integrating out the Fermions. ✓
- Equal time observables. (Green functions and Wicks theorem) ✓
- Sequential sampling.

All in all we have:

$$\left\langle \hat{O} \right\rangle = \frac{\sum_{\mathbf{s}_1\cdots\mathbf{s}_L} \prod_{\tau=1\cdots L} a(\mathbf{s}_\tau) \left\langle \Psi_T \middle| \hat{\mathbf{B}}(\mathbf{s}_L)\cdots\hat{\mathbf{B}}(\mathbf{s}_1) \middle| \Psi_T \right\rangle \left\langle \hat{O} \right\rangle(\mathbf{s})}{\sum_{\mathbf{s}_1\cdots\mathbf{s}_L} \prod_{\tau=1\cdots L} a(\mathbf{s}_\tau) \left\langle \Psi_T \middle| \hat{\mathbf{B}}(\mathbf{s}_L)\cdots\hat{\mathbf{B}}(\mathbf{s}_1) \middle| \Psi_T \right\rangle} = \frac{\sum_{\mathbf{s}_1\cdots\mathbf{s}_L} W(\mathbf{s}) \left\langle \hat{O} \right\rangle(\mathbf{s})}{\sum_{\mathbf{s}_1\cdots\mathbf{s}_L} W(\mathbf{s})}$$

Sum over HS fields → Metropolis importance sampling. Adopt a sequential single spin-flip upgrading scheme.

$$s_{i,\tau} \rightarrow s'_{i,\tau}$$

$$B(\mathbf{s}_\tau) \rightarrow B(\mathbf{s}'_\tau) = (1+\Delta)B(\mathbf{s}_\tau)$$

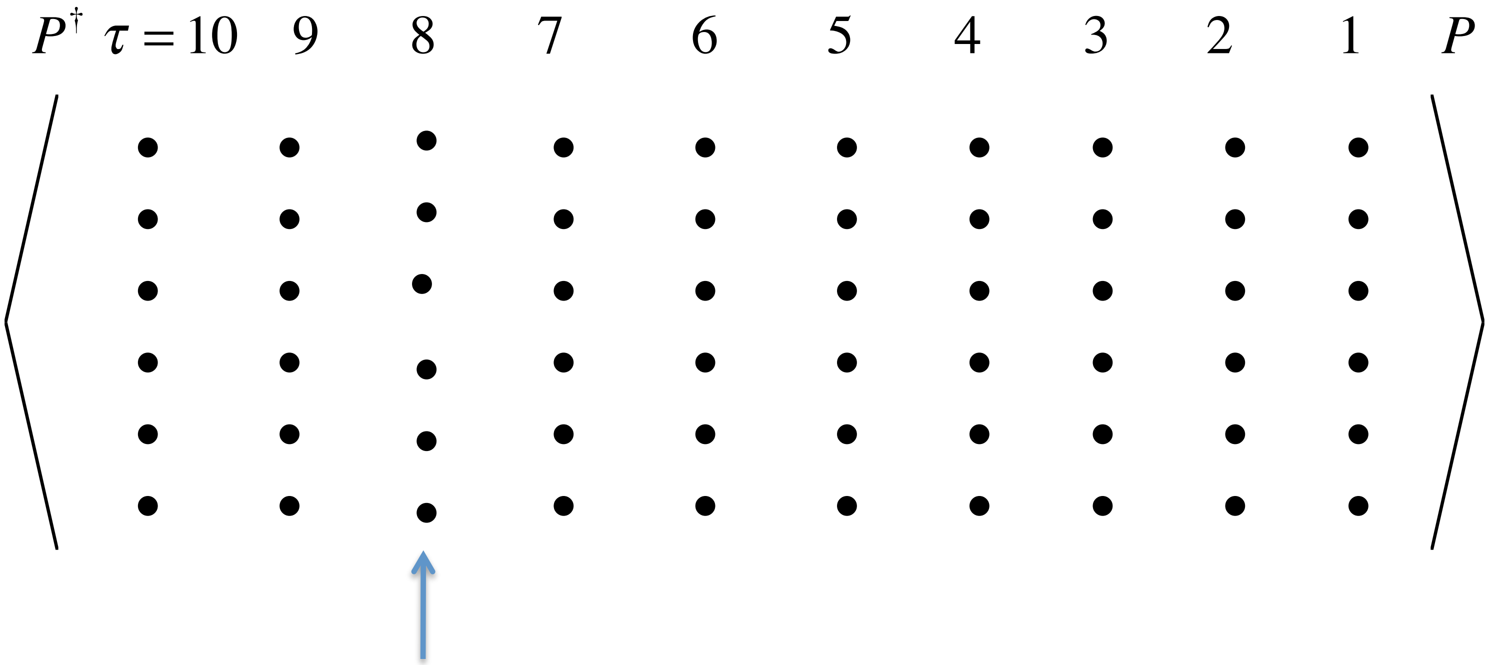
$$\frac{W(\mathbf{s}')}{W(\mathbf{s})} = \frac{a(\mathbf{s}')}{a(\mathbf{s})} \frac{\det\left(U^<_\tau\left(1+\Delta\right)U^>_\tau\right)}{\det\left(U^<_\tau U^>_\tau\right)} = \frac{\alpha(\mathbf{s}')}{\alpha(\mathbf{s})} \det\left[1+\Delta\left(1-G_{\mathbf{s}}(\tau)\right)\right]$$

The equal time Green function matrix is the central quantity of the algorithm. It determines

i) The Monte Carlo dynamics

ii) All equal time observables (Wick’s theorem)

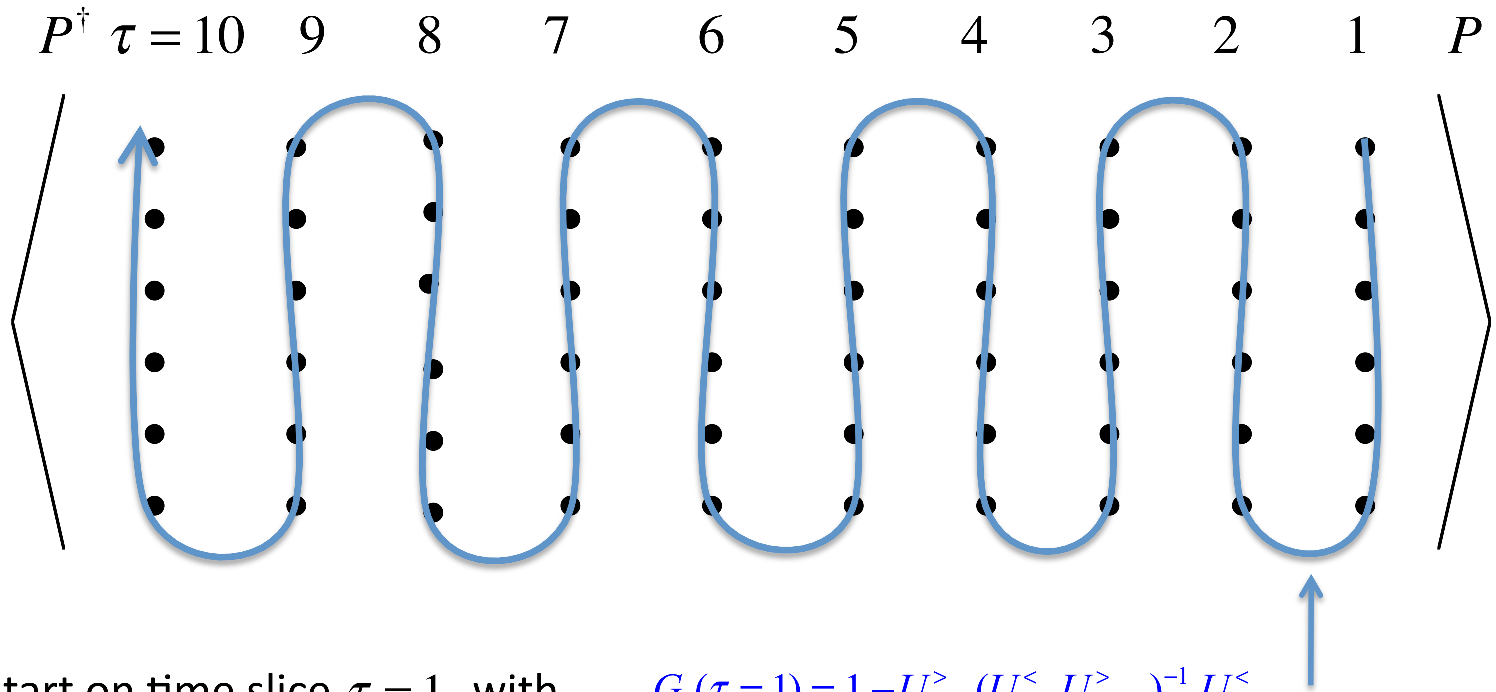
Organization of the code.



Real space lattice, with replica at each imaginary time slice.

Independent Hubbard Stratonovitch field at each imaginary time and lattice site. $s_{i,\tau}$

Organization of the code.



Start on time slice $\tau = 1$ with $G_{\mathbf{s}}(\tau = 1) = 1 - U^{>}_{\tau=1}(U^{<}_{\tau=1}U^{>}_{\tau=1})^{-1}\,U^{<}_{\tau=1}$

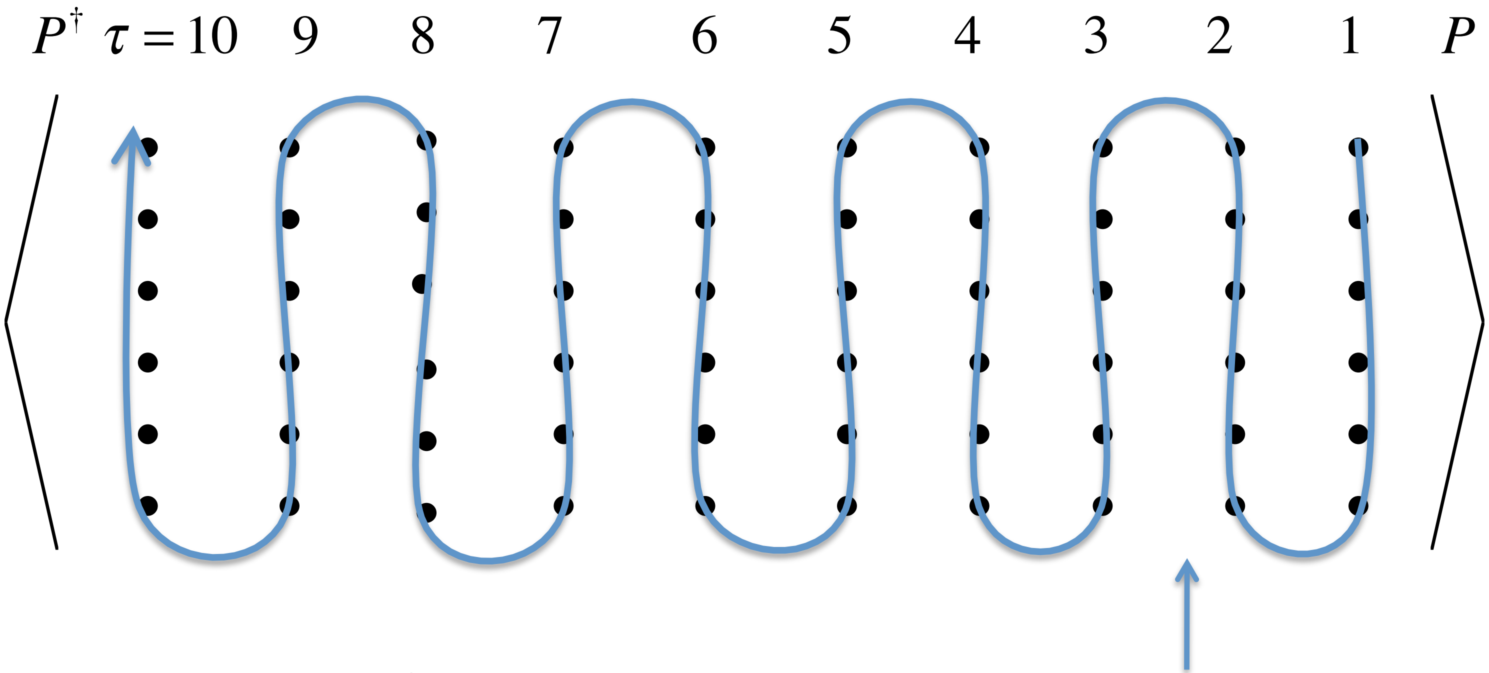
Scan through the real space lattice and flip spin sequentially Accept move with probability:

$$\frac{W(\mathbf{s}')}{W(\mathbf{s})} = \frac{\alpha(\mathbf{s}')}{\alpha(\mathbf{s})}\det\left[1+\Delta\left(1-G_{\mathbf{s}}(\tau=1)\right)\right]$$

If the move is accepted, upgrade the Green function.

$$G_{\mathbf{s}}(\tau = 1) \rightarrow G_{\mathbf{s}'}(\tau = 1)$$

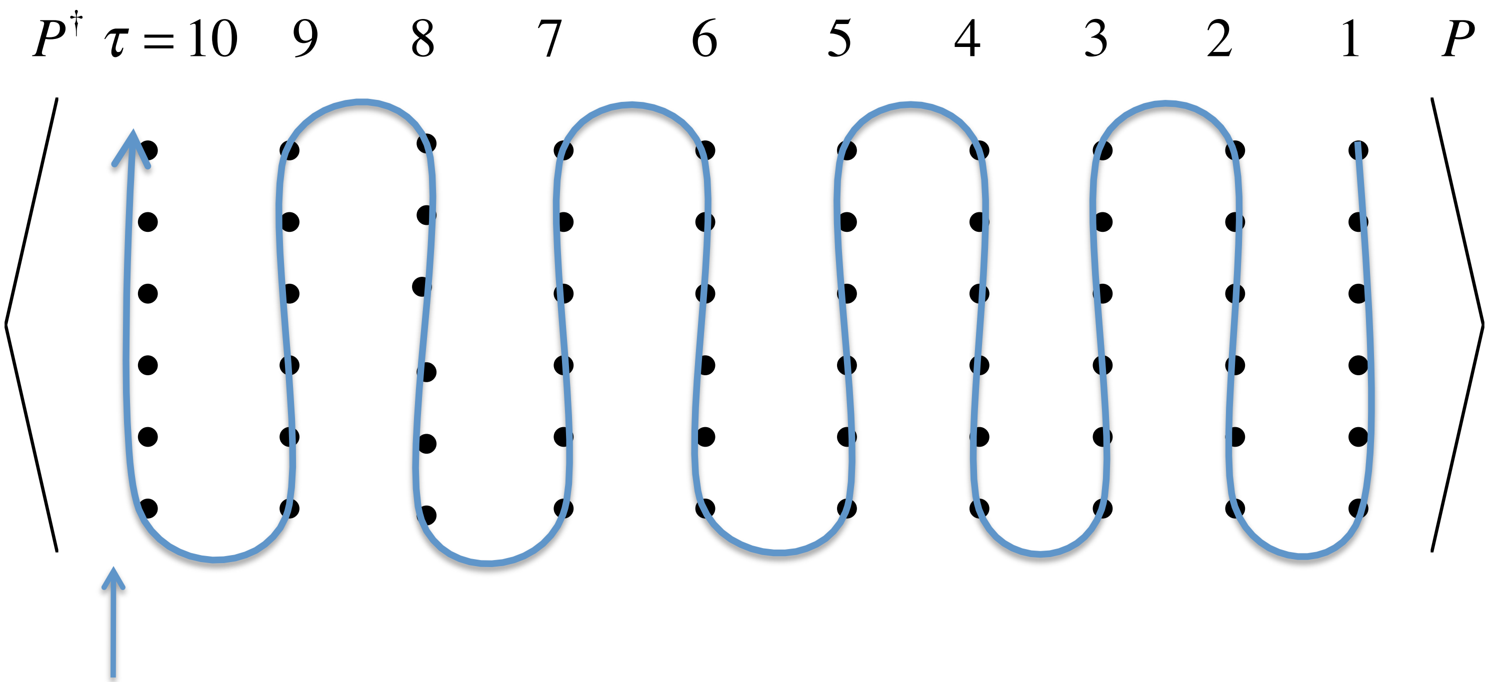
Organization of the code.



Propagate the Green function
from $\tau = 1$ to $\tau = 2$

$$G_{\mathbf{s}}(\tau = 2) = 1 - B(s_2)U^{>}_{\tau=1}(\underbrace{U^{<}_{\tau=1}U^{>}_{\tau=1}}_{=U^{<}_{\tau=2}U^{>}_{\tau=2}})^{-1}\,U^{<}_{\tau=1}B^{-1}(s_2) \;=\; B(s_2)G_{\mathbf{s}}(\tau = 1)B^{-1}(s_2)$$

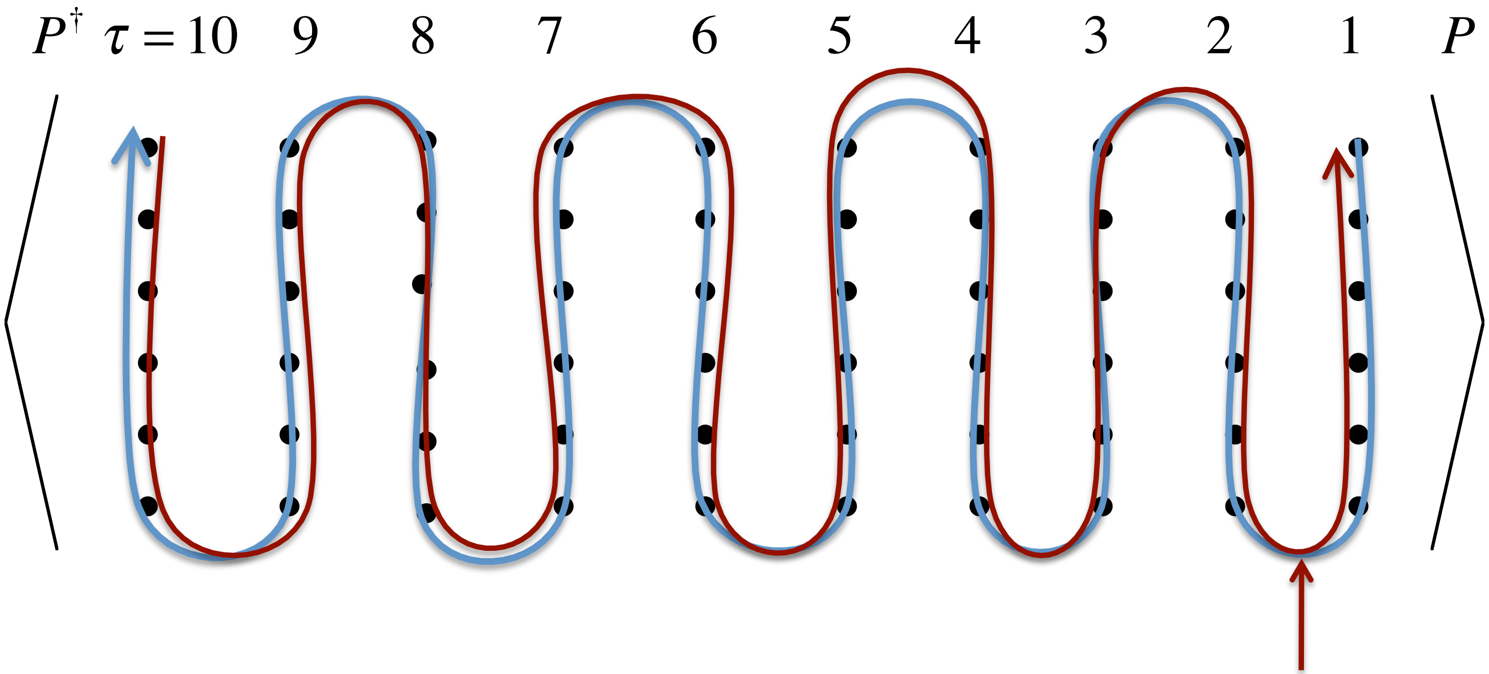
Organization of the code.



Repeat till $\tau = L = 10$ and do not forget to measure observables on the middle time slices.

$$G_{\mathbf{s}}(\tau+1) = 1 - B(s_{\tau+1})U^{>}_{\tau}\,(\underbrace{U^{<}_{\tau}U^{>}_{\tau}}_{=U^{<}_{\tau+1}U^{>}_{\tau+1}})^{-1}\,U^{<}_{\tau}B^{-1}(s_{\tau+1}) = B(s_{\tau+1})G_{\mathbf{s}}(\tau)B^{-1}(s_{\tau+1})$$

Organization of the code.



Retrace your steps back to $\tau = 1$

$$G_s(\tau-1) = 1 - B^{-1}(s_\tau)U^>_\tau \, (\underbrace{U^<_{\tau-1}U^>_{\tau-1}}_{=U^<_\tau U^>_\tau})^{-1} \, U^<_\tau B(s_\tau) \; = \; B^{-1}(s_\tau)G_s(\tau)B(s_\tau)$$

Making the algorithm work.

1) Fast updates. ✓

2) Numerical stabilization.

3) Imaginary time displaced correlation functions.

5) The choice of the trial wave function. Symmetries or overlaps ?

6) Absence of minus sign problem. Conditions for.

Fast updates:

$$e^{-\Delta\tau \hat{H}_U} = \frac{1}{2^N} e^{-\Delta\tau UN/4} \sum_{s_i=\pm 1} e^{-\alpha \sum_i s_i \left(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}\right)} = \frac{1}{2^N} e^{-\Delta\tau UN/4} \sum_{s_i=\pm 1} e^{\sum_{x,y} c_x^\dagger A_{xy}(\mathbf{s}) c_y}$$

Single spin-flip on time slice τ

$$\mathbf{s}_\tau = (s_{\tau,1},\cdots,s_{\tau,r},\cdots s_{\tau,N}) \rightarrow (s_{\tau,1},\cdots,-s_{\tau,r},\cdots s_{\tau,N}) = \mathbf{s}'_\tau$$

$$e^{A(\mathbf{s}')} = \left[1+\Delta^{(r)}\right] e^{A(\mathbf{s})}, \quad \Delta^{(r)}_{x,y} = \sum_\sigma \delta_{x,(r,\sigma)} \delta_{y,(r,\sigma)} \eta^{(r,\sigma)}, \quad \eta^{(r,\sigma)} = (e^{-2\alpha\sigma s_r} - 1)$$

$$B_{s'}(\tau,0) = B(s'_\tau) B(s_\tau) \cdots B(s_1) = (1+\Delta^{(r)}) B_s(\tau,0)$$

$$B_s(L,\tau) = B(s_L)\cdots B(s_{\tau+1})$$

Green function.

$$\Delta^{(z,z')}_{x,y} = \delta_{x,z}\,\delta_{y,z'}\eta^{(z,z')}$$

$$\left(\mathbf{A}+\mathbf{u}\otimes\mathbf{v}\right)^{-1} = \mathbf{A}^{-1} - \frac{\mathbf{A}^{-1}\mathbf{u}\otimes\mathbf{v}\mathbf{A}^{-1}}{1+\mathbf{v}\,\mathbf{A}^{-1}\mathbf{u}}$$

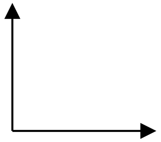
$$\begin{aligned} G_{s'}(\tau)_{x,y} &= \lim_{\theta\to\infty} \left[1 + B_{s'}(\tau,0) e^{-\theta(h_T - E_T)} B_{s'}(L,\tau)\right]^{-1}_{x,y} = \\ &= \lim_{\theta\to\infty} \left[1 + (1+\Delta) B_s(\tau,0) e^{-\theta(h_T - E_T)} B_s(L,\tau)\right]^{-1}_{x,y} \\ &= G_s(\tau)_{x,y} - \frac{G_s(\tau)_{x,z}\eta^{z,z'}\left(1-G_s(\tau)\right)_{z',y}}{\left(1-G_s(\tau)\right)_{z',z}\eta^{z,z'}} \end{aligned}$$

Making the algorithm work.

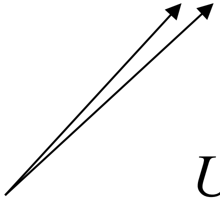
1) Fast updates. ✓
2) Numerical stabilization.
3) Imaginary time displaced correlation functions.
5) The choice of the trial wave function. Symmetries or overlaps ?
6) Absence of minus sign problem. Conditions for.

Numerical stabilization: Problem. $e^{-\beta H_t}$

$P:$

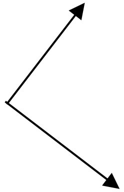


$U^{>} = B(s_l)\cdots B(s_1)P:$



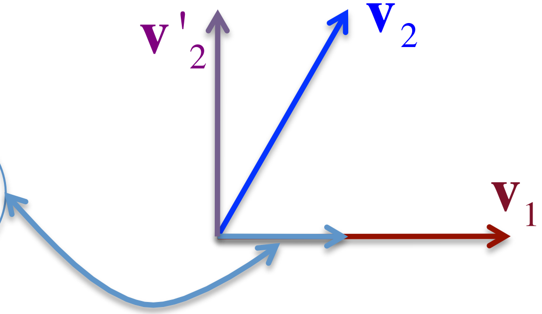
Gram Schmidt.

$U^{>} = \mathbf{U}^{>}\mathrm{d}^{>}\mathrm{v}^{>}$ $\quad \mathbf{U}^{>}:$



The Gram Schmidt orthogonalization.

$$\begin{aligned}
\boldsymbol{v}_1' &= \boldsymbol{v}_1 \\
\boldsymbol{v}_2' &= \boldsymbol{v}_2 - \frac{\boldsymbol{v}_2 \cdot \boldsymbol{v}_1'}{\boldsymbol{v}_1' \cdot \boldsymbol{v}_1'}\boldsymbol{v}_1' \\
&\cdot \\
&\cdot \\
\boldsymbol{v}_{N_p}' &= \boldsymbol{v}_{N_p} - \sum_{i=1}^{N_p-1} \frac{\boldsymbol{v}_{N_p} \cdot \boldsymbol{v}_i'}{\boldsymbol{v}_i' \cdot \boldsymbol{v}_i'}\boldsymbol{v}_i'.
\end{aligned}$$



Since $\boldsymbol{v}_n'$ depends only on the vectors $\boldsymbol{v}_n \cdots \boldsymbol{v}_1$ we can write,

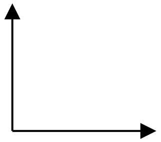
$$\left(\boldsymbol{v}_1', \cdots, \boldsymbol{v}_{N_p}'\right) = \left(\boldsymbol{v}_1, \cdots, \boldsymbol{v}_{N_p}\right) V_R^{-1}$$

where V_R is an upper unit triangular $N_p \times N_p$ matrix, that is the diagonal matrix elements are equal to unity. One can furthermore normalize the vectors $\boldsymbol{v}_1', \cdots, \boldsymbol{v}_{N_p}'$ to obtain:

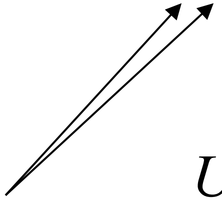
$$B^{\rangle} \equiv \left(\boldsymbol{v}_1, \cdots, \boldsymbol{v}_{N_p}\right) = \underbrace{\left(\frac{\boldsymbol{v}_1'}{|\boldsymbol{v}_1'|}, \cdots, \frac{\boldsymbol{v}_{N_p}'}{|\boldsymbol{v}_{N_p}'|}\right)}_{\equiv U^{\rangle}} D_R V_R$$

Numerical stabilization: Problem. $e^{-\beta H_t}$

$P:$

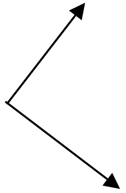


$U^{>} = B(s_l)\cdots B(s_1)P:$



Gram Schmidt.

$U^{>} = \mathbf{U}^{>} \mathrm{d}^{>} \mathrm{v}^{>}$ $\quad \mathbf{U}^{>}:$



Similarly: $U^{<} = \mathbf{U}^{<} \mathrm{d}^{<} \mathrm{v}^{<}$

Green functions remains invariant. $U^{>}\left(U^{<}U^{>}\right)^{-1}U^{<} = \mathbf{U}^{>}\left(\mathbf{U}^{<}\mathbf{U}^{>}\right)^{-1}\mathbf{U}^{<}$ ✓.

Since the algorithm depends only on the equal time Green function everything remains invariant!

Making the algorithm work.

1) Fast updates. ✓

2) Numerical stabilization. ✓

3) Imaginary time displaced correlation functions.

5) The choice of the trial wave function. Symmetries or overlaps ?

6) Absence of minus sign problem. Conditions for.

Measuring time displaced Green functions.

For a given HS field, we wish to evaluate:

$$G_{\boldsymbol{s}}(\tau_1,\tau_2)_{x,y} = \langle T c_x(\tau_1) c_y^\dagger(\tau_2)\rangle_{\boldsymbol{s}} = \begin{cases} \langle c_x(\tau_1) c_y^\dagger(\tau_2)\rangle_{\boldsymbol{s}} & \text{if } \tau_1 \geq \tau_2 \\ -\langle c_y^\dagger(\tau_2) c_x(\tau_1)\rangle_{\boldsymbol{s}} & \text{if } \tau_1 < \tau_2 \end{cases}$$

where T corresponds to the time ordering. Thus for $\tau_1 > \tau_2$ $G_{\boldsymbol{s}}(\tau_1,\tau_2)_{x,y}$ reduces to

Note: $\tau_1 > \tau_2$

$$\langle c_x(\tau_1) c_y^\dagger(\tau_2)\rangle_{\boldsymbol{s}} = \frac{\mathrm{Tr}\left[e^{-\Theta(\hat{H}_T - E_T)} \hat{B}_{\boldsymbol{s}}(\beta,\tau_1) c_x \hat{B}_{\boldsymbol{s}}(\tau_1,\tau_2) c_y^\dagger \hat{B}_{\boldsymbol{s}}(\tau_2,0)\right]}{\mathrm{Tr}\left[e^{-\Theta(\hat{H}_T - E_T)} \hat{B}_{\boldsymbol{s}}(\beta,0)\right]}$$

$$= \frac{\mathrm{Tr}\left[e^{-\Theta(\hat{H}_T - E_T)} \hat{B}_{\boldsymbol{s}}(\beta,\tau_2) \hat{B}_{\boldsymbol{s}}^{-1}(\tau_1,\tau_2) c_x \hat{B}_{\boldsymbol{s}}(\tau_1,\tau_2) c_y^\dagger \hat{B}_{\boldsymbol{s}}(\tau_2,0)\right]}{\mathrm{Tr}\left[e^{-\Theta(\hat{H}_T - E_T)} \hat{B}_{\boldsymbol{s}}(\beta,0)\right]}$$

Measuring time displaced Green functions.

Evaluating $\hat{B}^{-1}(\tau_1,\tau_2) c_x \hat{B}_{\boldsymbol{s}}(\tau_1,\tau_2)$ boils down to the calculation of

$$c_x(\tau) = e^{\tau \boldsymbol{c}^\dagger A \boldsymbol{c}} c_x e^{-\tau \boldsymbol{c}^\dagger A \boldsymbol{c}}$$

where A is an arbitrary matrix. Differentiating the above with respect to τ yields

$$\frac{\partial c_x(\tau)}{\partial \tau} = e^{\tau \boldsymbol{c}^\dagger A \boldsymbol{c}} \left[\boldsymbol{c}^\dagger A \boldsymbol{c}, c_x \right] e^{-\tau \boldsymbol{c}^\dagger A \boldsymbol{c}} = -\sum_{\boldsymbol{z}} A_{x,z} c_z(\tau).$$

Note:
$\tau_1 > \tau_2$

Thus,

$$c_x(\tau) = \left(e^{-A} \boldsymbol{c} \right)_x \quad \text{and similarly} \quad c_x^\dagger(\tau) = \left(\boldsymbol{c}^\dagger e^{A} \right)_x .$$

We can use the above equation successively to obtain:

$$\begin{aligned} \hat{B}_{\boldsymbol{s}}^{-1}(\tau_1,\tau_2) c_x \hat{B}_{\boldsymbol{s}}(\tau_1,\tau_2) &= \left(B_{\boldsymbol{s}}(\tau_1,\tau_2) \boldsymbol{c} \right)_x \\ \hat{B}_{\boldsymbol{s}}^{-1}(\tau_1,\tau_2) c_x^\dagger \hat{B}_{\boldsymbol{s}}(\tau_1,\tau_2) &= \left(\boldsymbol{c}^\dagger B_{\boldsymbol{s}}^{-1}(\tau_1,\tau_2) \right)_x \end{aligned}$$

Since B is a matrix and not a second quantized operator, we can pull it out of the trace to obtain:

Measuring time displaced Green functions.

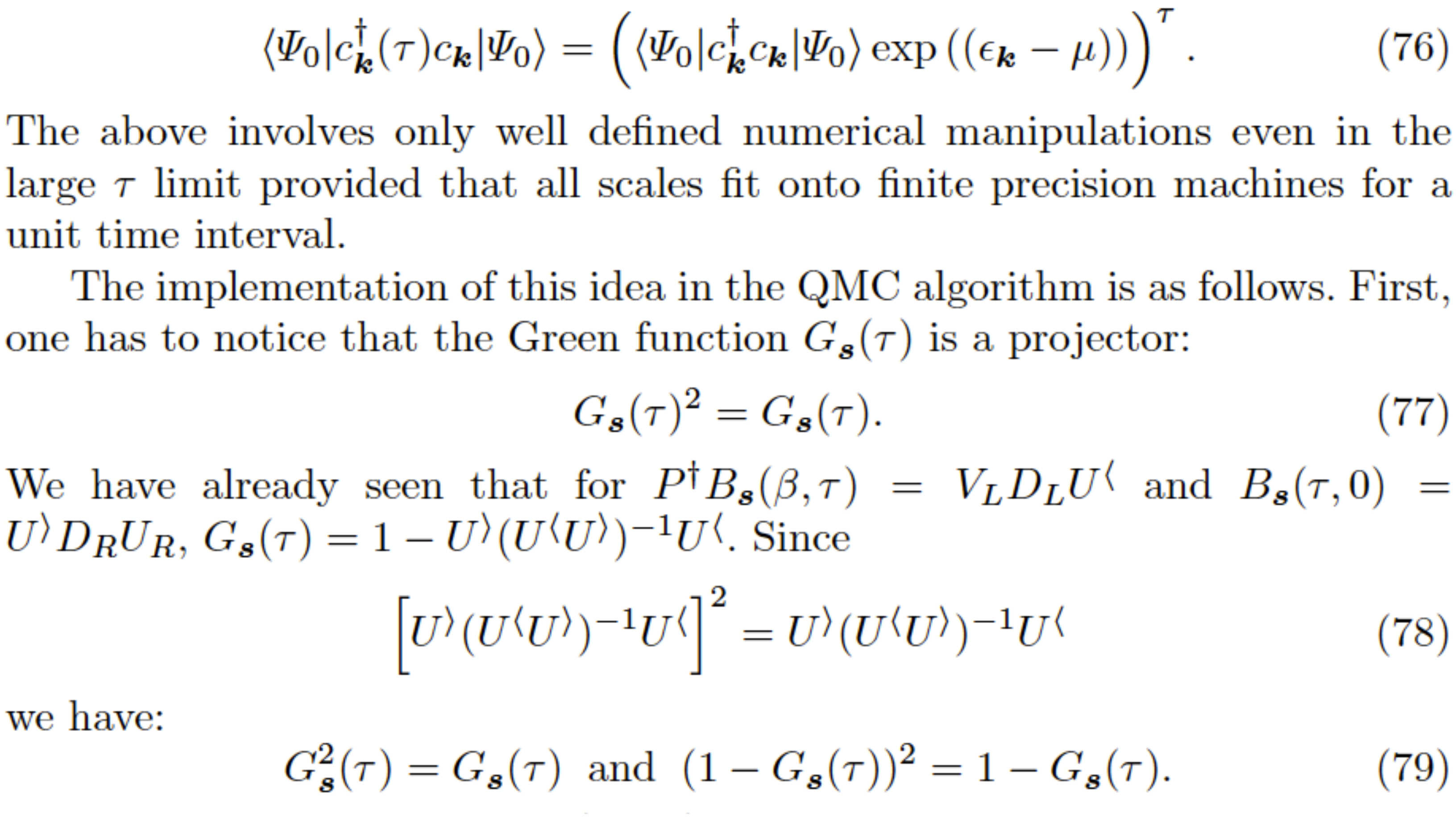
$$G_{\boldsymbol{s}}(\tau_1,\tau_2)_{x,y} = \langle c_x(\tau_1) c^{\dagger}_y(\tau_2)\rangle_{\boldsymbol{s}} = [B_{\boldsymbol{s}}(\tau_1,\tau_2) G_{\boldsymbol{s}}(\tau_2,\tau_2)]_{x,y} \quad \tau_1 > \tau_2$$

Note:
$\tau_1 > \tau_2$

$$G_{\boldsymbol{s}}(\tau_1,\tau_2)_{x,y} = -\langle c^{\dagger}_y(\tau_2) c_x(\tau_1)\rangle_{\boldsymbol{s}} = -\left[\left(1 - G_{\boldsymbol{s}}(\tau_1,\tau_1)\right) B^{-1}_{\boldsymbol{s}}(\tau_2,\tau_1)\right]_{x,y}.$$

Note:
$\tau_1 < \tau_2$

Consider the free electron case: $H_0 = \sum_k \varepsilon(k) c_k^+ c_k$ and assume that $\langle\psi_0|c_k^+ c_k|\psi_0\rangle = 0,1$ so that



$$\langle\Psi_0|c^\dagger_{\boldsymbol{k}}(\tau)c_{\boldsymbol{k}}|\Psi_0\rangle = \Big(\langle\Psi_0|c^\dagger_{\boldsymbol{k}}c_{\boldsymbol{k}}|\Psi_0\rangle \exp\left((\epsilon_{\boldsymbol{k}}-\mu)\right)\Big)^\tau . \tag{76}$$

The above involves only well defined numerical manipulations even in the large τ limit provided that all scales fit onto finite precision machines for a unit time interval.

The implementation of this idea in the QMC algorithm is as follows. First, one has to notice that the Green function $G_{\boldsymbol{s}}(\tau)$ is a projector:

$$G_{\boldsymbol{s}}(\tau)^2 = G_{\boldsymbol{s}}(\tau). \tag{77}$$

We have already seen that for $P^\dagger B_{\boldsymbol{s}}(\beta,\tau) = V_L D_L U^{\langle}$ and $B_{\boldsymbol{s}}(\tau,0) = U^{\rangle} D_R U_R$, $G_{\boldsymbol{s}}(\tau) = 1 - U^{\rangle}(U^{\langle}U^{\rangle})^{-1}U^{\langle}$. Since

$$\left[U^{\rangle}(U^{\langle}U^{\rangle})^{-1}U^{\langle}\right]^2 = U^{\rangle}(U^{\langle}U^{\rangle})^{-1}U^{\langle} \tag{78}$$

we have:

$$G^2_{\boldsymbol{s}}(\tau) = G_{\boldsymbol{s}}(\tau) \ \text{ and } \ (1 - G_{\boldsymbol{s}}(\tau))^2 = 1 - G_{\boldsymbol{s}}(\tau). \tag{79}$$

$$G_{\boldsymbol{s}}(\tau_1, \tau_3) = G_{\boldsymbol{s}}(\tau_1, \tau_2) G_{\boldsymbol{s}}(\tau_2, \tau_1). \tag{80}$$

In particular for $\tau_1 > \tau_2 > \tau_3$

$$\begin{aligned} G_{\boldsymbol{s}}(\tau_1, \tau_3) &= B_{\boldsymbol{s}}(\tau_1, \tau_3) G^2_{\boldsymbol{s}}(\tau_3) = G_{\boldsymbol{s}}(\tau_1, \tau_3) G_{\boldsymbol{s}}(\tau_3) \\ &= \underbrace{G_{\boldsymbol{s}}(\tau_1, \tau_3) B^{-1}_{\boldsymbol{s}}(\tau_2, \tau_3)}_{G_{\boldsymbol{s}}(\tau_1, \tau_2)} \underbrace{B_{\boldsymbol{s}}(\tau_2, \tau_3) G_{\boldsymbol{s}}(\tau_3)}_{G_{\boldsymbol{s}}(\tau_2, \tau_3)} \end{aligned}$$

A similar proof is valid for $\tau_3 > \tau_2 > \tau_1$

Using this composition property (80) we can break up a large τ interval into a set of smaller intervals of length $\tau = N\tau_1$ so that

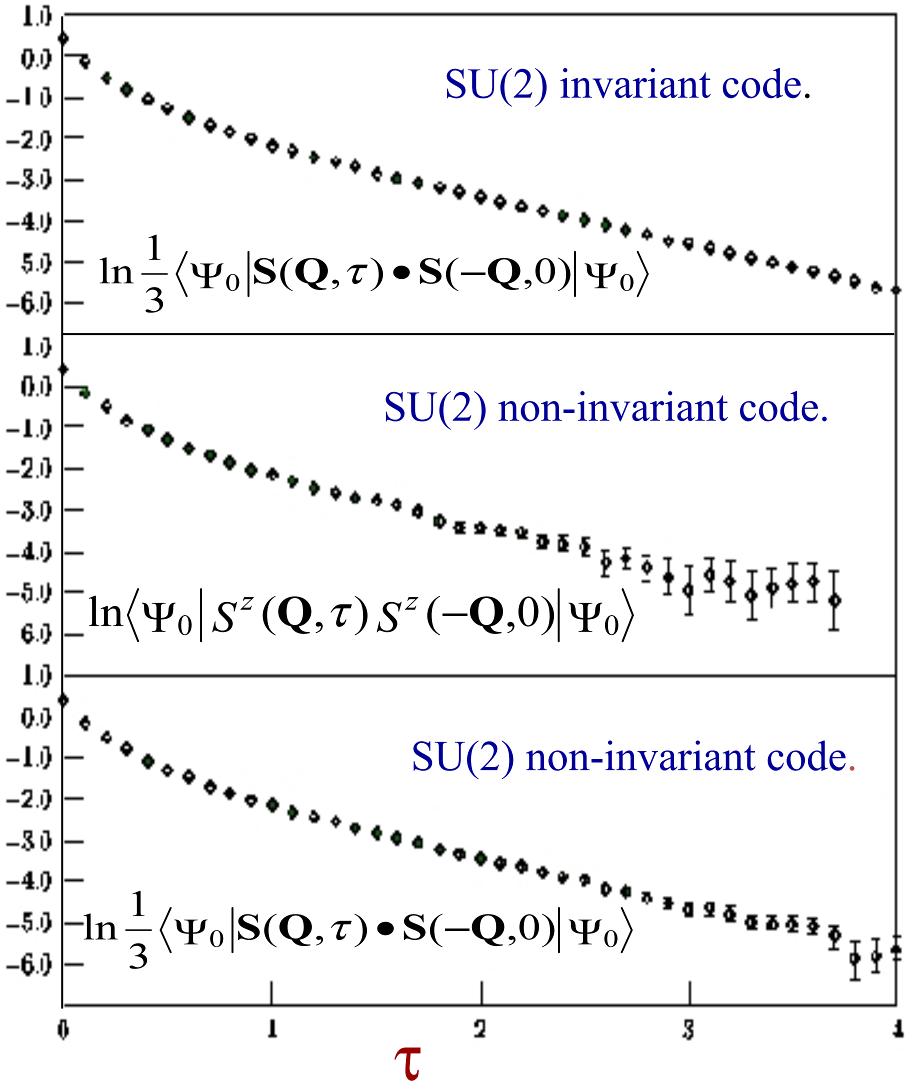
$$G_{\boldsymbol{s}}\left(\beta/2 + \frac{\tau}{2}, \beta/2 - \frac{\tau}{2}\right) = \prod_{n=0}^{N-1} G_{\boldsymbol{s}}\left(\beta/2 - \frac{\tau}{2} + [n+1]\,\tau_1, \beta/2 - \frac{\tau}{2} + n\tau_1\right) \tag{81}$$

The above equation is the generalization of Eq. (76). If τ_1 is *small* enough each Green function in the above product is accurate and has matrix elements bounded by order unity. The matrix multiplication is then numerically well defined.

Imaginary time displaced correlation functions.

Gaps. Dynamics (MaxEnt).

L=8, t-U-W model: W/t =0.35, U/t=2, <n>=1, T=0



$$e^{-\Delta\tau H_U} \sim \sum_{s=\pm1} e^{-i\alpha' s(n_\uparrow + n_\downarrow - 1)}$$

$$e^{-\Delta\tau H_U} \sim \sum_{s=\pm1} e^{-\alpha s(n_\uparrow - n_\downarrow)}$$

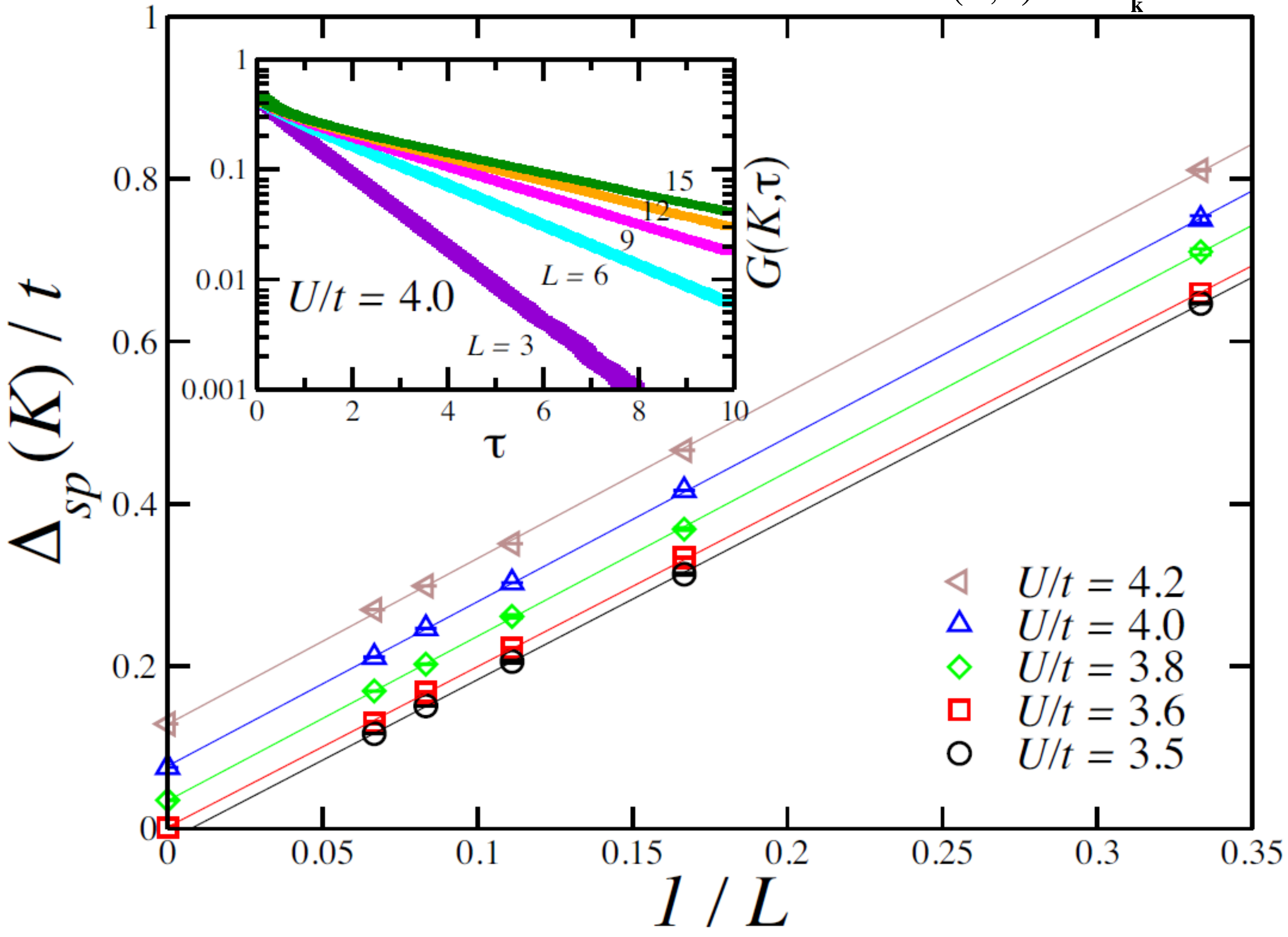
<u>Note</u>: Same CPU time for both simulations.

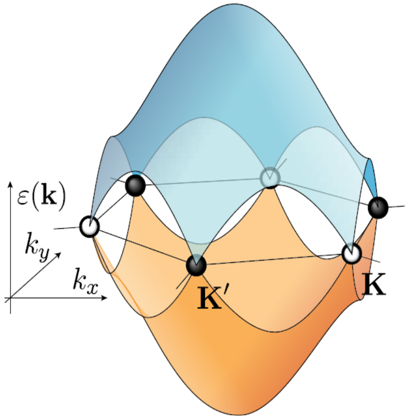
Single-Particle Gap

$$G(\vec{k},\tau) = \frac{1}{2}\sum_a \langle c^\dagger_{\vec{k}a\uparrow}(\tau)\, c_{\vec{k}a\uparrow}(0)\rangle$$

- Green's function

$$G(\vec{\mathbf{k}},\tau) \rightarrow Z_{\vec{\mathbf{k}}}\, e^{-\Delta_{sp}(\vec{\mathbf{k}})\tau}$$





Single particle gap opens beyond

$U\,/\,t > 3.6$

Making the algorithm work.

1) Fast updates. ✓

2) Numerical stabilization. ✓

3) Imaginary time displaced correlation functions. ✓

5) The choice of the trial wave function. Symmetries or overlaps ?

6) Absence of minus sign problem. Conditions for.

PHYSICAL REVIEW B, VOLUME 63, 155114

Spin and charge dynamics of the ferromagnetic and antiferromagnetic two-dimensional half-filled Kondo lattice model

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(Received 26 October 2000; published 30 March 2001)

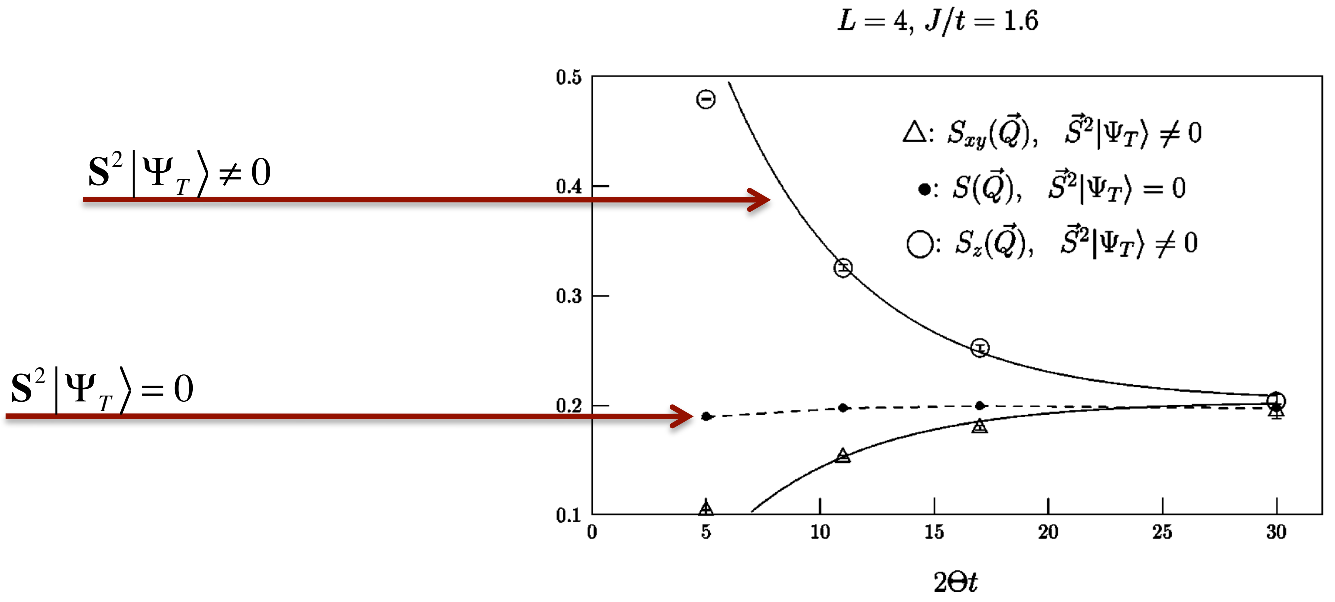

FIG. 1. Spin-spin correlations as a function of the projection parameter Θ. Here, $S(\vec{Q})=\frac{4}{3}\langle\vec{S}^f(\vec{Q})\cdot\vec{S}^f(-\vec{Q})\rangle$, $S^f_z(\vec{Q})=4\langle\vec{S}^f_z(\vec{Q})\cdot\vec{S}^f_z(-\vec{Q})\rangle$, and $S^f_{xy}(\vec{Q})=2(\langle\vec{S}^f_x(\vec{Q})\cdot\vec{S}^f_x(-\vec{Q})\rangle+\langle\vec{S}^f_y(\vec{Q})\cdot\vec{S}^f_y(-\vec{Q})\rangle)$. The trial wave function with $\vec{S}^2|\Psi_T\rangle\neq 0$ ($\vec{S}^2|\Psi_T\rangle=0$) corresponds to the ground state of the Hamiltonian in Eq. (27) [Eq. (17)]. In the *large* Θ limit, the results are independent on the choice of the trial wave function. In particular, starting from a broken-symmetry state the symmetry is restored at *large* values of Θt. For this system, the spin gap is given by $\Delta_{sp}=0.169\pm0.004$ (Ref. 31). Starting with a trial wave function with $\vec{S}^2|\Psi_T\rangle\neq 0$, convergence to the ground state follows approximately the form: $a+be^{-\Delta_{sp}2\Theta}$. The solid lines correspond to a least-square fit to this form.

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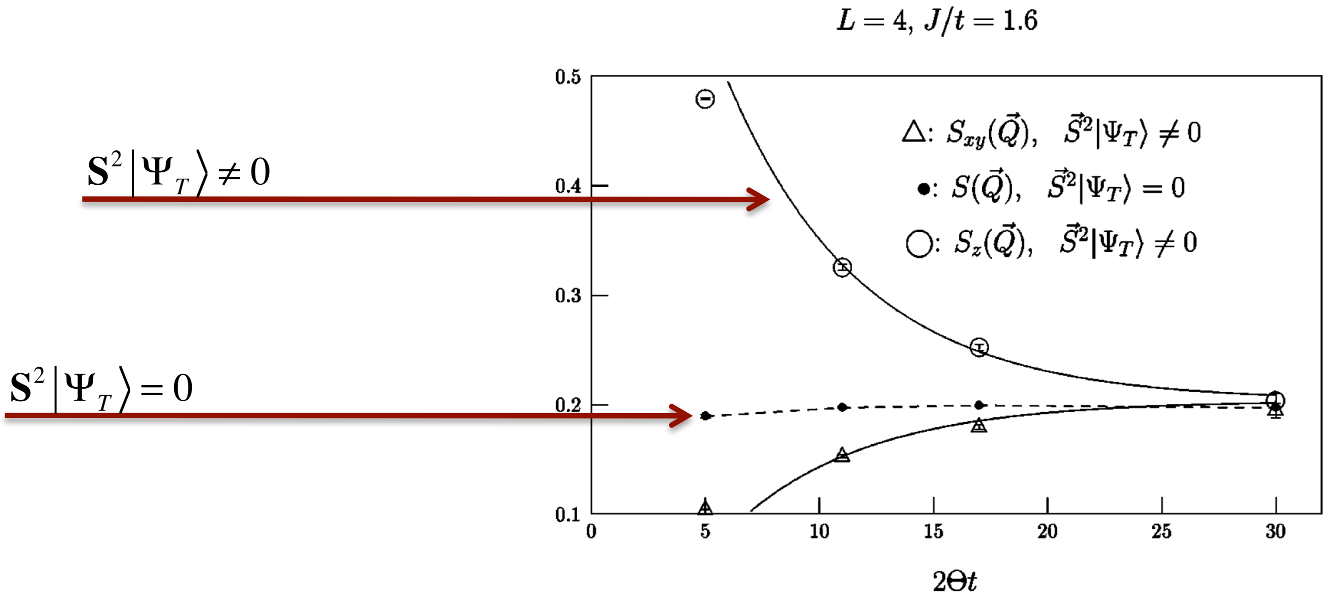

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Optimized Hartree-Fock trial wave functions at finite doping.

N. Furukawa and M. Imada, J. Phys. Soc. Jpn. 60, 3669 (1991).

Making the algorithm work.

1) Fast updates. ✓
2) Numerical stabilization. ✓
3) Imaginary time displaced correlation functions. ✓
5) The choice of the trial wave function. Symmetries or overlaps ? ✓
6) Absence of minus sign problem. Conditions for.

Absence of minus sign problem: conditions for.

$$e^{-\Delta\tau \hat{H}_U} = \frac{1}{2^N} e^{-\Delta\tau U N/4} \sum_{s_i=\pm 1} e^{-\alpha \sum_i s_i \left(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}\right)}$$

$$\left|\psi_T\right\rangle\left\langle\psi_T\right| = \lim_{\theta_T \to \infty} e^{-\theta_T(\hat{H}_T - E_T)} = e^{-\theta_T(\sum_\sigma c^\dagger_\sigma h_\sigma c_\sigma - E_\sigma)}$$

$$\hat{H}_t = \sum_\sigma \hat{\mathbf{c}}^\dagger_\sigma T_\sigma \hat{\mathbf{c}}_\sigma$$

$$Z_0 = \mathrm{Tr}\left[e^{-\theta_T(\hat{H}_T - E_T)} e^{-\beta\hat{H}}\right] = C \sum_s \prod_\sigma \underbrace{\mathrm{Tr}\left[e^{-\theta_T(\mathbf{c}^\dagger h_\sigma \mathbf{c} - E_\sigma)} \prod_{\tau=1}^{L} e^{-\Delta\tau \hat{\mathbf{c}}^\dagger T_\sigma \hat{\mathbf{c}}} e^{\sigma\alpha \sum_i s_{i,\tau}\left(\hat{n}_i - 1/2\right)}\right]}_{W_\sigma(s)}$$

$$\overline{W_{\uparrow,\downarrow}(s)} = \overline{\mathrm{Tr}\left[e^{-\theta_T \left(\sum_{i,j} c_i^\dagger h_{\uparrow\downarrow i,j} c_j - E_{\uparrow\downarrow}\right)} \prod_{\tau=1}^{L} e^{-\Delta\tau \sum_{i,j} \hat{c}_i^\dagger T_{\uparrow\downarrow,i,j}\, \hat{c}_j}\, e^{-\alpha \sum_i s_{i,\tau}\left(\hat{c}_{\boldsymbol{i}}^\dagger \hat{c}_i^\dagger \;-1/2\right)} \right]}$$

Canonical transformation $\quad c_i \rightarrow (-1)^i c_i^\dagger$

$$\overline{W_\uparrow(s)} =$$

$$\overline{\mathrm{Tr}\left[e^{-\theta_T \left(\sum_{i,j} c_j^\dagger (-1)^{i+j+1} h_{\uparrow i,j} c_j - \left(E_\uparrow - \sum_i h_{\uparrow,i,i}\right)\right)} \prod_{\tau=1}^{L} e^{-\Delta\tau \sum_{i,j} \hat{c}_j^\dagger (-1)^{i+j+1} T_{\uparrow,i,j}\, \hat{c}_i}\, e^{-\alpha \sum_i s_{i,\tau}\left(\hat{c}_{\boldsymbol{i}}^\dagger \hat{c}_i^\dagger \;-1/2\right)} \right]}$$

$$W_\downarrow(s)$$

If

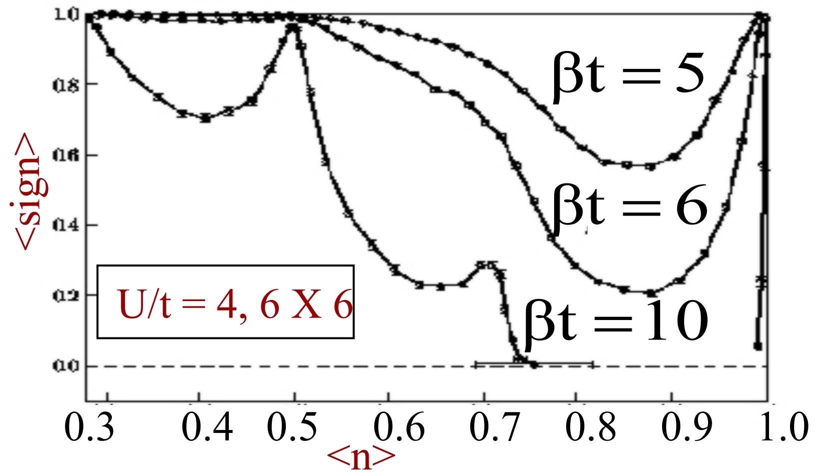
$$(-1)^{i+j+1}\,\overline{h_{\uparrow i,j}} = h_{\downarrow j,i} \qquad E_\uparrow - \sum_i h_{\uparrow,i,i} = E_\downarrow$$

$$(-1)^{i+j+1}\,\overline{T_{\uparrow,i,j}} = T_{\downarrow,j,i}$$

This includes, bipartite lattices with hopping only between sub-lattices. Orbital magnetic field does not generate a sign problem. Zeeman term can also be included.
~~Chemical potential~~

Away from half-filling.

$$e^{-\Delta\tau \hat{H}_U} \sim \sum_{s=\pm 1} e^{-\alpha s (n_\uparrow - n_\downarrow)}$$



Never use.

$$e^{-\Delta\tau \hat{H}_U} \sim \sum_{s=\pm 1} e^{-\alpha i s (n_\uparrow + n_\downarrow - 1)}$$

Making the algorithm work.

1) Fast updates. ✓
2) Numerical stabilization. ✓
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5) The choice of the trial wave function. Symmetries or overlaps ? ✓
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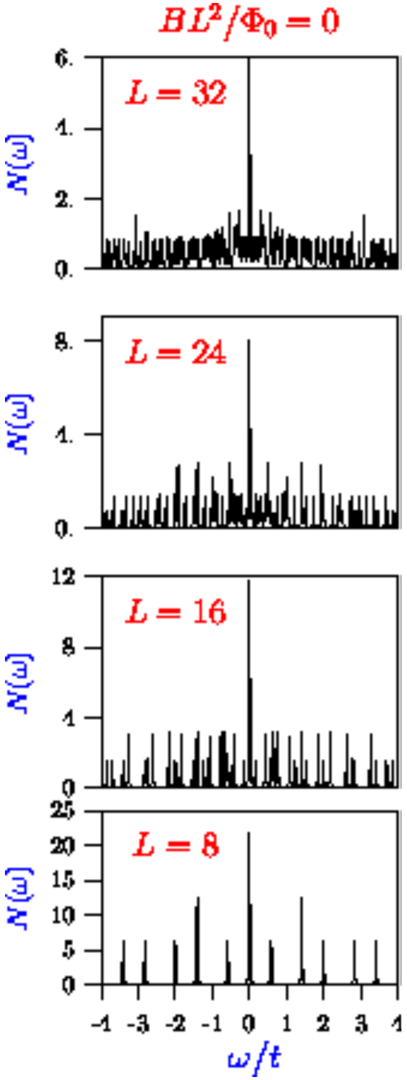
Size effects. Algorithm scales as V³ -> Hard to reach large lattice sizes.

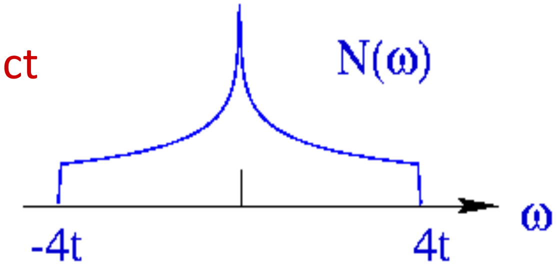
Ex. 2D tight binding.

$$H=-t\sum_{<i,j>} c_i^{+} c_j$$

$$H=-t\sum_{<i,j>} e^{\frac{2\pi i}{\Phi_0}\int_i^j \mathbf{A}\,d\mathbf{l}} c_i^{+} c_j$$



Exact



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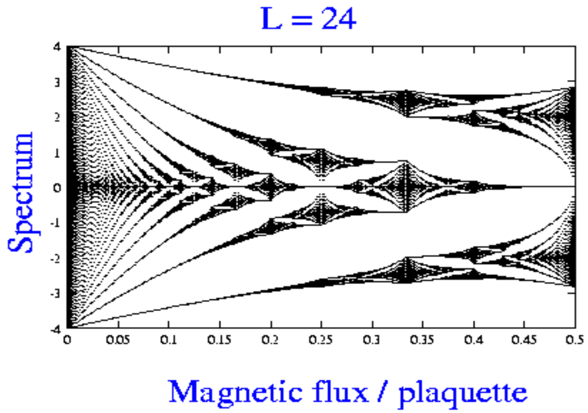
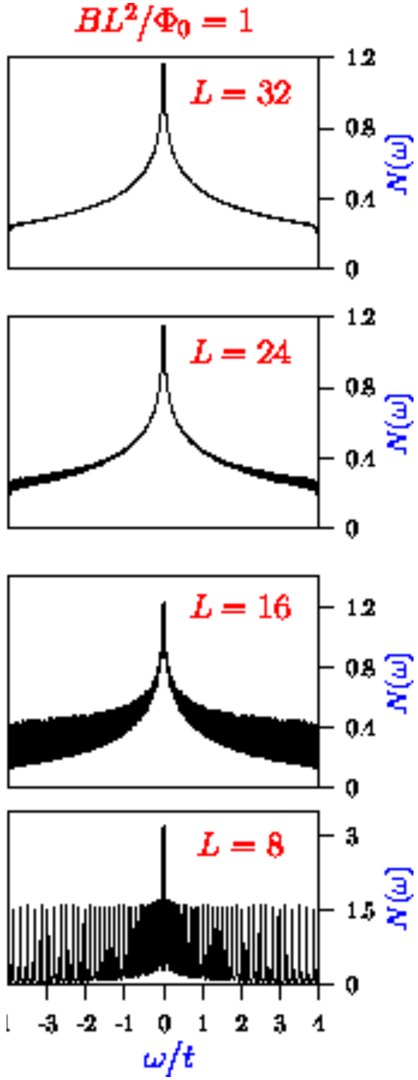


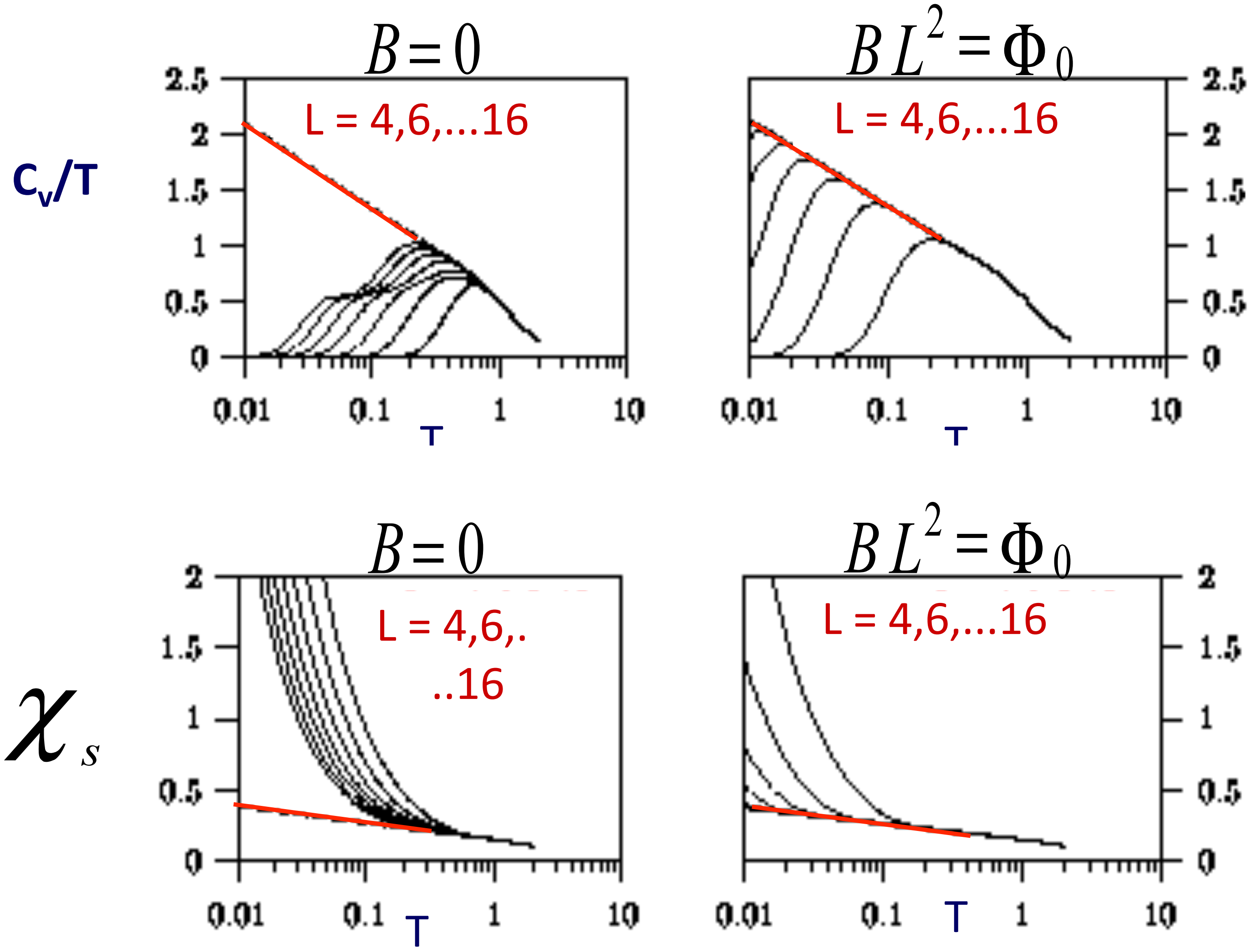


$$\delta = 0.01\,t$$

Scaling:

$$B=\Phi_0 / L^2$$

Thermodynamic quantities.



<u>L=16:</u> More than an order of magnitude gain in temperature before results get dominated by size effects.

FFA. Phys. Rev. B 65 115104 (2002)

Auxiliary field quantum Monte Carlo at work.

F. F. Assaad.

School on Quantum Monte methods at work for no s of matter
ICTP Trieste January 23, 2012 to January 27, 2

Thank you for your attention.

Outline:

- Cl hich one can solve.
- The thod with details of the projective method.
  (All the relevant calculations can be done on the blackboard)
- Selected applications (novel phases of matter)

http://www.physik.uni-wuerzburg.de/~assaad/pub.html Publication # 58