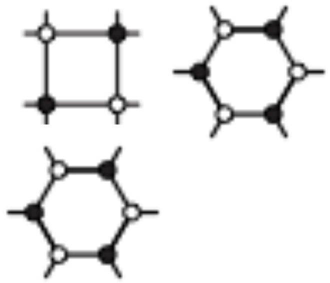
SU(N) Hubbard Heisenberg Models on the Honeycomb and Square Lattices.

F. F. Assaad (KITP November 18, 2010)

Outline

- Quantum Monte Carlo → BSS (R. Blankenbecler, D. J. Scalapino, and R. L. Sugar 1981)
- Spin liquids, solids, magnets, and semi-metals.



- Kane-Mele Hubbard.
- Conclusions.

In Collaboration with: Z. Meng, T. Lang, S. Wessel, A. Muramatsu, and M. Hohenadler

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SU(N) Hubbard-Heisenberg model on bipartite lattices.

$$\hat{H}_N = -t \sum_{<i,j>} \hat{\mathbf{c}}_i^{+} \hat{\mathbf{c}}_j + H.c. - \frac{J}{2N} \sum_{<i,j>} (\hat{\mathbf{c}}_i^{+}\hat{\mathbf{c}}_j)(\hat{\mathbf{c}}_j^{+}\hat{\mathbf{c}}_i) + (\hat{\mathbf{c}}_j^{+}\hat{\mathbf{c}}_i)(\hat{\mathbf{c}}_i^{+}\hat{\mathbf{c}}_j) + \frac{U}{N}\sum_i \left(\hat{\mathbf{c}}_i^{+}\hat{\mathbf{c}}_i - \frac{N}{2}\right)^2$$

$$\sim J \sum_{<i,j>} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \qquad \sim U \sum_i n_{i,\uparrow} n_{i,\downarrow} \quad \text{(N=2)}$$

$$\mathbf{c}_i^{+} = (c_{i,1}^{+} \cdots c_{i,N}^{+})$$

Band-filling, half-filling $\langle \mathbf{c}_i^{+}\mathbf{c}_i \rangle = \frac{N}{2}$

N=4 Two orbitals per unit cell.

t: Diagonal hopping

J: Exchange

Note: $U \rightarrow \infty$, $\mathbf{c}_i^{+}\mathbf{c}_i = N/2$ antisymmetric self-adjoint rep.

Auxiliary Field QMC for SU(N) tUJ.

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

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

1) Trotter decomposition → Introduces a systematic error of order $(\Delta\tau)^2$

$$Z = \text{Tr}[e^{-\beta \hat{H}_N}] = \text{Tr}\left[\prod_{n=1}^{m} e^{-\Delta\tau \hat{H}_t} e^{-\Delta\tau \hat{H}_U} e^{-\Delta\tau \hat{H}_J}\right] + O\left(\Delta\tau^2\right), \qquad m\Delta\tau = \beta$$

Auxiliary Field QMC for SU(N) tUJ.

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

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

2) Hubbard Stratonovich [conserves SU(N) symmetry].

Generic

$$e^{\Delta\tau \hat{A}^2} = \frac{1}{\sqrt{2\pi}} \int d\phi \; e^{-\phi^2/2 + \sqrt{2\Delta\tau}\,\phi\,\hat{A}} \longrightarrow$$

Efficient: Discrete variables.

$$e^{\Delta\tau \hat{A}^2} = \sum_{l=\pm1,\pm2} \gamma(l)\, e^{\sqrt{\Delta\tau}\,\eta(l)\,\hat{A}} + O(\Delta\tau^4)$$

$$\gamma(l) = \gamma(-l) > 0, \quad \eta(l) = -\eta(-l)$$

Auxiliary Field QMC for SU(N) tUJ.

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

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

$$Z \propto \int \prod_{i,\tau} d\Phi_i(\tau) \prod_{b,\tau} d\,\mathrm{Re}\, z_b(\tau) d\,\mathrm{Im}\, z_b(\tau) \; e^{-N\, S(\{\Phi\},\{z\})}$$

with

$$S(\{\Phi\},\{z\}) = \int d\tau \; J\sum_b |z_b(\tau)|^2 + U\sum_i |\Phi_i(\tau)|^2/4 \; - \ln \overbrace{\mathrm{Tr}\left[T e^{-\int_0^\beta d\tau \hat{h}(\tau)} \right]}^{\text{Fermionic Det.}}$$

and

$$\underbrace{\hat{h}(\tau) = -\sum_{<i,j>} [t + J\,\overline{z}_{<i,j>}(\tau)]\hat{c}_i^+ \hat{c}_j + H.c. \; - iU\sum_i \Phi_i(\tau)[\hat{c}_i^+ \hat{c}_i - 1/2]}_{\text{Single particle Hamiltonian for only one fermionic flavor.}}$$

Auxiliary Field QMC for SU(N) tUJ.

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

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Sign problem.

$$\overline{\mathrm{Tr}[T e^{-\int_0^\beta d\tau \hat{h}(\tau)}]} = \mathrm{Tr}[T e^{-\int_0^\beta d\tau \hat{h}(\tau)}]$$

$$\uparrow$$

$$\hat{c}_i^+ \rightarrow (-1)^{i_x + i_y} \hat{c}_i$$

Fermionic det. is real → no sign problem for *even* values of N.

Auxiliary Field QMC for SU(N) tUJ.

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

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

$$Z \propto \int \prod_{i,\tau} d\Phi_i(\tau) \prod_{b,\tau} d\,\mathrm{Re}\, z_b(\tau)\, d\,\mathrm{Im}\, z_b(\tau)\; e^{-N\, S(\{\Phi\},\{z\})}$$

with

$$S(\{\Phi\},\{z\}) = \int d\tau\; J \sum_b |z_b(\tau)|^2 + U\sum_i |\Phi_i(\tau)|^2/4 \; - \ln \overbrace{\mathrm{Tr}\left[T e^{-\int_0^\beta d\tau\, \hat{h}(\tau)} \right]}^{\text{Fermionic Det.}}$$

Monte Carlo : Sequential updating.

CPU time for a sweep : $V^3\beta$ (Does not depend on N)

Projective versus finite temperature approaches

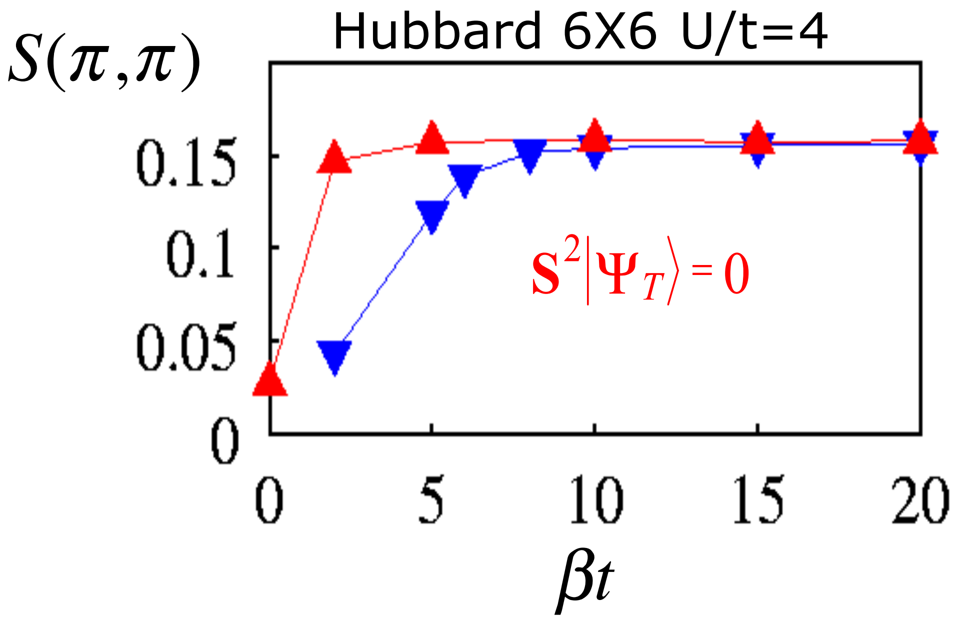
Ground state.

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

$$\langle \psi_T | \psi_0 \rangle \neq 0$$

Finite temperature.

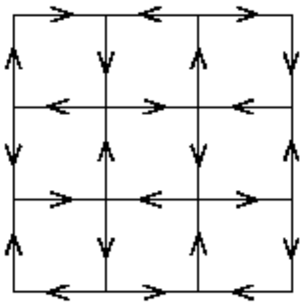
$$\langle O \rangle = \frac{\mathrm{Tr}\left[e^{-\beta H} O \right]}{\mathrm{Tr}\left[e^{-\beta H} \right]}$$



Imaginary time displaced correlation functions ✔

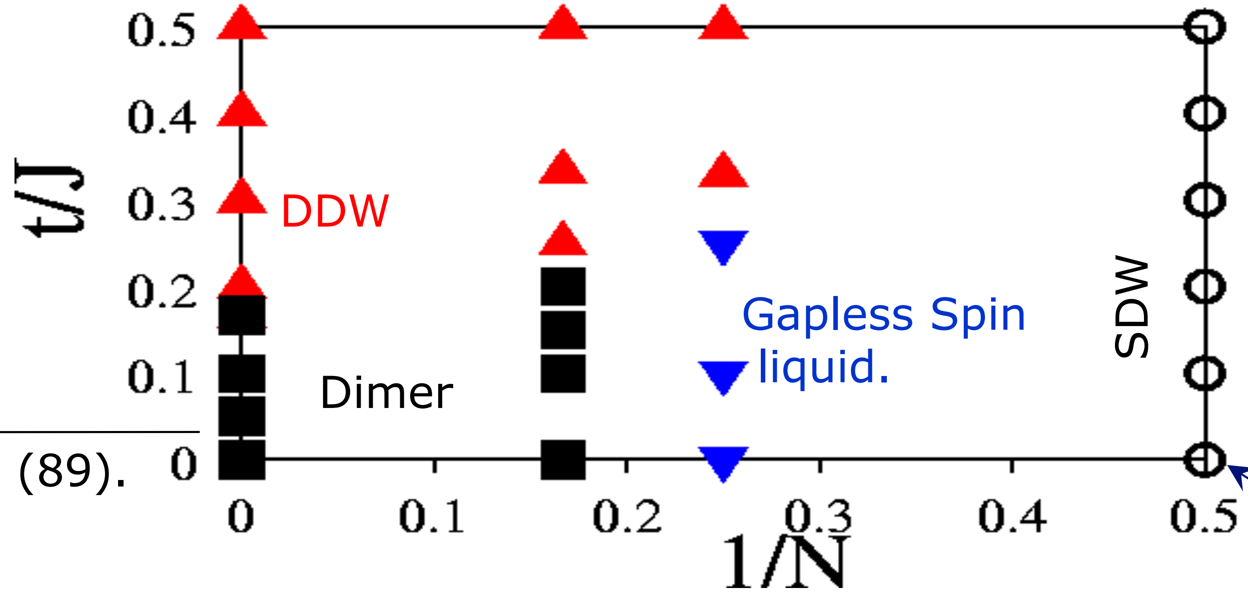
F. F. Assaad and H. G. Evertz, in ComputationalMany Particle Physics, Vol. 739 of Lecture Notes in Physics, Springer Verlag, Berlin, 2008

Phase diagram of SU(N) Hubbard-Heisenberg model at half band-filling.

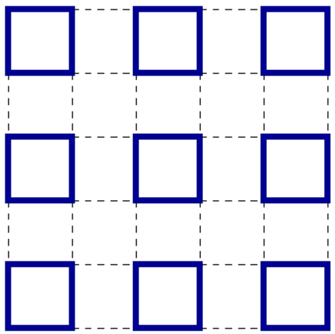


DDW.
Broken time
and lattice symmetries.
Semimetal. Nodes at $k=(\pi/2,\pi/2)$

T=0, (U/J=0)



Affleck-Marston (89).



Dimer: Broken
lattice symmetries.
Insulator.
Spin gap.

Heisenberg

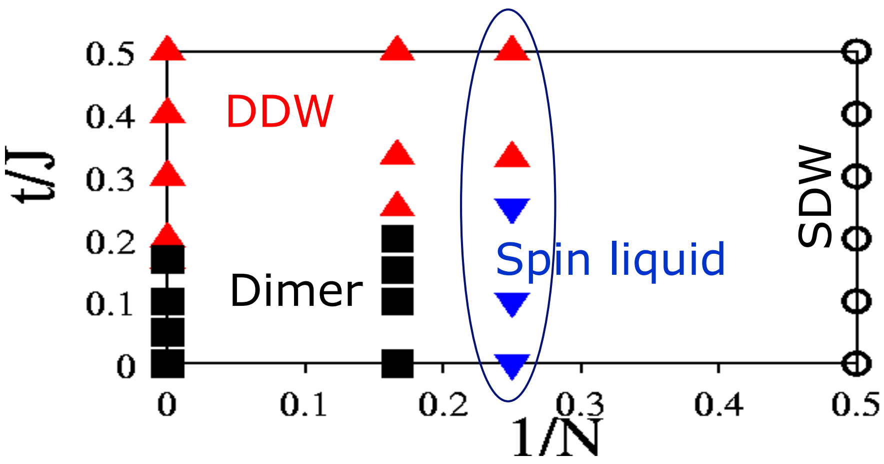
$$H = \frac{J}{N}\sum_{\substack{\langle \mathbf{i},\mathbf{j}\rangle \\ \alpha,\beta}} S_{\mathbf{i}}^{\alpha,\beta}\, S_{\mathbf{j}}^{\beta,\alpha}$$

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

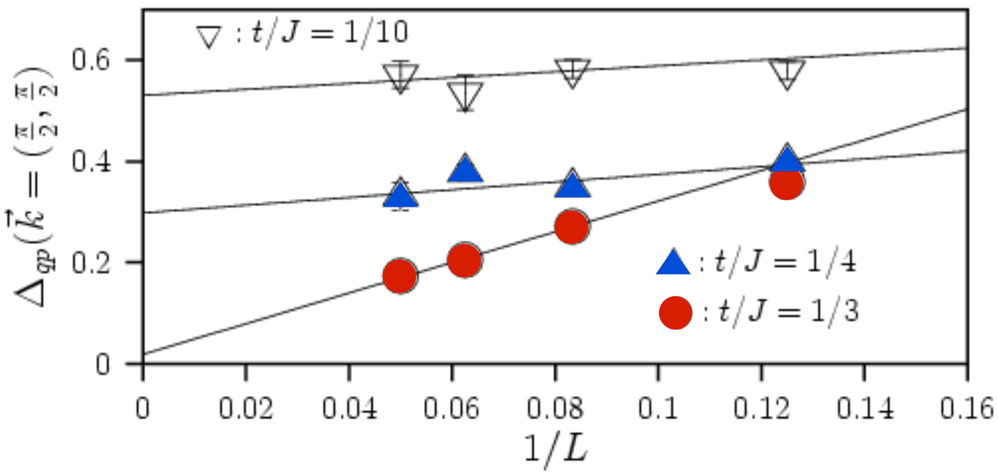
$$\mathbf{c}_i^{+}\mathbf{c}_i = N/2$$

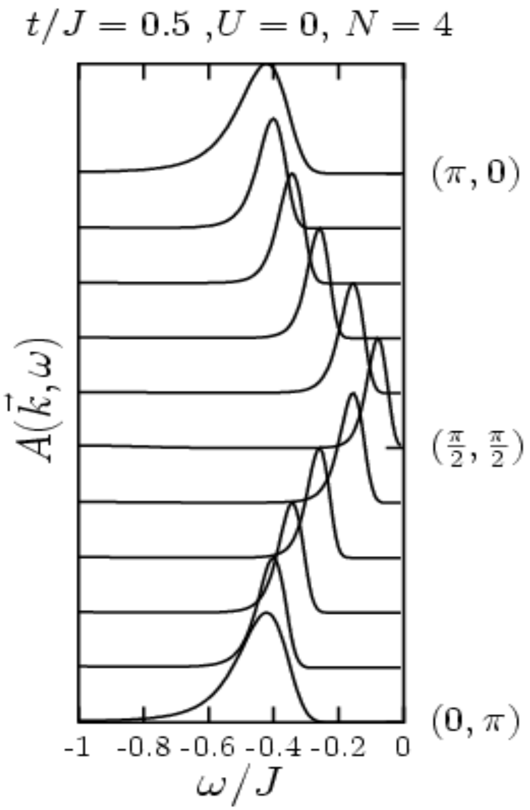
FFA PRB (2005)

N=4.

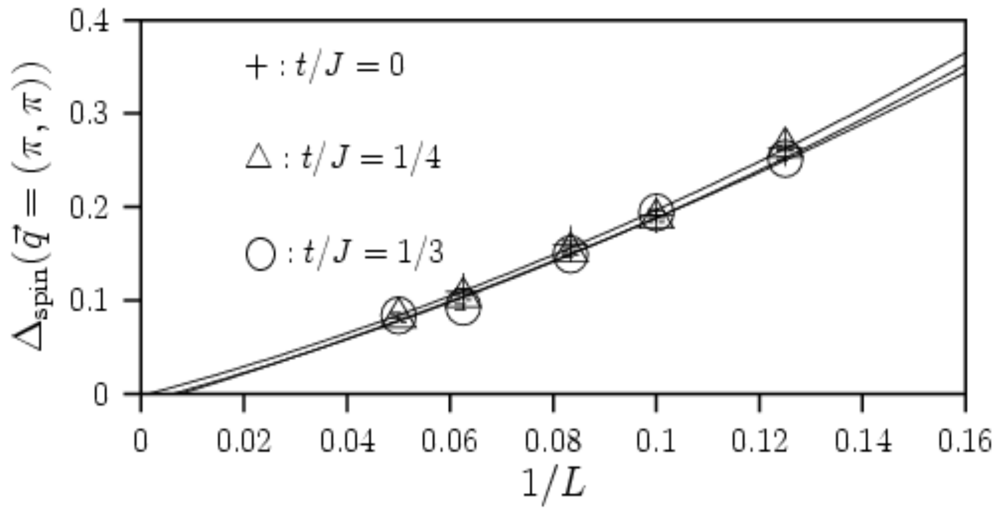


Quasi-particle gap at k=(π/2,π/2)



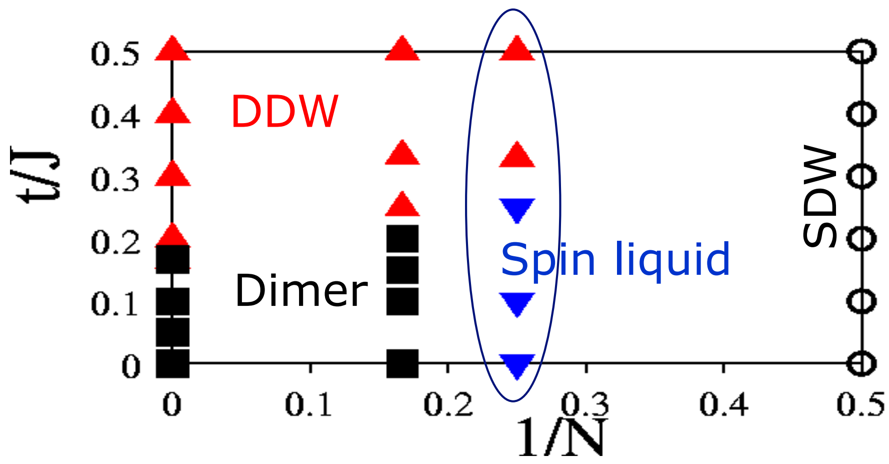


Spin Gap **q** = (π,π)

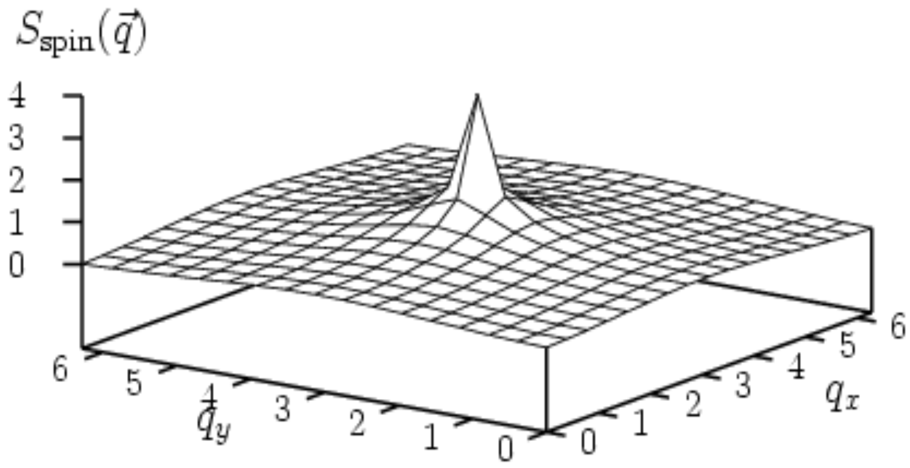


No dimer order. No spin order.

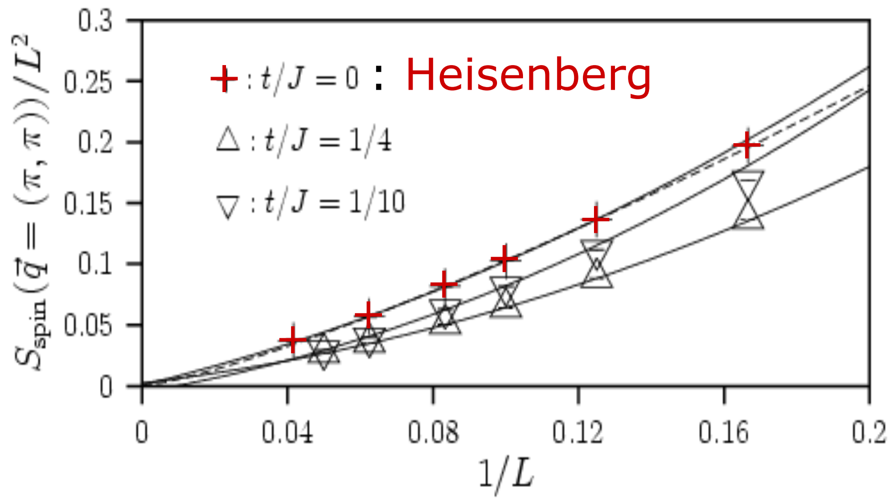
N=4.



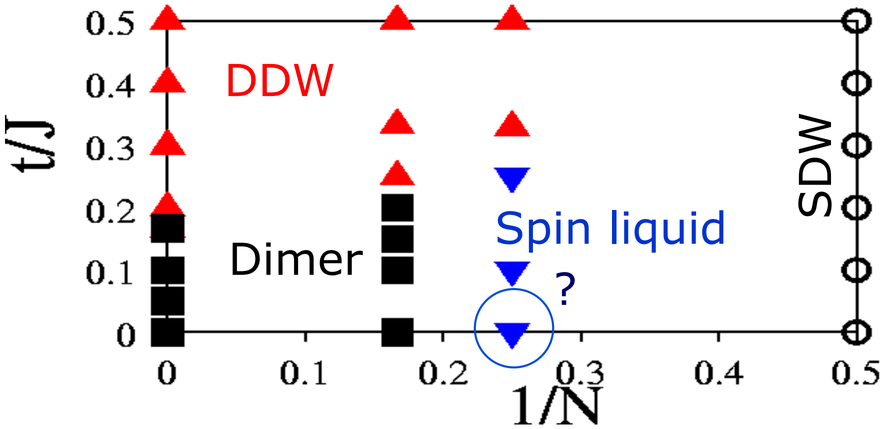
Equal-time spin correlations (Heisenberg)



Spin correlations **q**=(π,π)

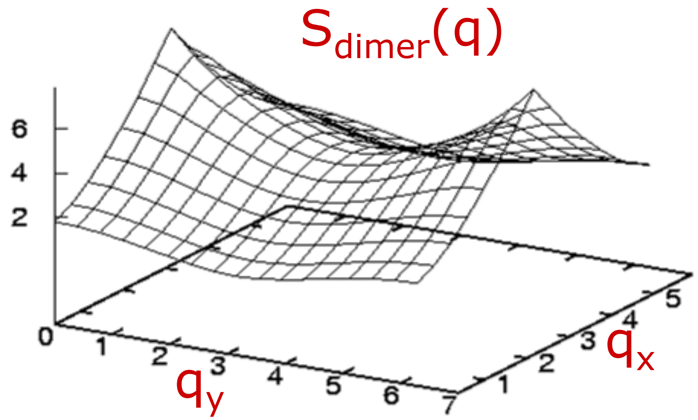


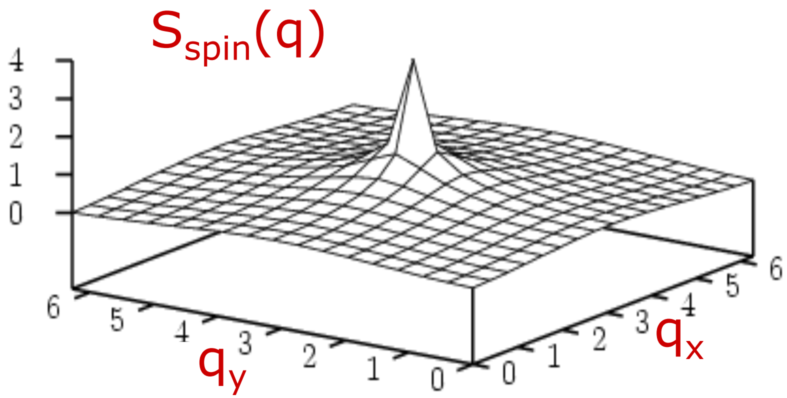
Dashed line: $S_{spin}(\mathbf{r}) \sim e^{i\mathbf{Qr}} r^{-1.2}$



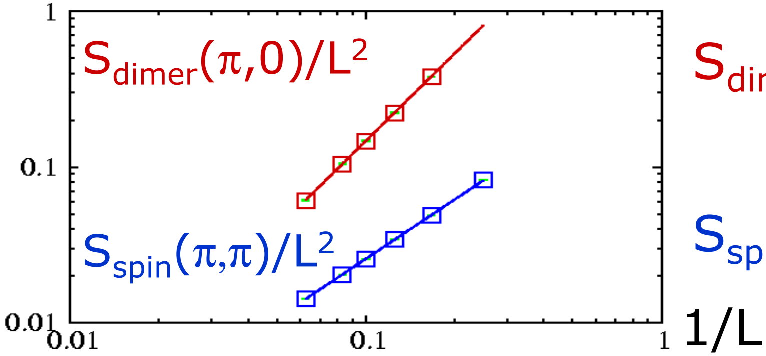
Mean-field SU(4) → ∏-flux phase.

In continuum limit ∏-flux phase has a larger symmetry, SU(8), which unifies competing spin and dimer fluctuations.
(M. Hermele, T. Senthil, M. P. A. Fisher, Phys. Rev. B 72, 104404 (2005))





Prediction of SU(8) symmetry: same large distance behavior of $(\pi,0)$ dimer and (π,π) spin fluctuations.

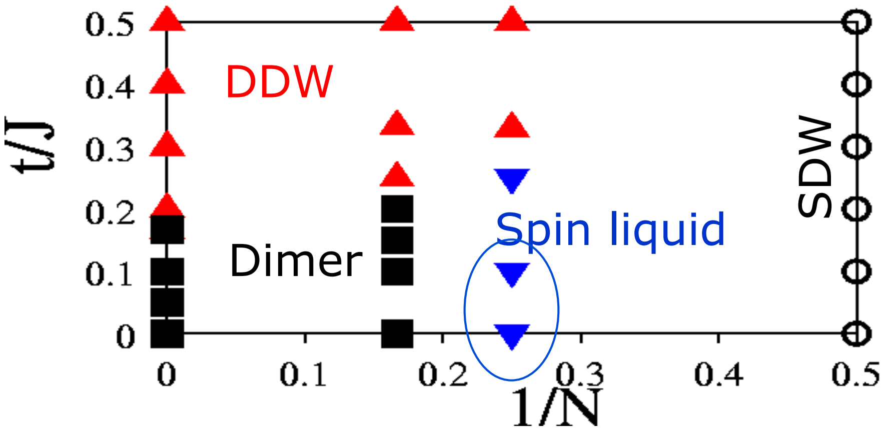


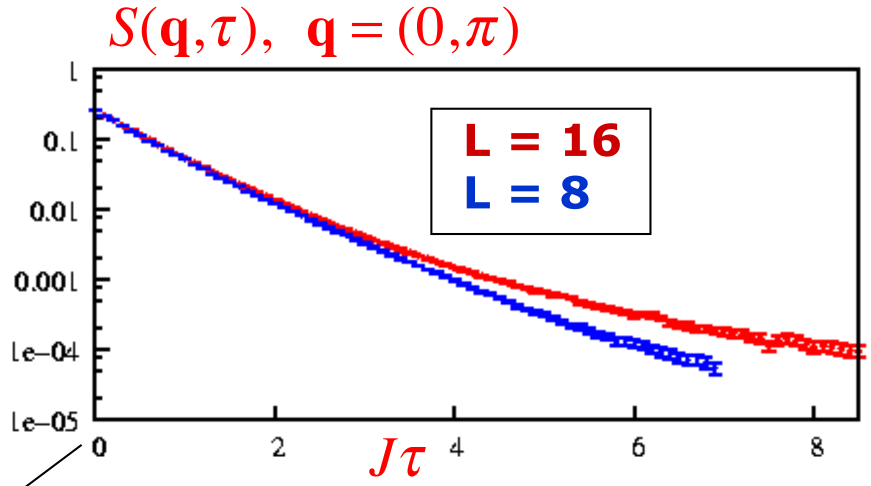
$S_{dimer}(\mathbf{r}) \sim e^{i\mathbf{qr}}\, r^{-1.8}$ $q=(\pi,0)$

$S_{spin}(\mathbf{r}) \sim e^{i\mathbf{qr}}\, r^{-1.2}$ $q=(\pi,\pi)$

N=4.

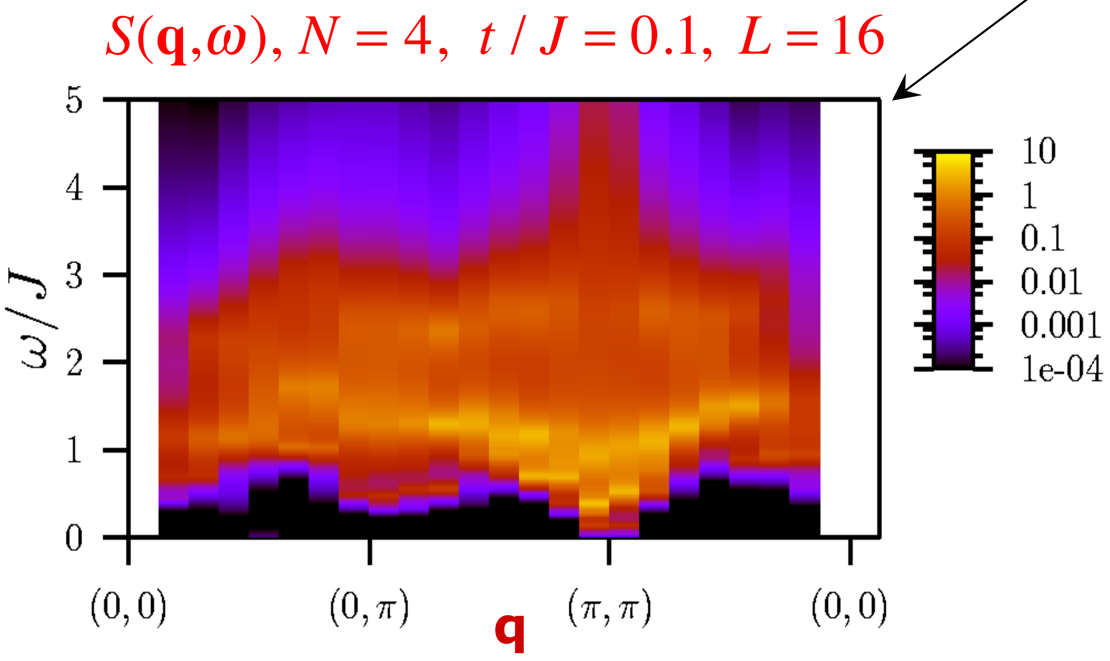
Spin Dynamics





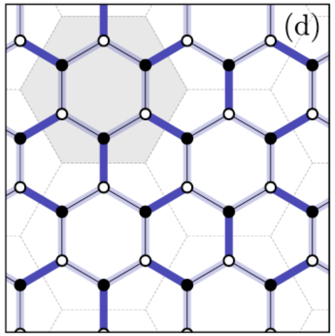
Stochastic analytical continuation.

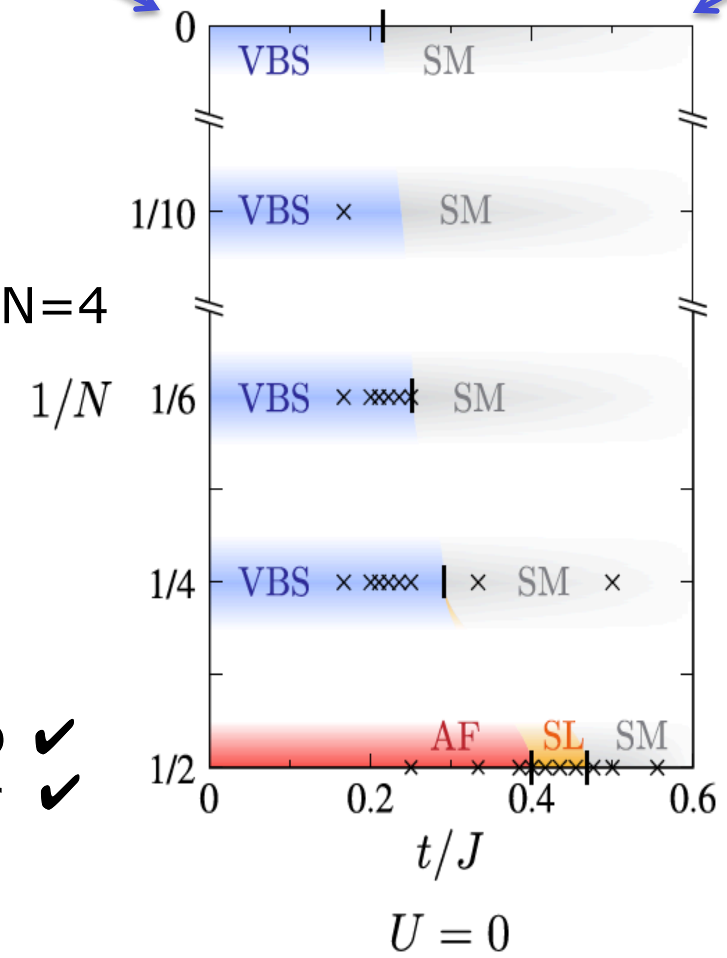
(Beach cond-mat/0403055)

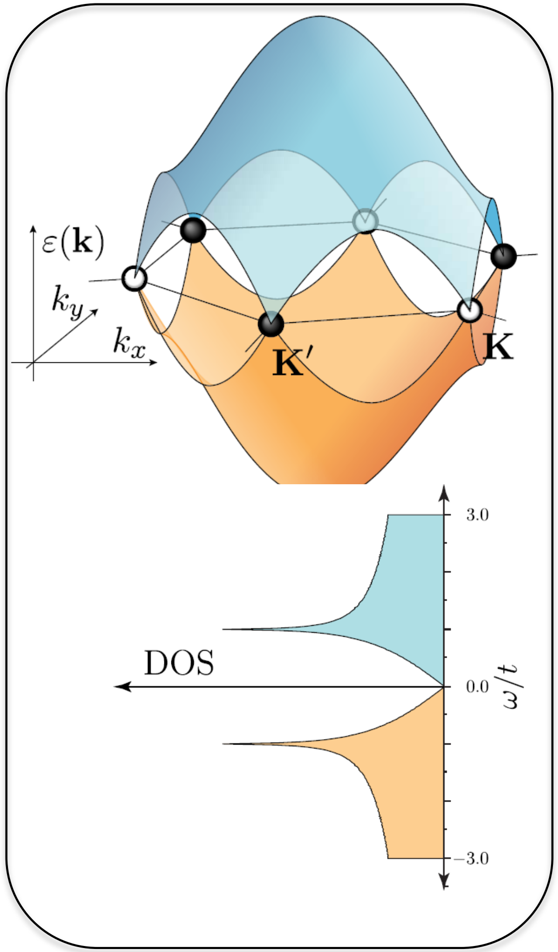


Continuum!

SU(N) Hubbard-Heisenberg model on the Honeycomb lattice.



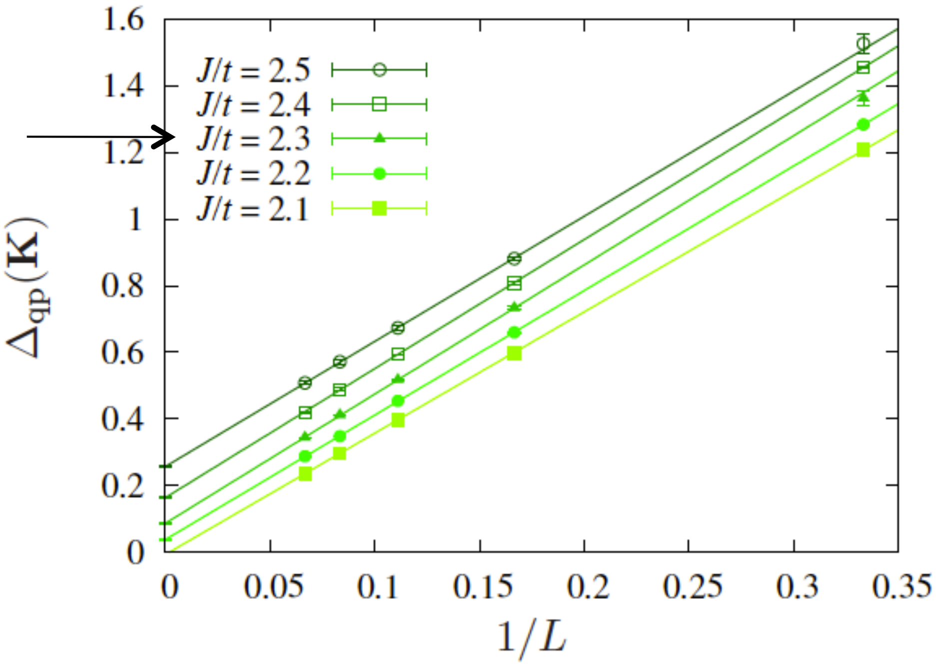


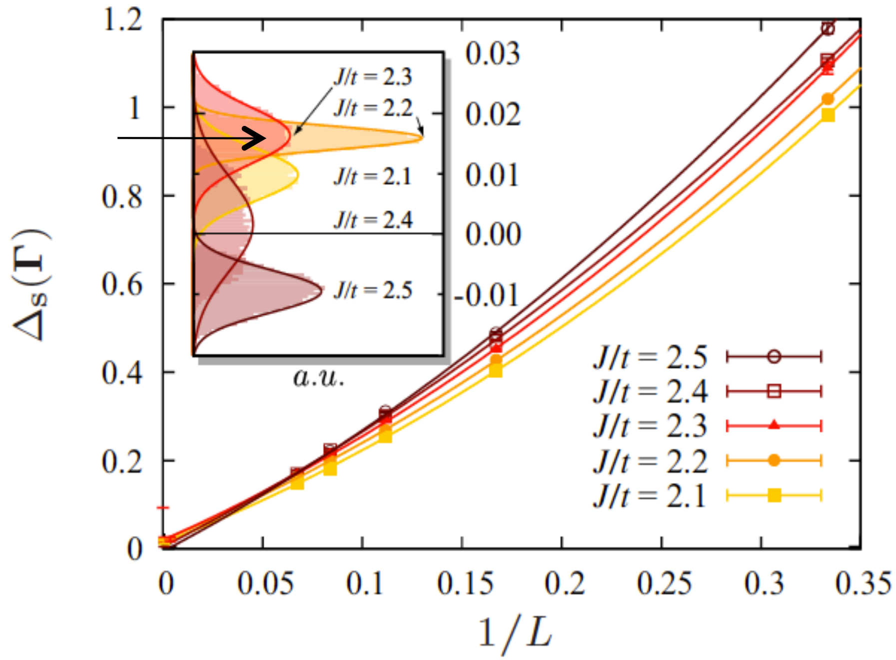


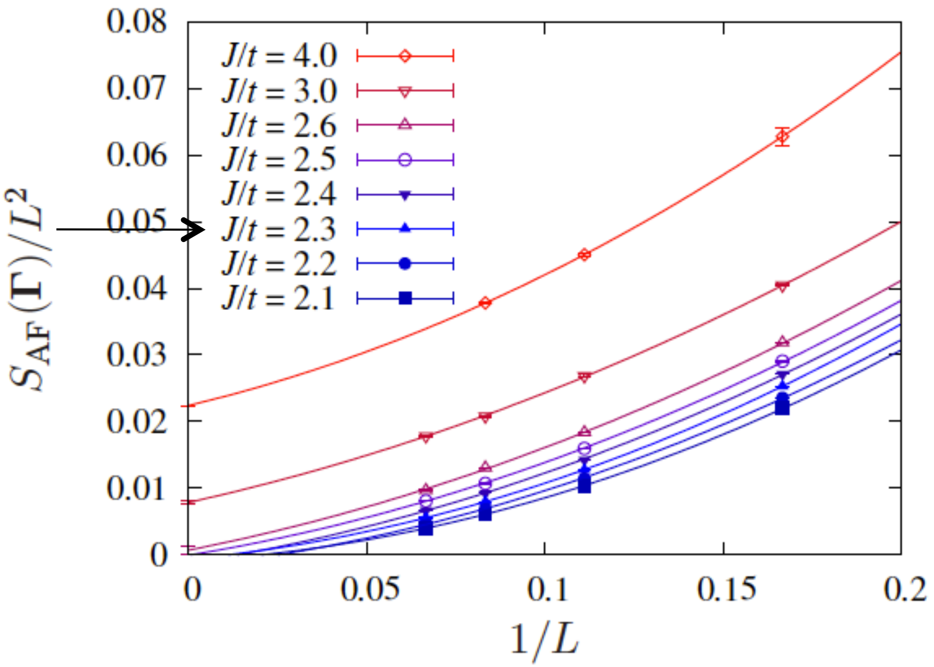
Mean-field down to N=4

Spin-liquid at N=2

Single-particle gap ✔
No magnetic order ✔
Spin-Gap ~





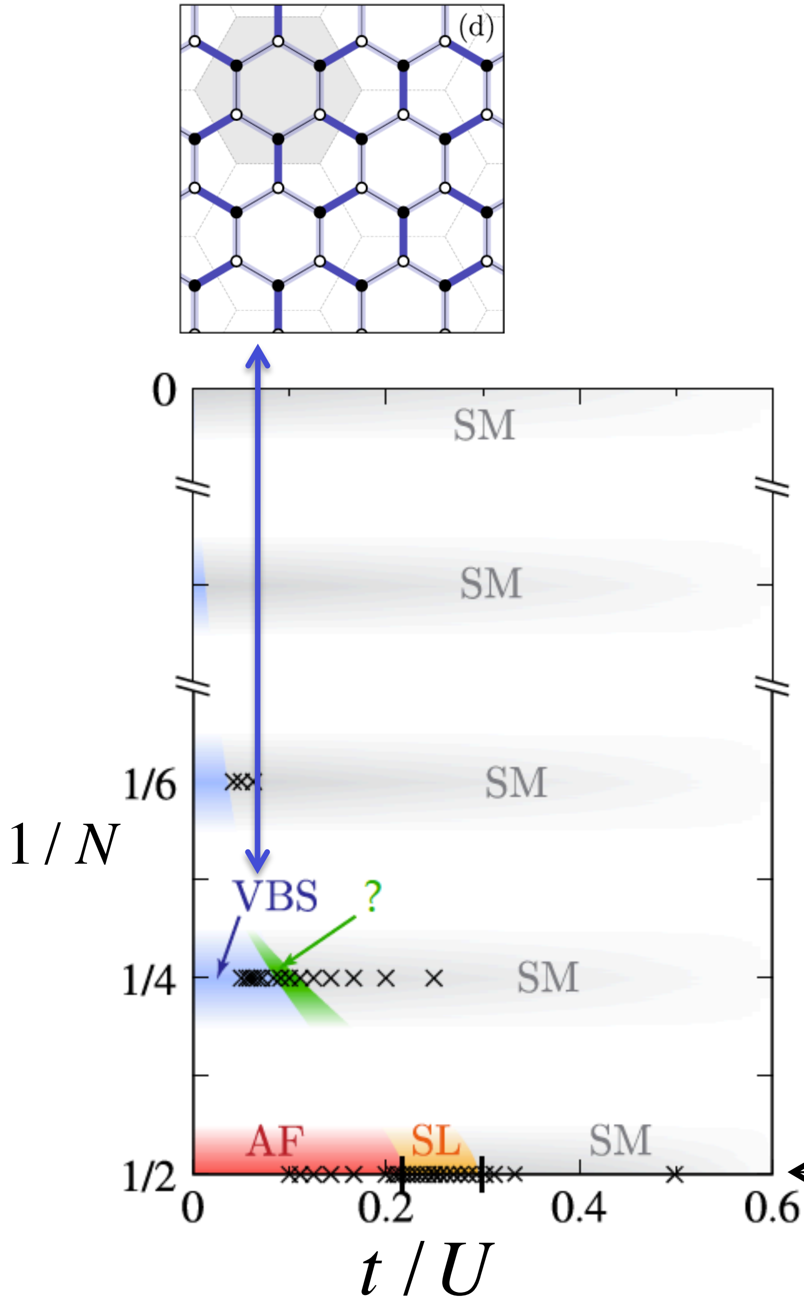


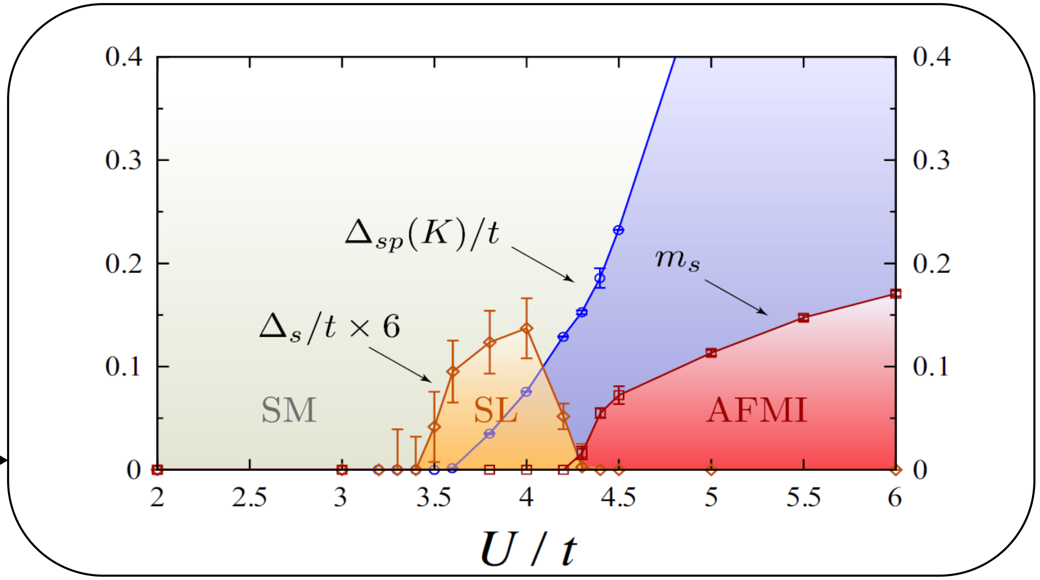
<u>Absence of.</u>

Dimer-dimer.

Superconductivity... etc.

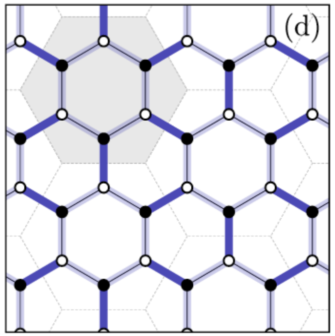
SU(N) Hubbard-model on the Honeycomb lattice.

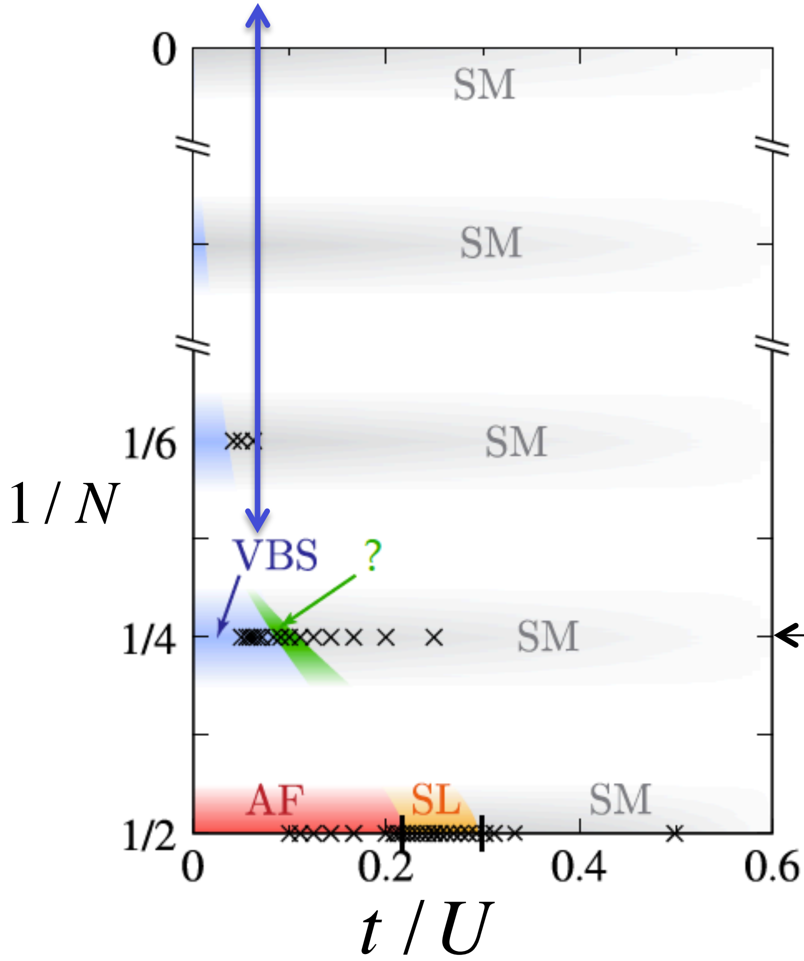




Meng et al. Nature 2010

SU(N) Hubbard-model on the Honeycomb lattice.

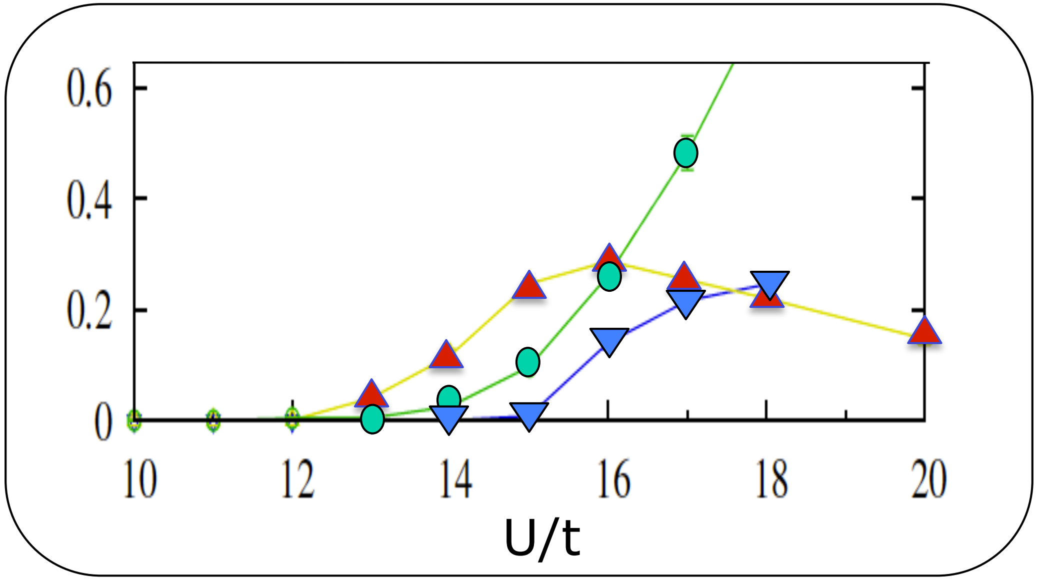




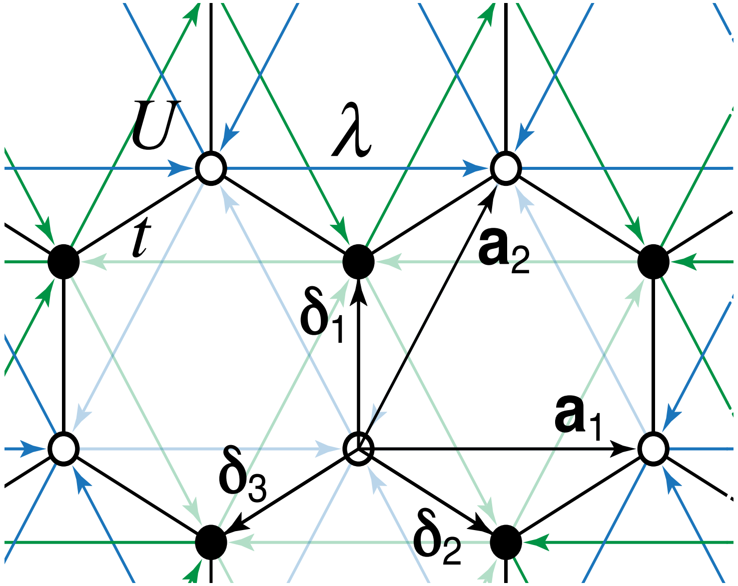
Single particle gap.

Spin gap.

Dimer order parameter.



The Kane-Mele Hubbard Model on the Honeycomb lattice.



$$H = H_{KM} + H_U$$

$$H_{KM} = -t \sum_{\langle \vec{i},\vec{j} \rangle} c^{\dagger}_{\vec{i}} c_{\vec{j}} + i\lambda \sum_{\langle\langle \vec{i},\vec{j} \rangle\rangle} c^{\dagger}_{\vec{i}} \vec{e}_{\langle\langle \vec{i},\vec{j} \rangle\rangle} \cdot \vec{\boldsymbol{\sigma}} c_{\vec{j}}$$

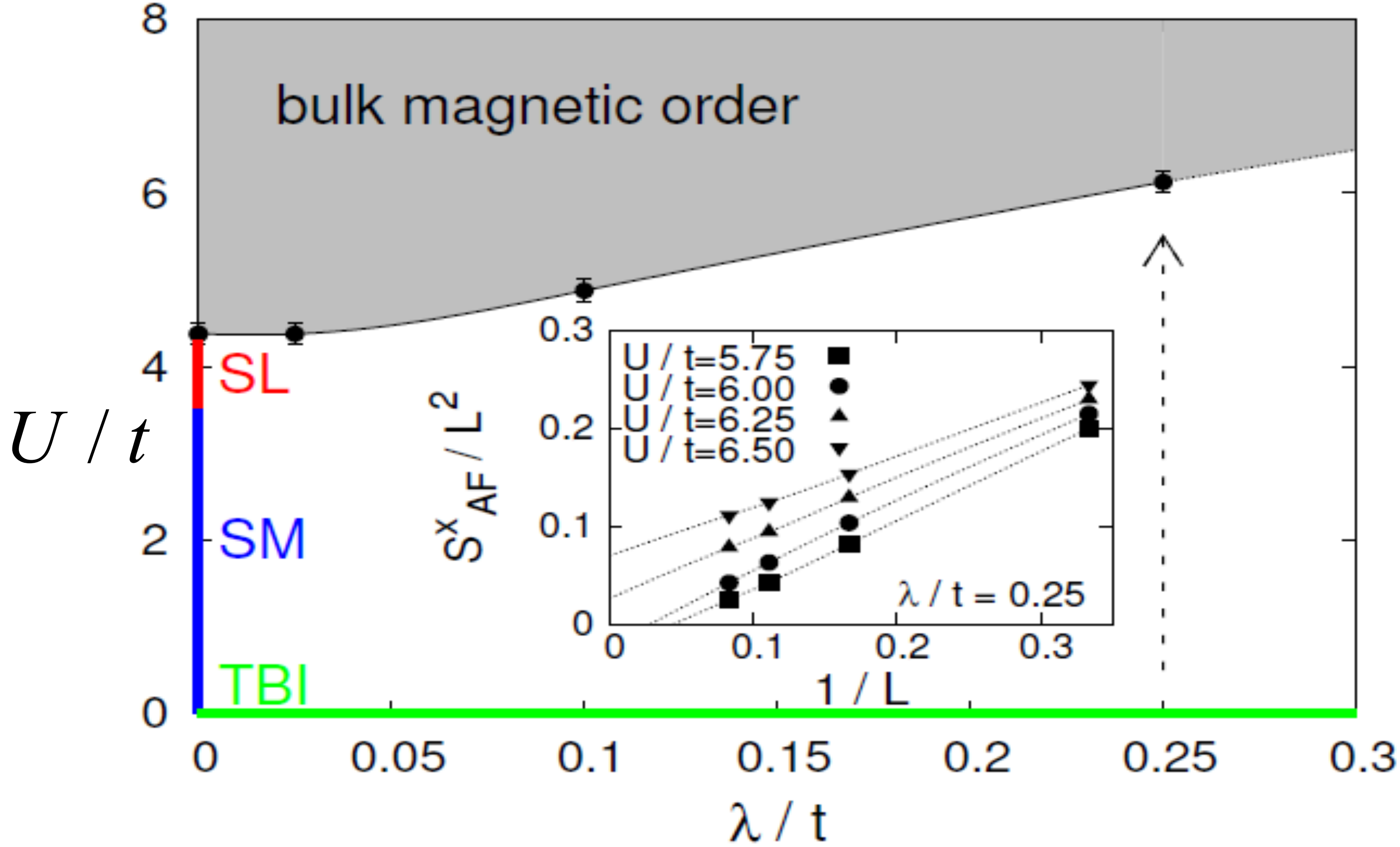
$$H_U = \frac{U}{2} \sum_{\vec{i}} \left(c^{\dagger}_{\vec{i}} c_{\vec{i}} - 1 \right)^2$$

$$c_i^{\dagger} = (c_{i,\uparrow}^{\dagger}, c_{i,\downarrow}^{\dagger})$$

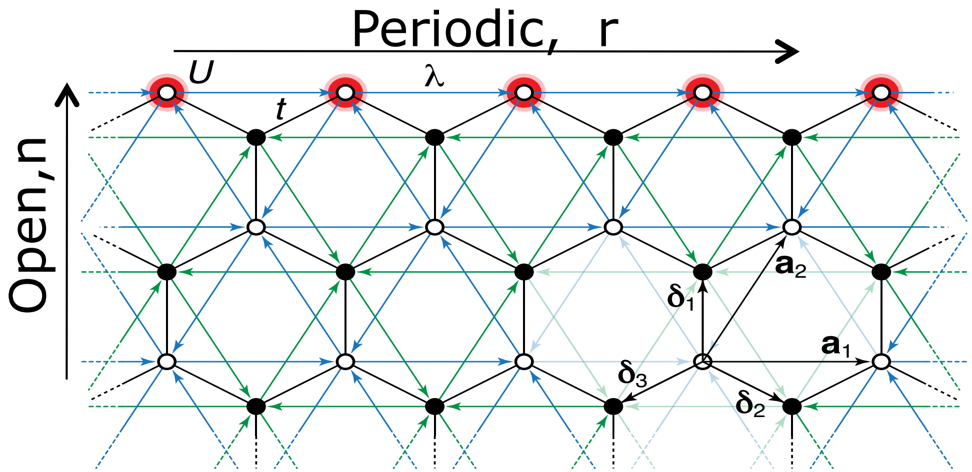
$$e_{\langle\langle i,j \rangle\rangle} = \delta_i \times \delta_j / \left| \delta_i \times \delta_j \right|$$

Sign-free simulations are possible.

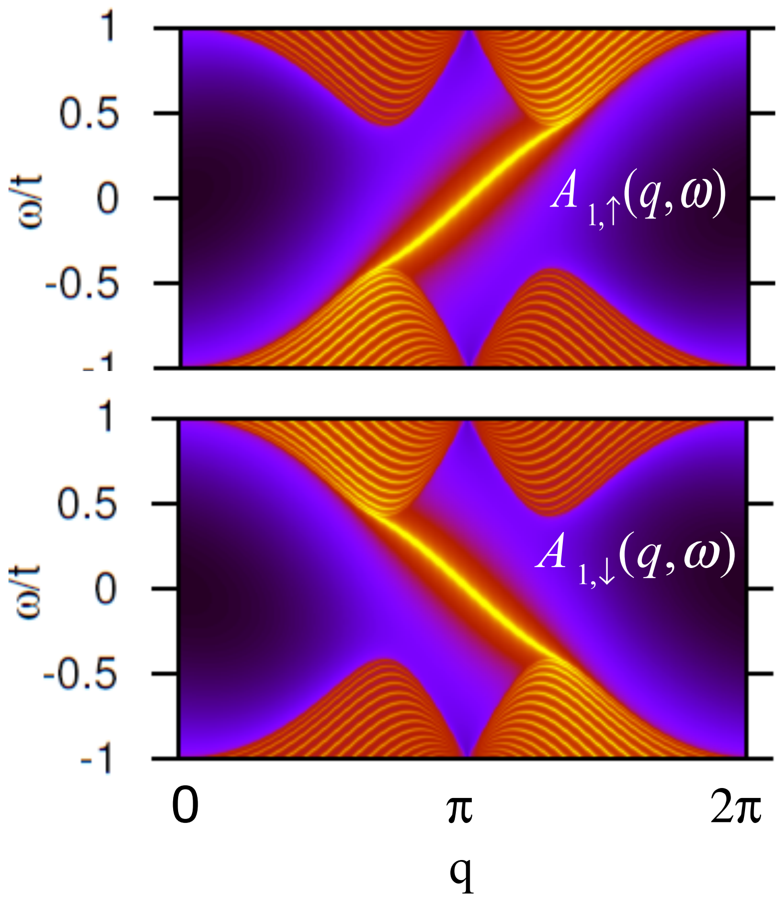
$$S^x_{AF} = \left\langle \sum_{\mathbf{i}} (-1)^{\mathbf{i}} S^x_{\mathbf{i}} S^x_{\mathbf{0}} \right\rangle$$



Edge states @ U/t=0, $\lambda / t = 0.25$



Time reversal symmetry protects edge state against weak interactions.

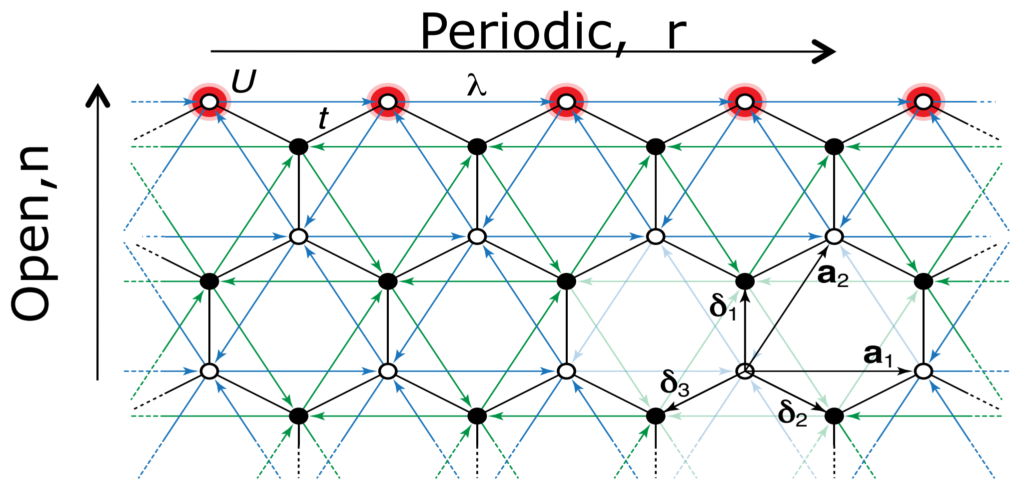


$$G_{n,\sigma}(q,\omega) = -i\int_0^\infty dt\, e^{i(\omega+i\delta)t} \left\langle \left\{ c_{n,\sigma,q}(t), c^\dagger_{n,\sigma,q} \right\} \right\rangle$$

$$A_{n,\sigma}(q,\omega) = -\frac{1}{\pi} \operatorname{Im} G_{n,\sigma}(q,\omega)$$

Nature of edge state in the paramagnetic phase?

→ Retain Hubbard U only along one edge, integrate out the bulk.



$$S=\int_0^\beta d\tau\int_0^\beta d\tau' \sum_{r,r',\sigma} c^\dagger_{r,\sigma}(\tau)\underbrace{G^{-1}_{0,\sigma}(r-r',\tau-\tau')}c_{r,\sigma}(\tau') \;+\; U\int_0^\beta d\tau\,\left(n_{r,\uparrow}(\tau)-\frac{1}{2}\right)\left(n_{r,\downarrow}(\tau)-\frac{1}{2}\right)$$

Green function of the KM model on the ribbon.

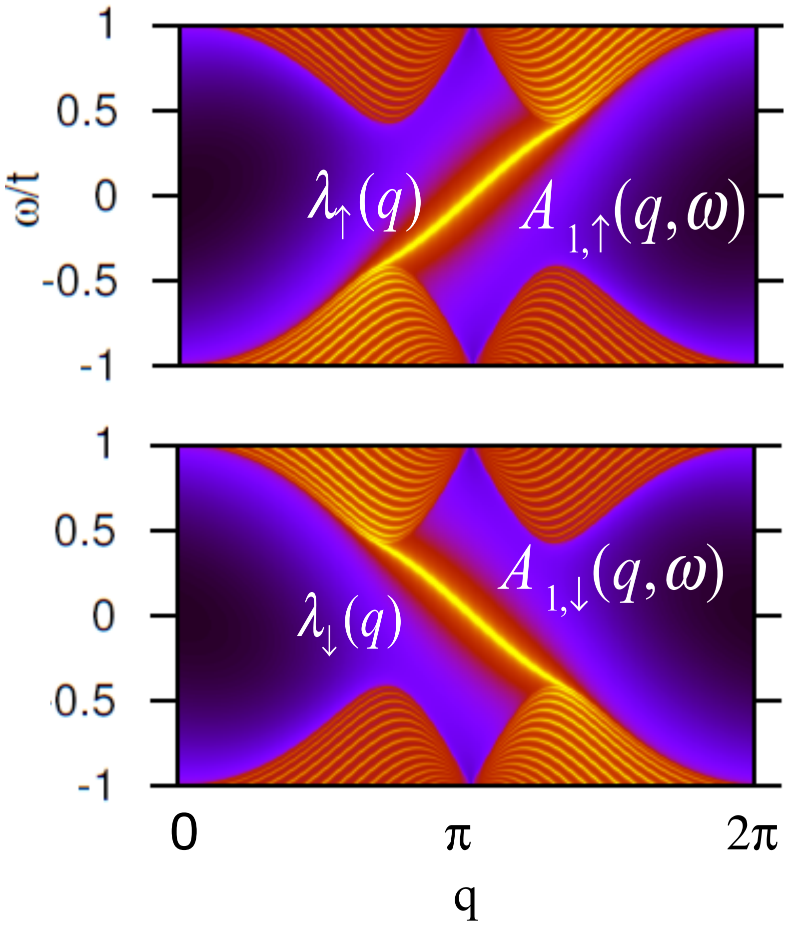
→ Solve with CTQMC (arbitrary large ribbons)

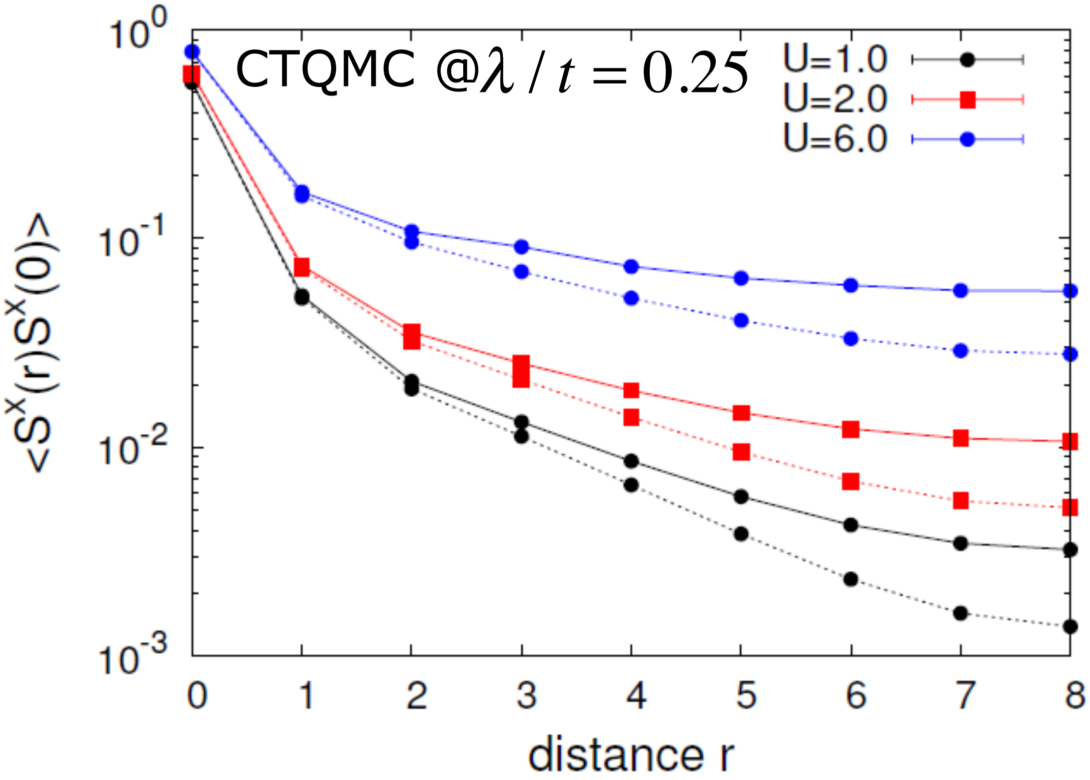
<u>Equal spin-spin correlations along the edge.</u>

At U=0, $\lambda_{\uparrow}(q) = -\lambda_{\downarrow}(q)$ leads to

nesting → ferromagnetic instability

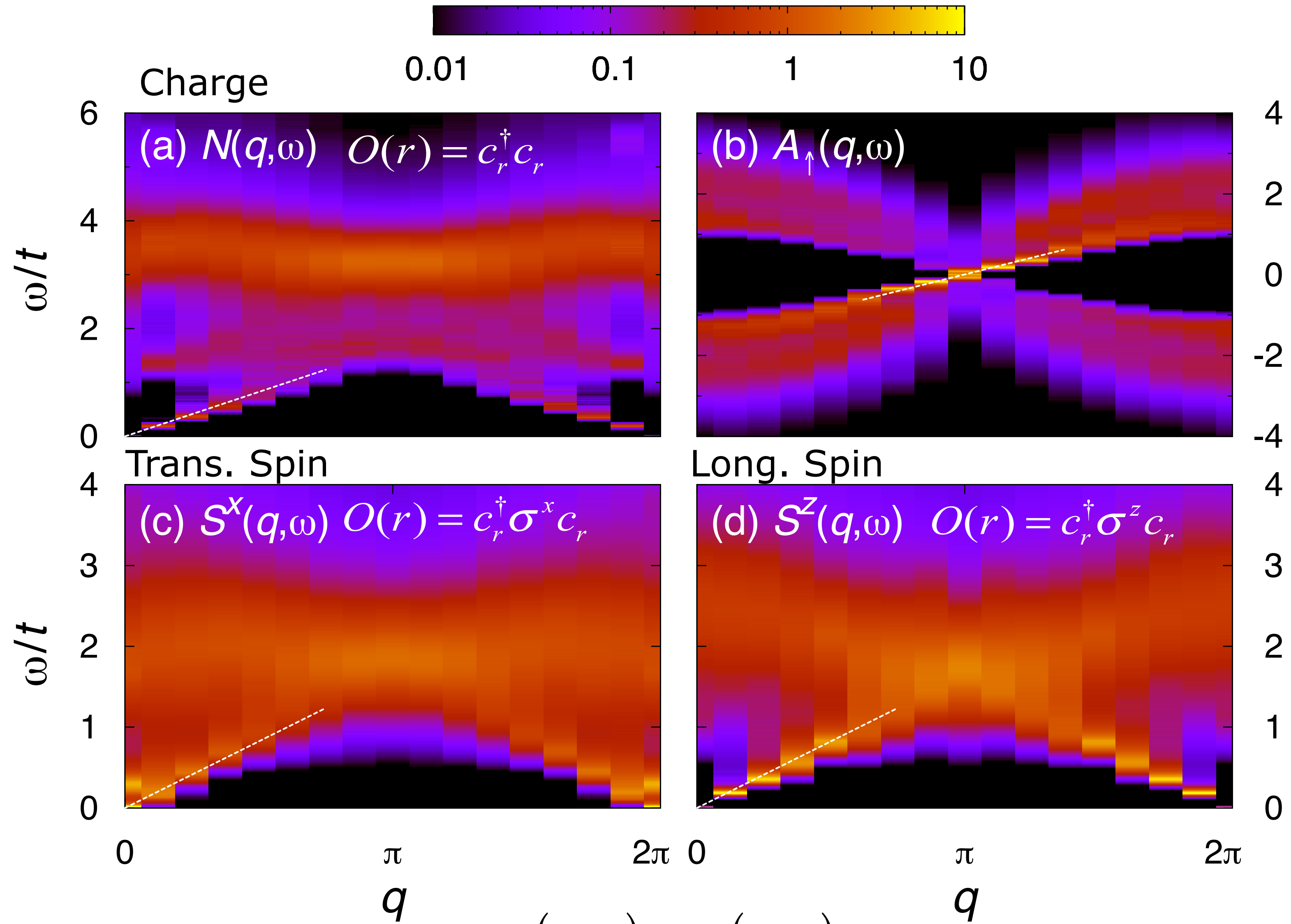
in xy plane.





$L = 16, \ \beta t = 20, 40$

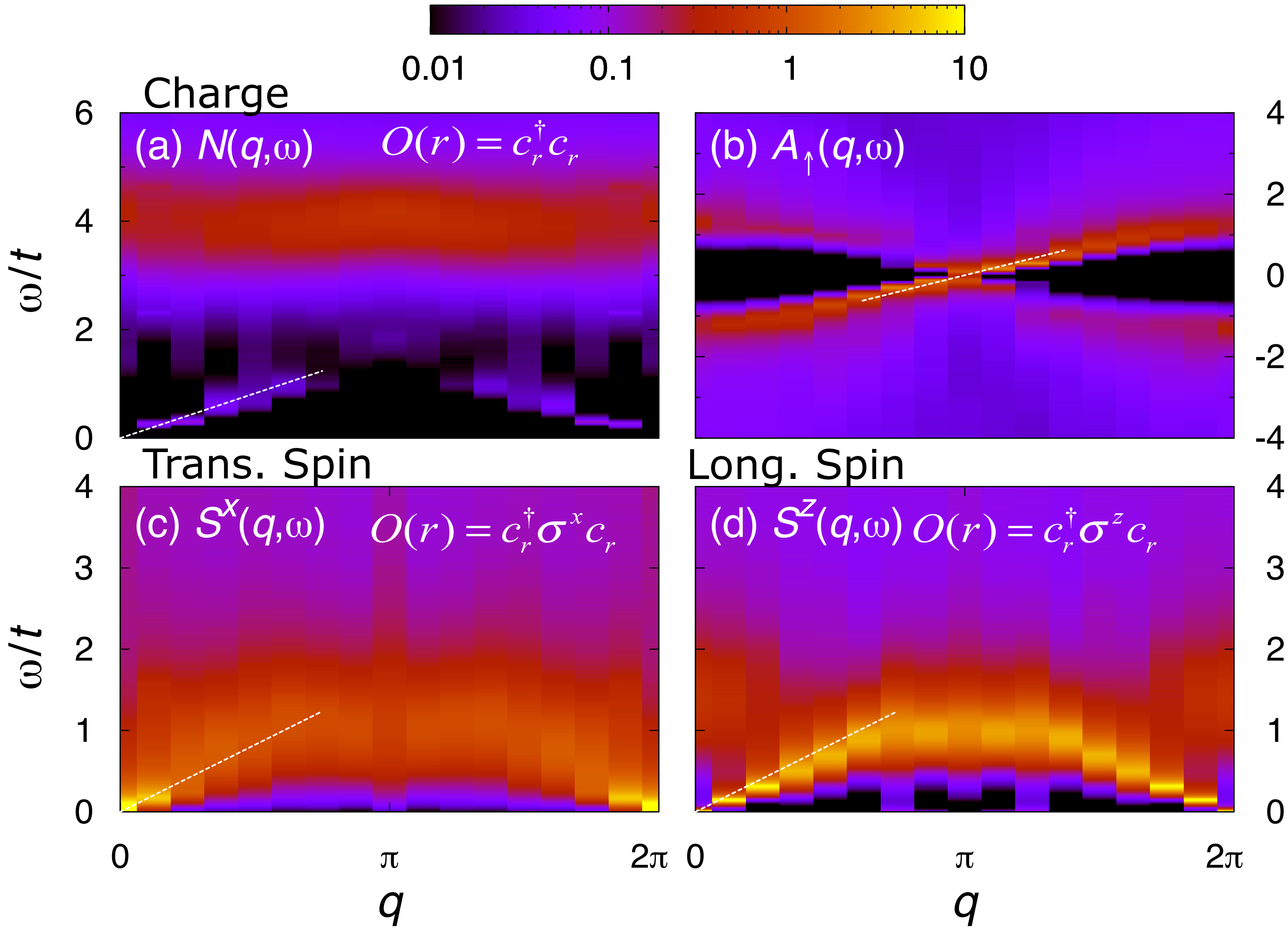
Dynamics@ $U/t = 2,\ \beta t = 40,\ \lambda = 0.25t$.



In the absence of interactions: $N(q,\omega) = S^z(q,\omega)$

$$O(q,\omega) = \frac{1}{Z}\sum_{n,m} e^{-\beta E_n} \left|\langle m | O(q) | n \rangle\right|^2 \delta(E_m - E_n - \omega)$$

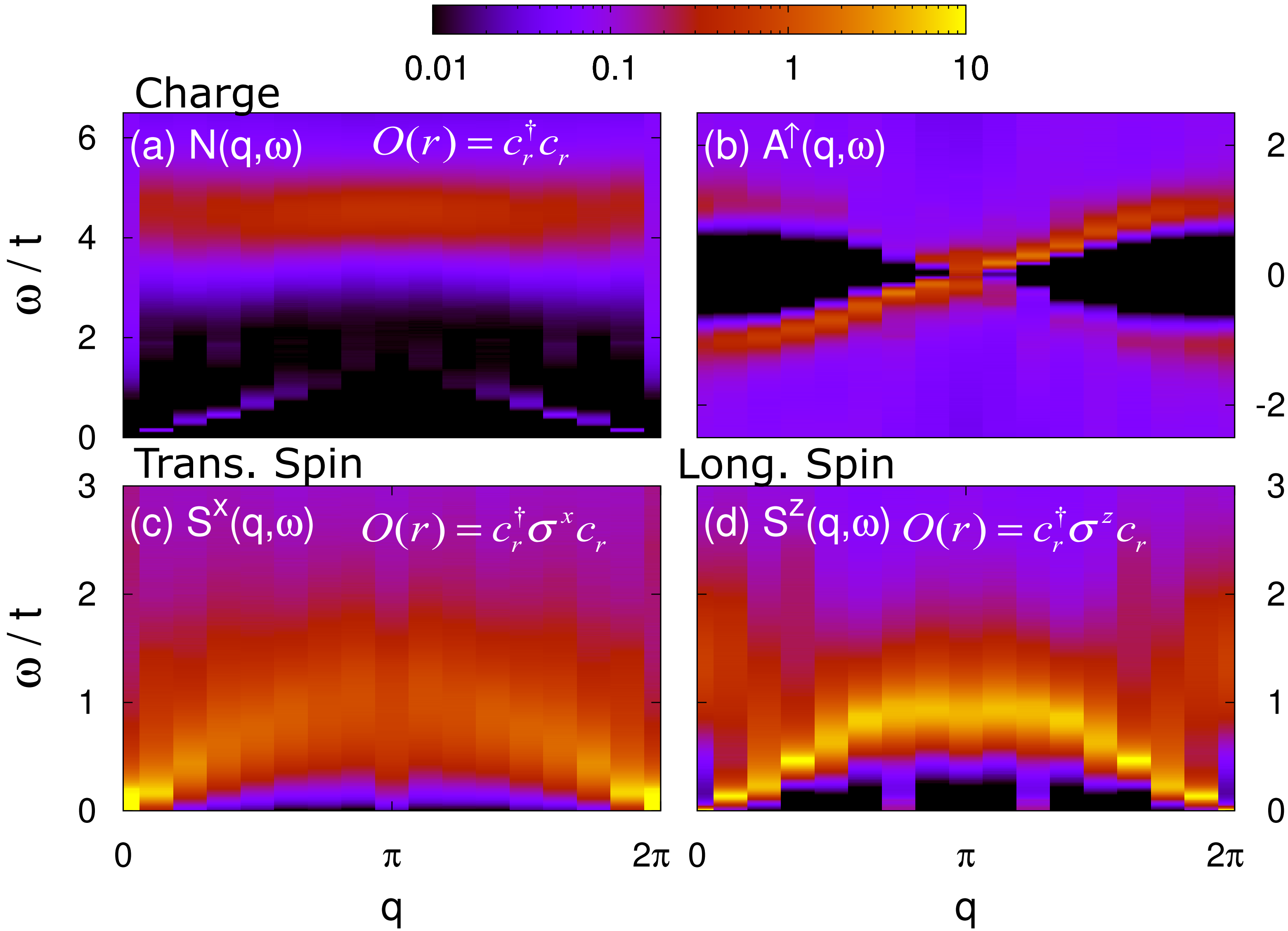
Dynamics @ $U/t = 5,\ \beta t = 40,\ \lambda = 0.25t$.



Velocities are independent on U/t.

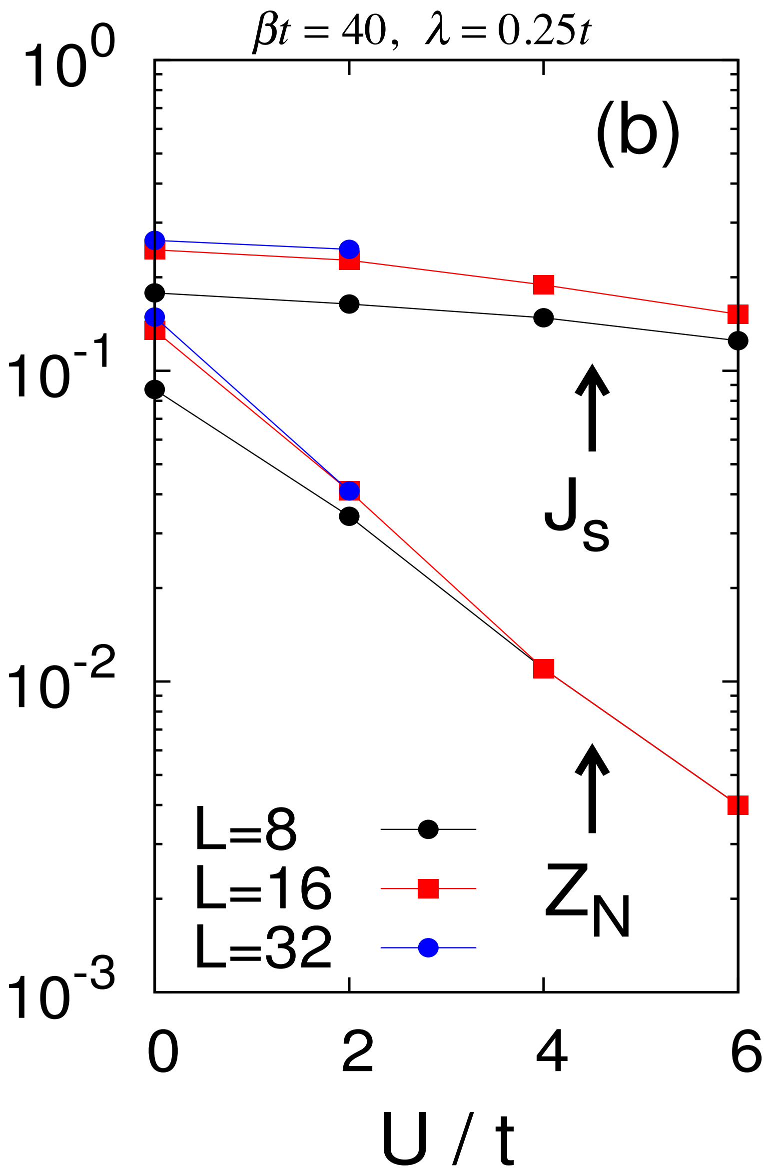
Loss of spectral weight in the low energy charge sector.

Dynamics @ $U/t = 6,\ \beta t = 40,\ \lambda = 0.25t$.



Velocities are independent on U/t.

Loss of spectral weight in the low energy charge sector.



Spin currents remain robust.

$$J_s = \frac{1}{L}\sum_k \sin(ka)(c^\dagger_{k\uparrow}c_{k\uparrow} - c^\dagger_{k\downarrow}c_{k\downarrow})$$

Drude, Z_N, weight is suppressed by orders of magnitudes.

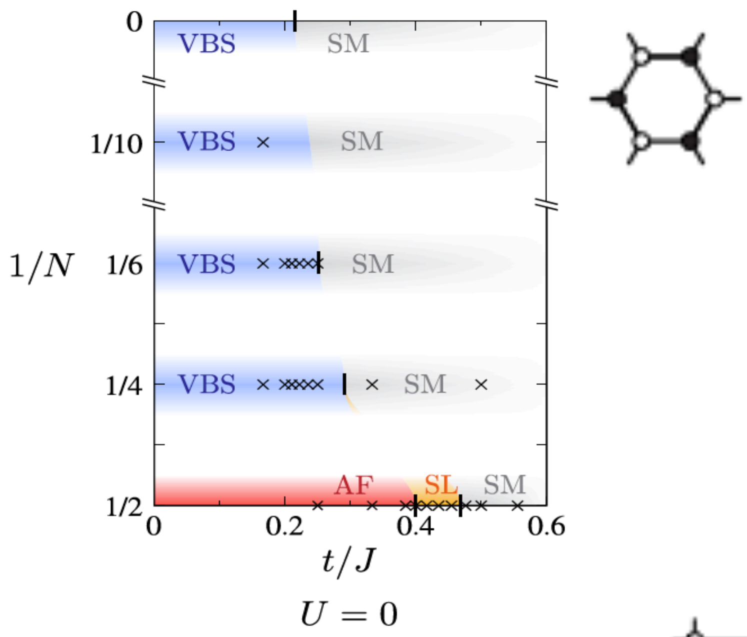
<u>Note</u>

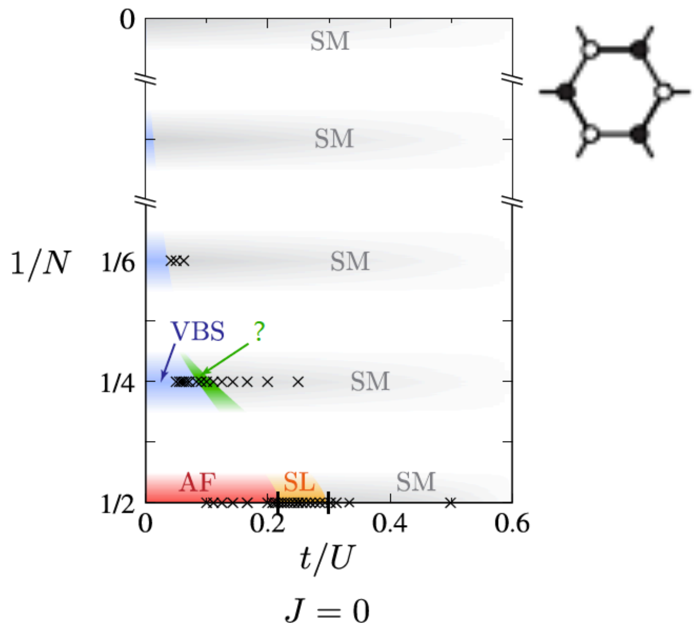
$$\sigma'_{xx}(q,\omega) = \frac{\omega}{q^2}\left(1 - e^{-\beta\omega}\right)N(q,\omega)$$

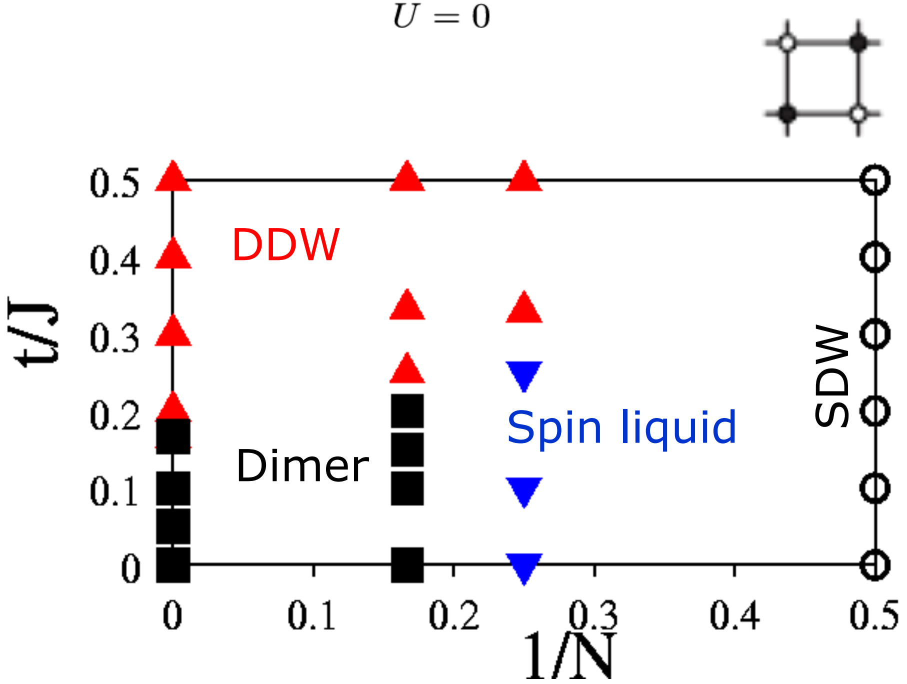
$$N(q,\omega) \propto q\, Z_N \delta(\omega - v_c q), \quad q = 2\pi / L$$

$$\lim_{q\to 0}\sigma'_{xx}(q,\omega) \propto Z_N \delta(\omega)$$

Conclusions. Exotic phases between ordered phases.







SU(2) Kane-Mele Hubbard