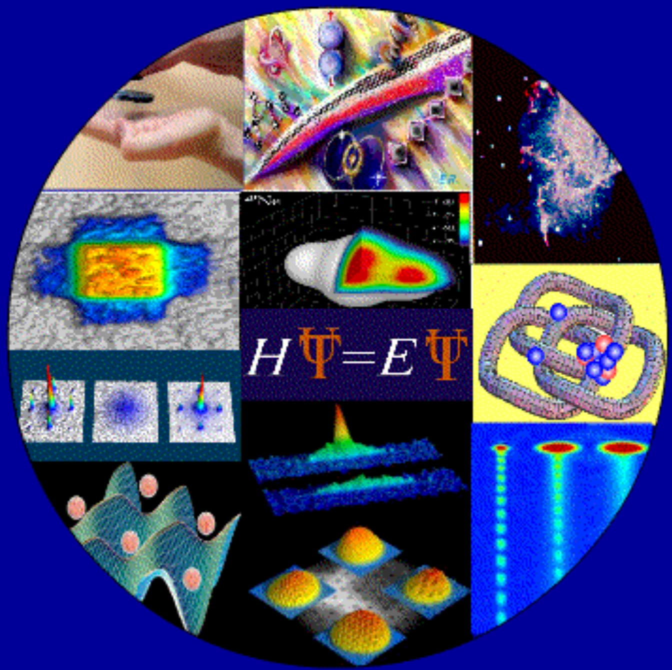
Intertwined orders in 2D strongly correlated fermion systems

"Computational Challenges in Nuclear and Many--Body Physics"
Nordita program - October 2014



Olivier Juillet, Alexandre Leprévost, Raymond Frésard

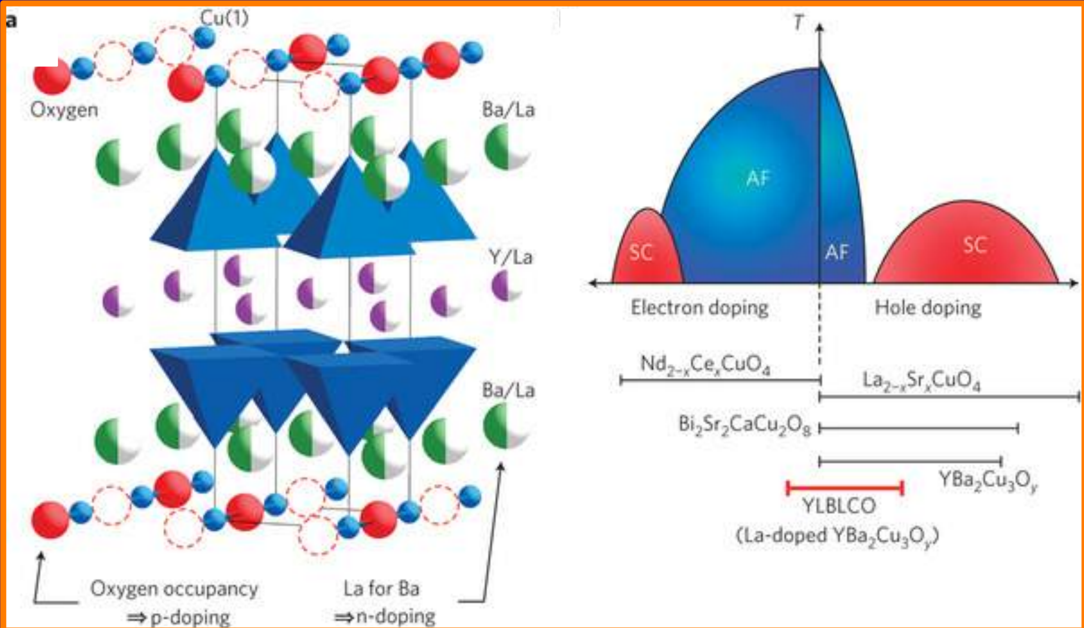
LPC Caen & CRISMAT

The Hubbard model

$$\hat{H} = -t \sum_{\substack{\langle \vec{r},\vec{r}' \rangle \\ \sigma=\uparrow,\downarrow}} \hat{c}^{+}_{\vec{r}\sigma} \hat{c}_{\vec{r}'\sigma} + U \sum_{\vec{r}} \hat{n}_{\vec{r}\uparrow} \hat{n}_{\vec{r}\downarrow}$$

Nearest neighbour hopping

On-site interaction



Cuprates

Low energy effective model of electrons in CuO_2 planes

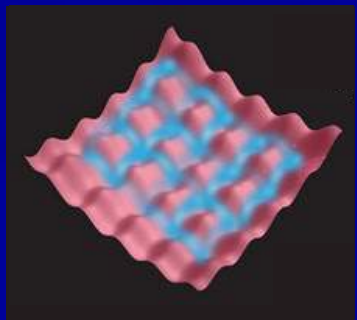
The half-filled Hubbard model

$$\hat{H} = -t \sum_{\langle \vec{r},\vec{r}' \rangle,\sigma} \hat{c}^{+}_{\vec{r}\sigma} \hat{c}_{\vec{r}'\sigma} + U \sum_{\vec{r}} \hat{n}_{\vec{r}\uparrow} \hat{n}_{\vec{r}\downarrow}$$

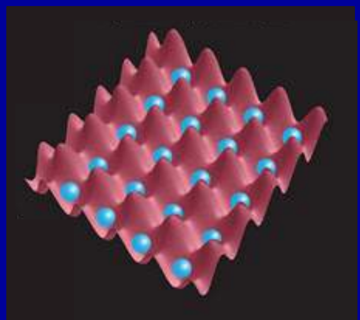
Fermionic atoms loaded in optical lattices

$U = 0$

Delocalized states

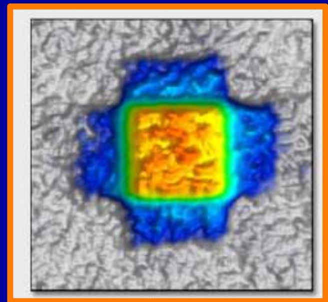


$U >> t$

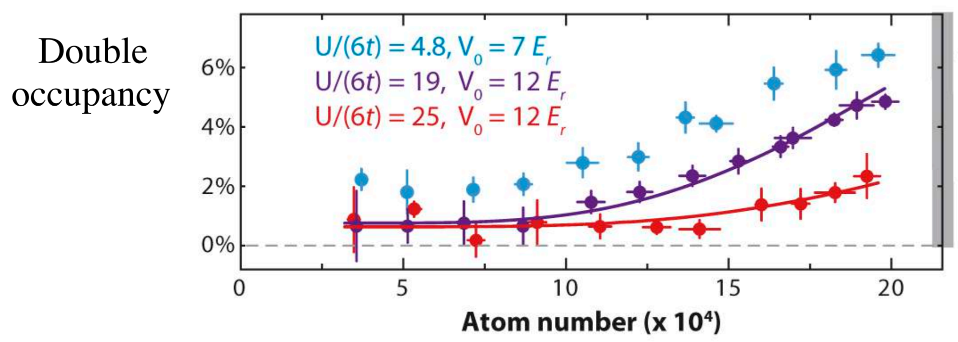


Mott insulator
One atom per site

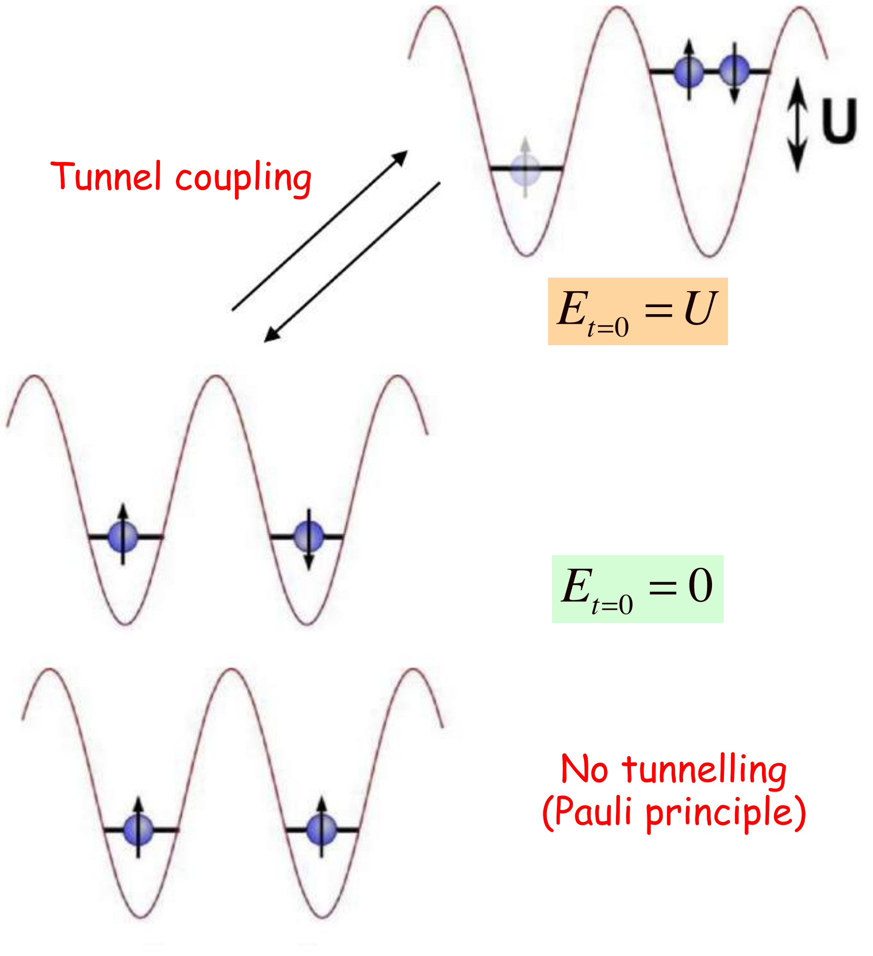
M. Köhl & al, Phys. Rev. Lett. (2005)



R. Jördens & al, Nature (2008)

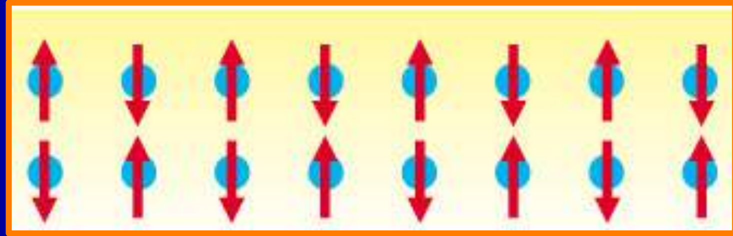


The half-filled Hubbard model



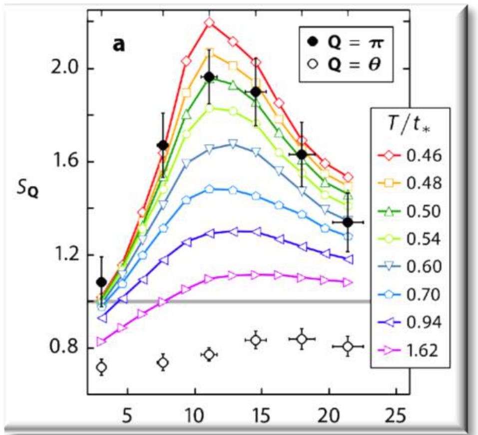
$$\hat{H} = -t \sum_{\langle \vec{r},\vec{r}'\rangle,\sigma} \hat{c}^{+}_{\vec{r}\sigma}\hat{c}_{\vec{r}'\sigma} + U\sum_{\vec{r}} \hat{n}_{\vec{r}\uparrow}\hat{n}_{\vec{r}\downarrow} \ , \ U >> t$$

Antiferromagnetic order



$$\left\langle \hat{\vec{S}}_{\vec{0}} \cdot \hat{\vec{S}}_{\vec{r}} \right\rangle \propto (-1)^{x+y} = \cos(\pi x + \pi y)$$

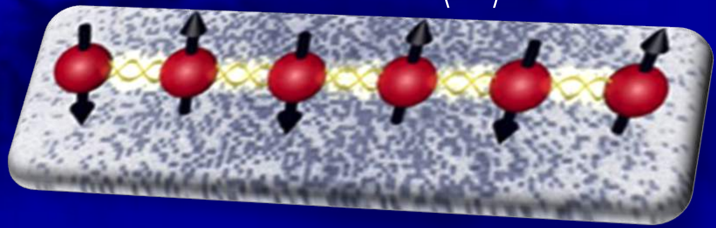
$$S(\vec{q}) = \sum_{\vec{r}} \exp(i\vec{q}\,\vec{r}) \left\langle \hat{\vec{S}}_{\vec{0}} \cdot \hat{\vec{S}}_{\vec{r}} \right\rangle \text{ peaked at } \vec{q} = (\pi,\pi)$$



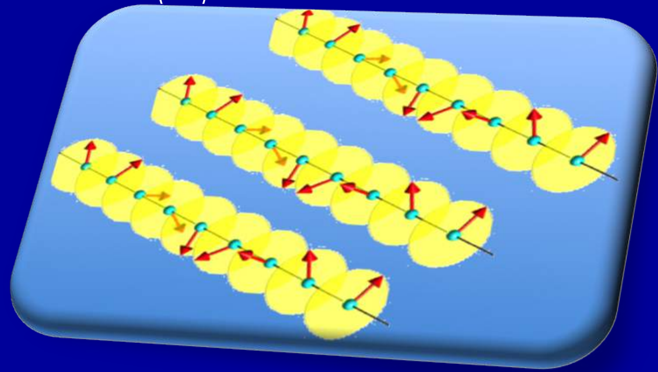
R. A. Hart et *al*., arxiv/cond-mat (2014)

The hole-doped Hubbard model

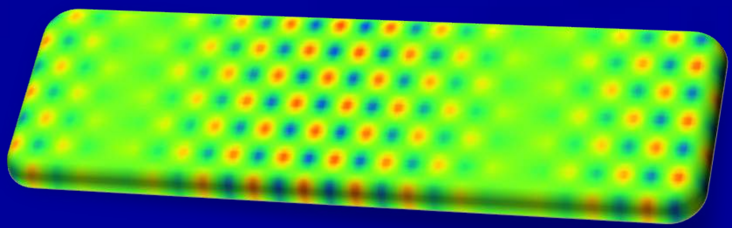
Antiferromagnetism : $\left\langle \hat{\vec{S}}_{\vec{r}} \right\rangle \propto (-1)^{x+y}\,\vec{u}_z$



Spiral magnetism : $\left\langle \hat{\vec{S}}_{\vec{r}} \right\rangle \propto \cos\left(\vec{q}_{Spiral}\cdot\vec{r}\right)\vec{u}_x + \sin\left(\vec{q}_{Spiral}\cdot\vec{r}\right)\vec{u}_y$

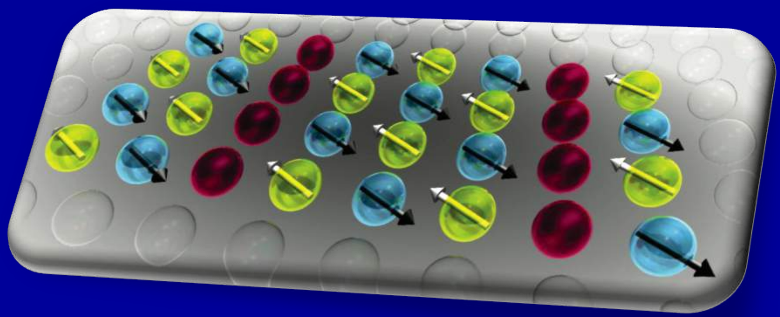


Spin density waves : $\left\langle \hat{\vec{S}}_{\vec{r}} \right\rangle \propto \cos\left(\vec{q}_{SDW}\cdot\vec{r}\right)\vec{u}_z$

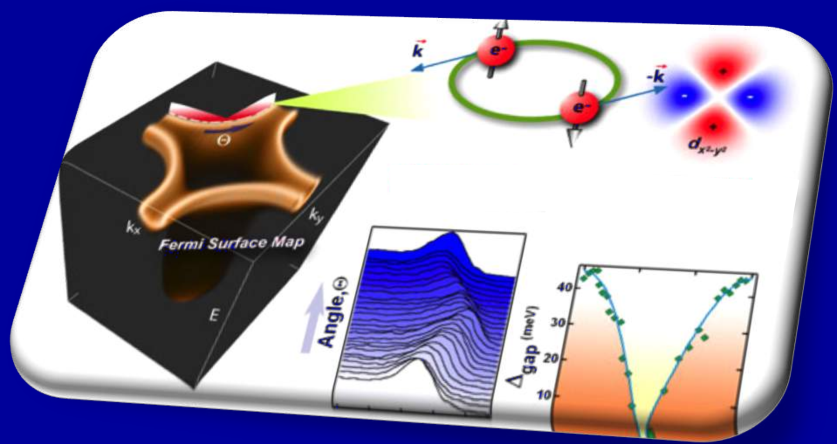


and many others ....

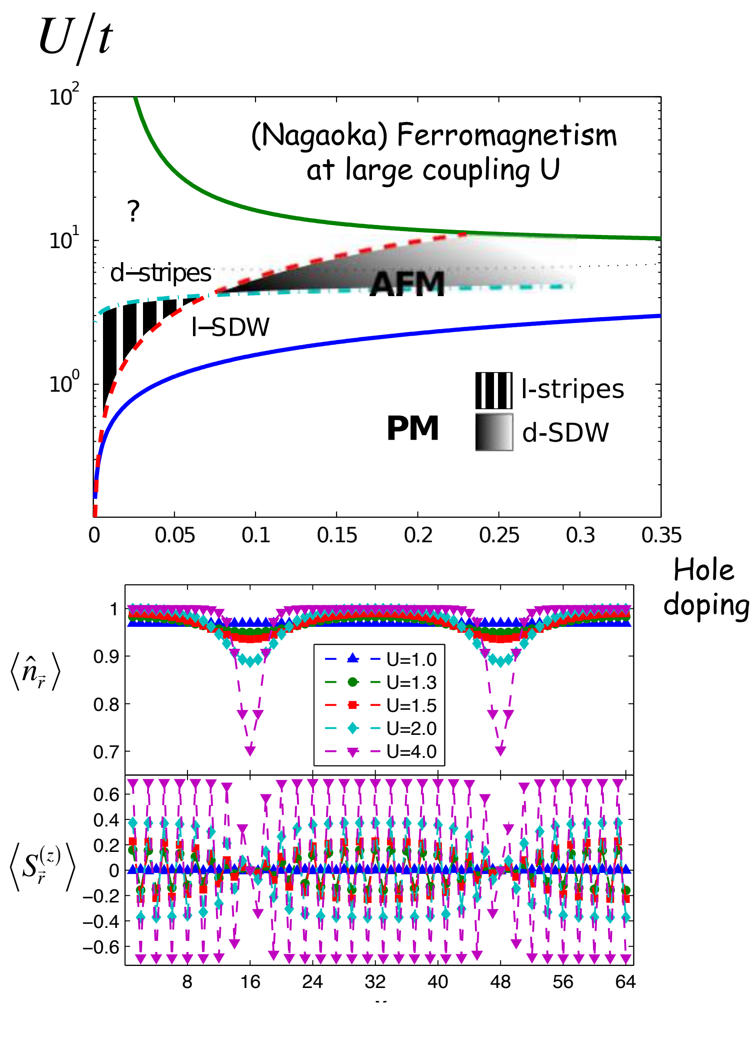
Stripes : $\left\langle \hat{\vec{S}}_{\vec{r}} \right\rangle \propto \cos\left(\vec{q}_{SDW}\cdot\vec{r}\right)\vec{u}_z, \left\langle \hat{n}_{\vec{r}} \right\rangle \propto \cos\left(\vec{q}_{CDW}\cdot\vec{r}\right)$



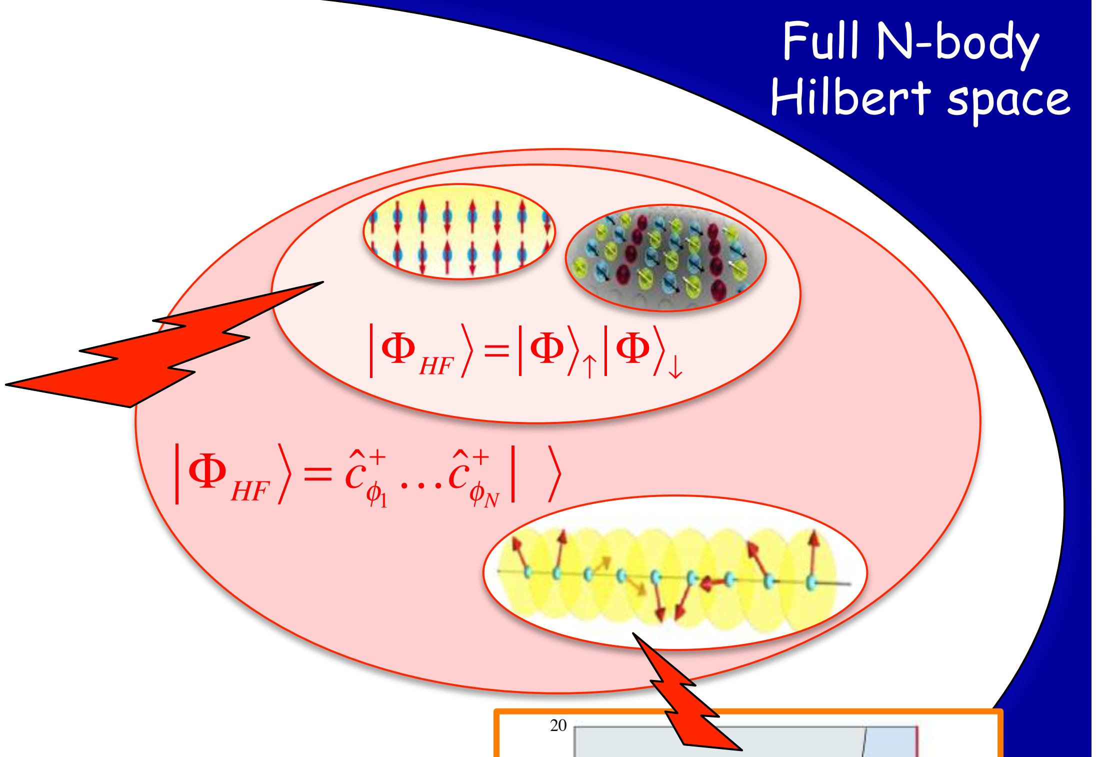
d-wave superconductivity : $\left\langle \hat{c}_{\vec{r}}\hat{c}_{\vec{r}+\vec{u}_x} \right\rangle = -\left\langle \hat{c}_{\vec{r}}\hat{c}_{\vec{r}+\vec{u}_y} \right\rangle \neq 0$

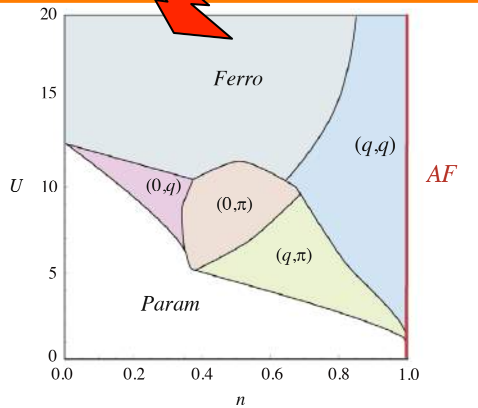


Conventional variational approaches to the Hubbard model



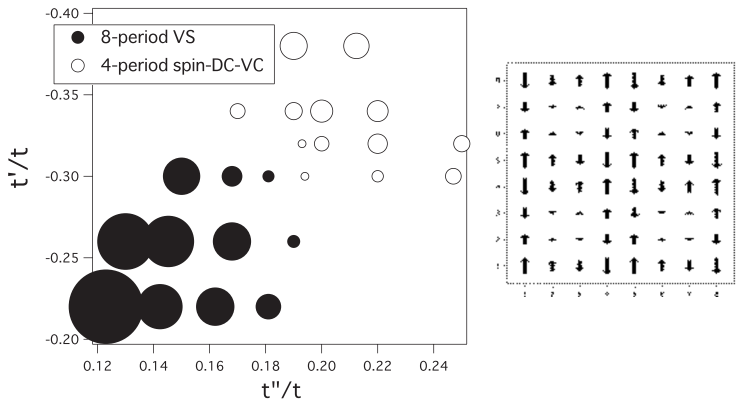
J. Xu, C-C. Chang, E. J. Walter & S. Zhang, J. Phys. Cond. Matter (2011)



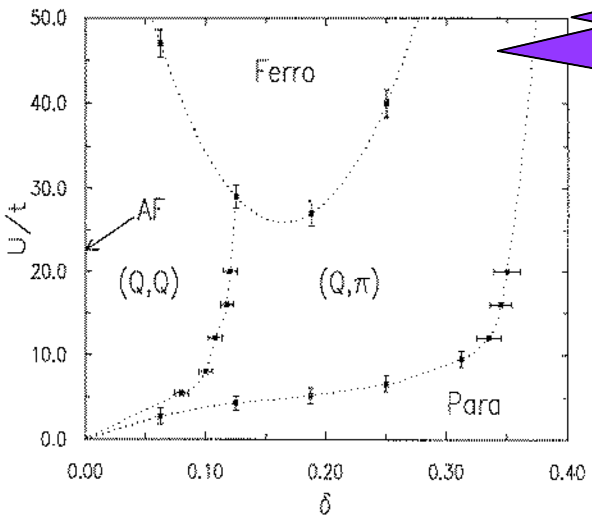


J.D. Gouveia, R.G. Dias, Solid State Comm. (2014)

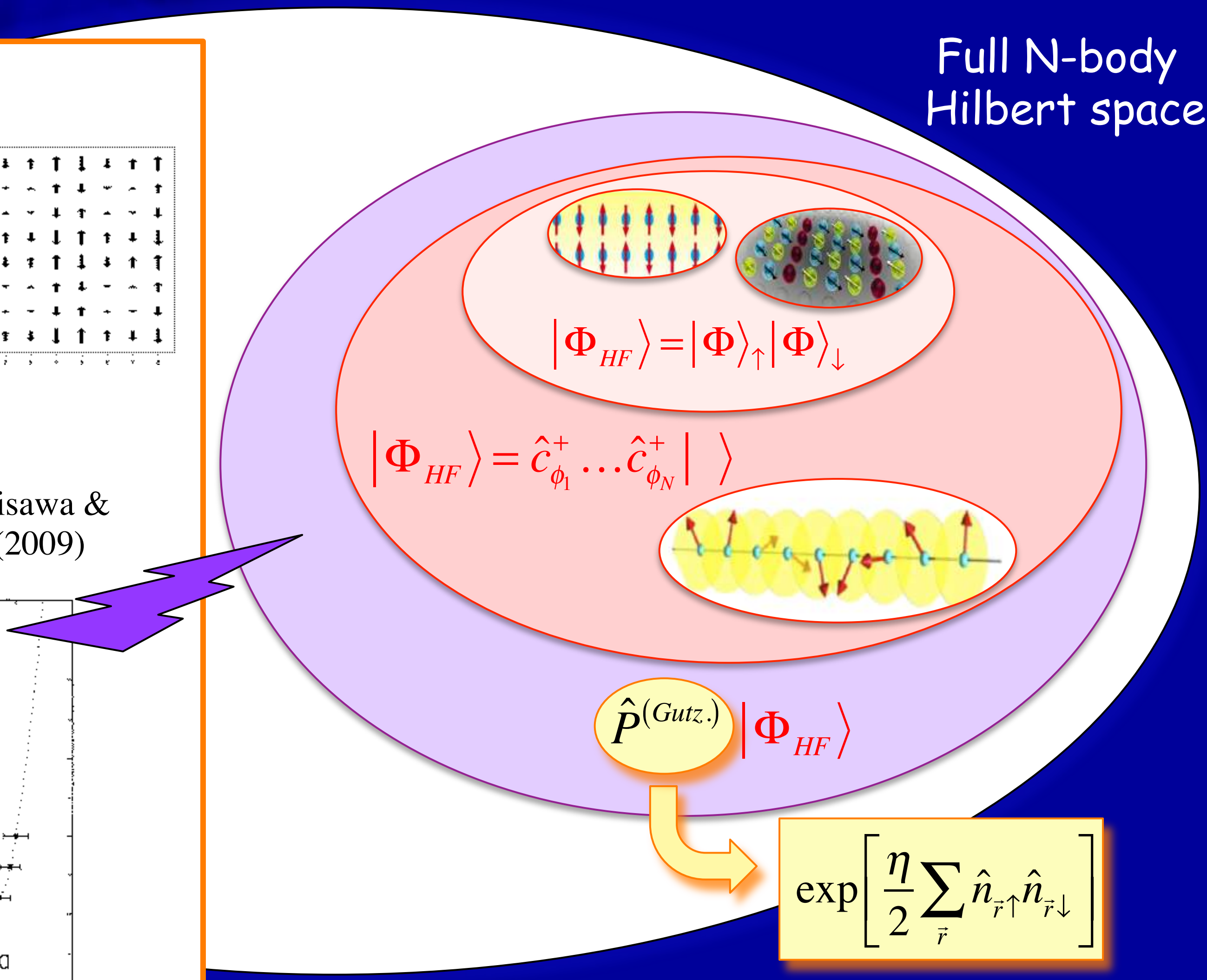
Conventional variational approaches to the Hubbard model



M. Miyazaki, K. Yamaji, T. Yanagisawa & R. Kadano, J. Phys. Soc. Japan (2009)

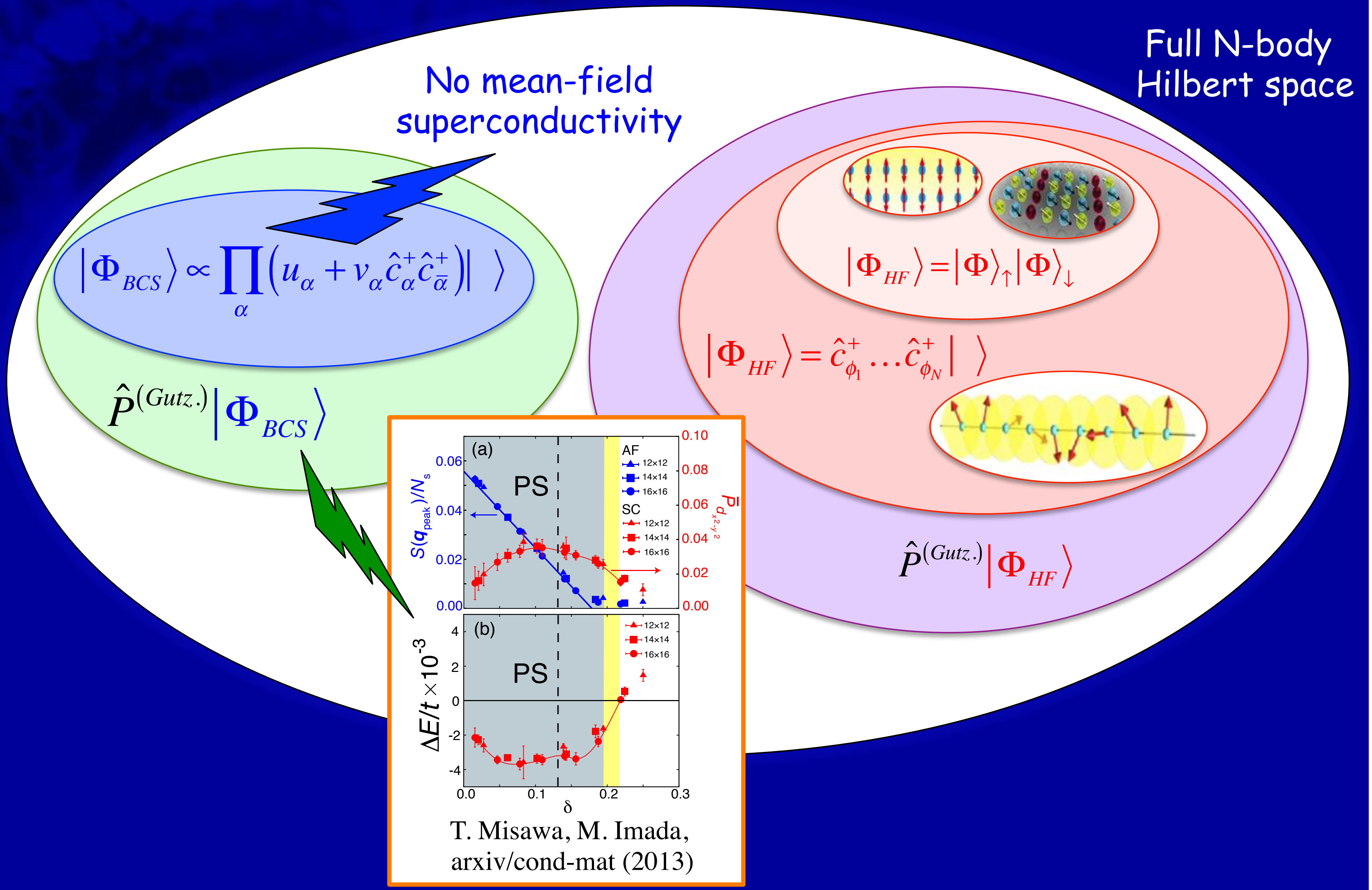


M. Dzierzawa & R. Frésard, Z. Phys B. (1993)



Two-body correlator to reduce double occupancy

Conventional variational approaches to the Hubbard model



The symmetry-projected Hartree-Fock/BCS wavefunction

No assumed charge, spin or superconducting orders

Totally unrestricted orthonormal single-particle states

$$\prod_{i=1}^{N} \hat{c}^{+}_{\phi_i} | \ \rangle$$

$$\text{with } \hat{c}^{+}_{\phi_i} = \sum_{\vec{r}\sigma} \phi_{i,\vec{r}\sigma} \hat{c}^{+}_{\vec{r}\sigma}$$

General unitary Bogoliubov transformation

$$\propto \prod_{\vec{r}\sigma} \hat{\gamma}_{\vec{r}\sigma} | \ \rangle$$

$$\text{with } \hat{\gamma}_{\vec{r}\sigma} = \sum_{\vec{r}'\sigma'} \left(U^{*}_{\vec{r}'\sigma',\vec{r}\sigma} \hat{c}_{\vec{r}'\sigma'} + V^{*}_{\vec{r}'\sigma',\vec{r}\sigma} \hat{c}^{+}_{\vec{r}'\sigma'} \right)$$

$$\left| \Psi_0^{(\Gamma)} \right\rangle \to \left| \Phi^{(\Gamma)}_{HF-BCS} \right\rangle = \hat{P}^{(\Gamma)} \left(c_{HF} \left| \Phi_{HF} \right\rangle + c_{BCS} \left| \Phi_{BCS} \right\rangle \right)$$

Exact ground state characterized by several quantum numbers Γ reflecting symmetries of the Hamiltonian

$$\Gamma = \left(N, \vec{K}, S, S_z, \cdots \right)$$

$$\hat{P}^{(\Gamma)} \propto \sum_{g} \left(\chi_g^{(\Gamma)} \right)^{*} \hat{U}_g$$

Quantum number projection by superposition of symmetry related wavefunctions

Correlations from restoration of deliberately broken symmetries by projection before variation

$$\delta E^{(\Gamma)} = \delta \left\langle \hat{H} \right\rangle_{\Phi^{(\Gamma)}} = 0$$

The symmetry-projected Hartree-Fock/BCS wavefunction

Generalized eigenvalue problem for the amplitudes

$$\sum_b \boxed{\left\langle \Phi_a \middle| \hat{H}\hat{P}^{(\Gamma)} \middle| \Phi_b \right\rangle} c_b = E^{(\Gamma)} \sum_b \boxed{\left\langle \Phi_a \middle| \hat{P}^{(\Gamma)} \middle| \Phi_b \right\rangle} c_b$$

$$\sum_g \left(\chi_g^{(\Gamma)}\right)^* \mathcal{N}_g^{(a,b)} \mathcal{E}\left[\mathcal{R}_g^{(a,b)}\right]$$

$$\sum_g \left(\chi_g^{(\Gamma)}\right)^* \mathcal{N}_g^{(a,b)} \text{ with } \mathcal{N}_g^{(a,b)} = \left\langle \Phi_a \middle| \Phi_{b,g} \right\rangle$$

Wick's theorem for matrix elements between mean-field states

One-body transition density matrix

Overlap between HF and/or BCS wave-functions (Determinant or pfaffian)

$$\mathcal{R}_g^{(a,b)} = \begin{pmatrix} \rho_g^{(a,b)} & \kappa_g^{(a,b)} \\ \tilde{\kappa}_g^{(a,b)} & \tilde{\rho}_g^{(a,b)} \end{pmatrix}$$

with
$$\begin{pmatrix} \left[\rho_g^{(a,b)}\right]_{\vec{r}\sigma,\vec{r}'\sigma'} & \left[\kappa_g^{(a,b)}\right]_{\vec{r}\sigma,\vec{r}'\sigma'} \\ \left[\tilde{\kappa}_g^{(a,b)}\right]_{\vec{r}\sigma,\vec{r}'\sigma'} & \left[\tilde{\rho}_g^{(a,b)}\right]_{\vec{r}\sigma,\vec{r}'\sigma'} \end{pmatrix} = \frac{1}{\mathcal{N}_g^{(a,b)}} \left\langle \Phi_a \middle| \begin{pmatrix} \hat{c}^+_{\vec{r}'\sigma'}\hat{c}_{\vec{r}\sigma} & \hat{c}_{\vec{r}'\sigma'}\hat{c}_{\vec{r}\sigma} \\ \hat{c}^+_{\vec{r}'\sigma'}\hat{c}^+_{\vec{r}\sigma} & \hat{c}_{\vec{r}'\sigma'}\hat{c}^+_{\vec{r}\sigma} \end{pmatrix} \middle| \Phi_{b,g} \right\rangle$$

The symmetry-projected Hartree-Fock/BCS wavefunction

Optimal single-particle states and BCS quasiparticles

$$\mathcal{Q}^{(\Gamma,a,b)} = \begin{pmatrix} L^{(\Gamma,a,b)} & \Lambda^{(\Gamma,a,b)} \\ \tilde{\Lambda}^{(\Gamma,a,b)} & \tilde{L}^{(\Gamma,a,b)} \end{pmatrix} = \sum_g \left(\chi_g^{(\Gamma)}\right)^* \mathcal{N}_g^{(a,b)} \left[\left(1-\mathcal{R}_g^{(a,b)}\right) \boxed{\mathcal{H}\left[\mathcal{R}_g^{(a,b)}\right]} \mathcal{R}_g^{(a,b)} + \mathcal{R}_g^{(a,b)}\left(\mathcal{E}\left[\mathcal{R}_g^{(a,b)}\right]-E^{(\Gamma)}\right)\right]$$

Hartree-Fock-Bogoliubov Hamiltonian expressed in terms of the one-body transition density matrix

$$\begin{pmatrix} h_g^{(a,b)} & \Delta_g^{(a,b)} \\ \tilde{\Delta}_g^{(a,b)} & \tilde{h}_g^{(a,b)} \end{pmatrix}$$

$$\text{with} \begin{pmatrix} \left[h_g^{(a,b)}\right]_{\vec{r}\sigma,\vec{r}'\sigma'} & \left[\Delta_g^{(a,b)}\right]_{\vec{r}\sigma,\vec{r}'\sigma'} \\ \left[\tilde{\Delta}_g^{(a,b)}\right]_{\vec{r}\sigma,\vec{r}'\sigma'} & \left[\tilde{h}_g^{(a,b)}\right]_{\vec{r}\sigma,\vec{r}'\sigma'} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial\mathcal{E}}{\partial\left[\rho_g^{(a,b)}\right]_{\vec{r}'\sigma',\vec{r}\sigma}} & \dfrac{\partial\mathcal{E}}{\partial\left[\tilde{\kappa}_g^{(a,b)}\right]_{\vec{r}'\sigma',\vec{r}\sigma}} \\ \dfrac{\partial\mathcal{E}}{\partial\left[\kappa_g^{(a,b)}\right]_{\vec{r}'\sigma',\vec{r}\sigma}} & \dfrac{\partial\mathcal{E}}{\partial\left[\tilde{\rho}_g^{(a,b)}\right]_{\vec{r}'\sigma',\vec{r}\sigma}} \end{pmatrix}$$

$$\begin{cases} c_{HF} L^{(\Gamma,HF,HF)} + c_{BCS} L^{(\Gamma,HF,BCS)} = 0 \\ c_{HF} \mathcal{Q}^{(\Gamma,BCS,HF)} + c_{BCS} \mathcal{Q}^{(\Gamma,BCS,BCS)} = 0 \end{cases}$$

A. Leprévost, O. Juillet, R. Frésard, to be published (2014).

Technical comments

- Energy minimization by the conjugate gradient method through Thouless parameterization of HF and BCS wavefunctions
- We use a 16x4 supercell with antiperiodic/periodic boundary conditions

  ↳ **$\sim 10^4$ complex variables to be simultaneously determined**
- Translational invariance and lattice symmetries (C_{2v} group) are restored
  + Particle number projection for the BCS state
  + Spin rotational invariance partially restored during the optimization :

$$S_z \text{ and spin-parity } \varpi_S = (-1)^S \text{ projections}$$

  ↳ **The variational N-body state corresponds to the superposition of $\sim 7.10^4$ symmetry related wavefunctions**
- Full spin projection after basis optimization

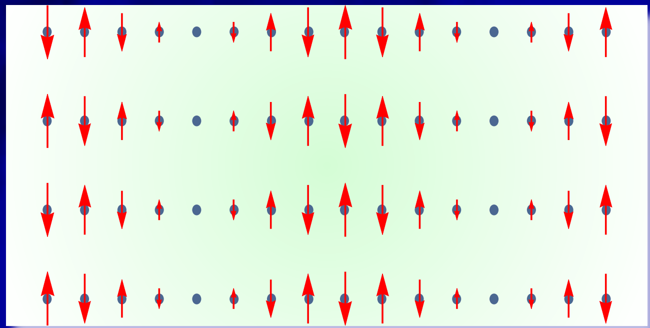
Same unprojected basis states

$$\hat{P}^{(N,\vec{K},\varpi_S,S_z,\Gamma_{latt.})}\left(c_{HF} \boxed{|\Phi_{HF}\rangle} + c_{BCS} \boxed{|\Phi_{BCS}\rangle} \right) \rightarrow \hat{P}^{(N,\vec{K},S,S_z,\Gamma_{latt.})}\left(c'_{HF} \boxed{|\Phi_{HF}\rangle} + c'_{BCS} \boxed{|\Phi_{BCS}\rangle} \right)$$

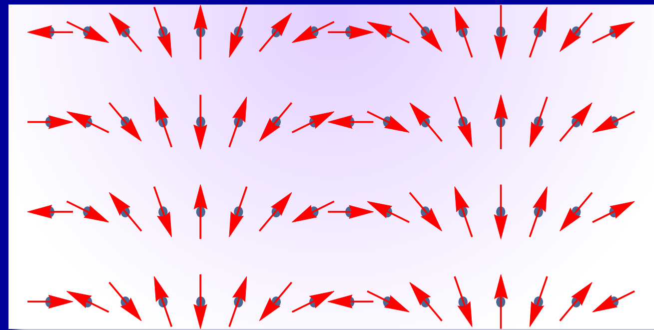
New amplitudes from eigenvalue equation with totally projected states

Signatures of spin-density wave and spiral orderings

Classical SDW : $\vec{S}_{\vec{r}} \propto \cos(\vec{q}_S \cdot \vec{r})\vec{u}_z$



Classical spiral : $\vec{S}_{\vec{r}} \propto \cos(\vec{q}_S \cdot \vec{r})\vec{u}_x + \sin(\vec{q}_S \cdot \vec{r})\vec{u}_y$



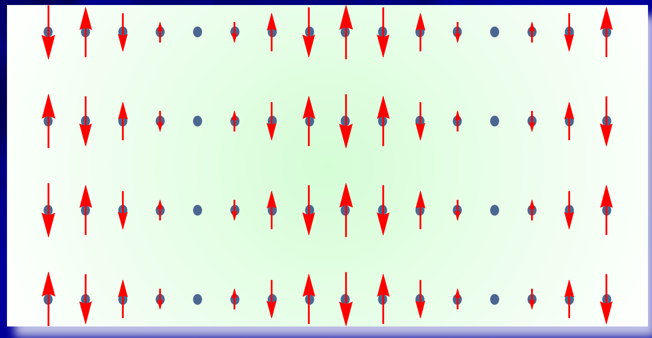
$\propto \cos(\vec{q}_S \cdot \vec{r})$	$\vec{S}_{\vec{0}} \cdot \vec{S}_{\vec{r}}$	$\propto \cos(\vec{q}_S \cdot \vec{r})$
$\vec{0}$	$\vec{V}_{\vec{r}} = \vec{S}_{\vec{r}} \wedge \left(\vec{S}_{\vec{r}+\vec{u}_x} + \vec{S}_{\vec{r}+\vec{u}_y}\right)$	$\propto \left(\cos q_y - \cos q_x\right)\vec{u}_z = Cte$

$$S(\vec{q}) = \sum_{\vec{r}} \exp(i\vec{q}.\vec{r})\left\langle \hat{\vec{S}}_{\vec{0}} \cdot \hat{\vec{S}}_{\vec{r}} \right\rangle \text{ peaked at } \vec{q} = \vec{q}_s$$

$$\mathscr{V}(\vec{r}) = \left\langle \hat{\vec{V}}_{\vec{0}} \cdot \hat{\vec{V}}_{\vec{r}} \right\rangle \xrightarrow[r\to\infty]{} Cte \Rightarrow \overline{\mathscr{V}(\vec{r})}_{r\to\infty} = \begin{cases} 0 \to \text{Spin density wave} \\ > 0 \to \text{Spiral} \end{cases}$$

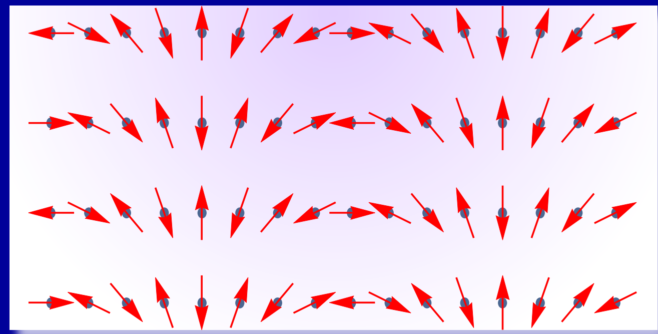
Signatures of spin-density wave and spiral orderings

SDW with wavevector $\vec{q}_S$



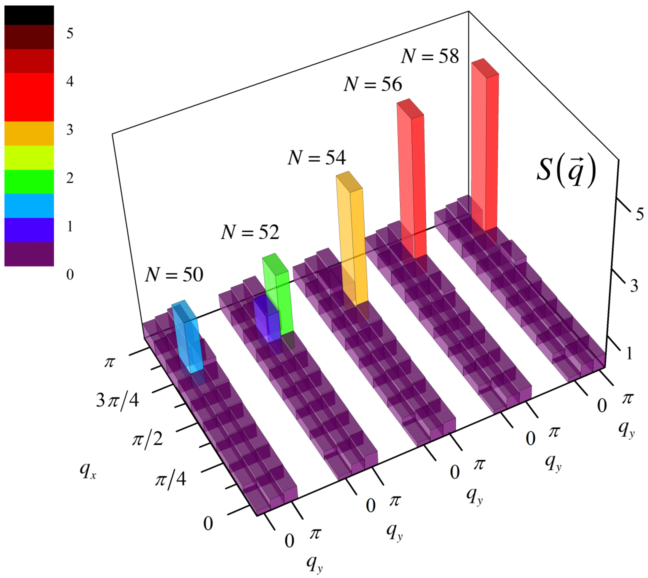
$$S(\vec{q}) \propto \delta_{\vec{q},\vec{q}_S} \text{ and } \overline{\mathscr{V}(\vec{r})}_{r\to\infty} = 0$$

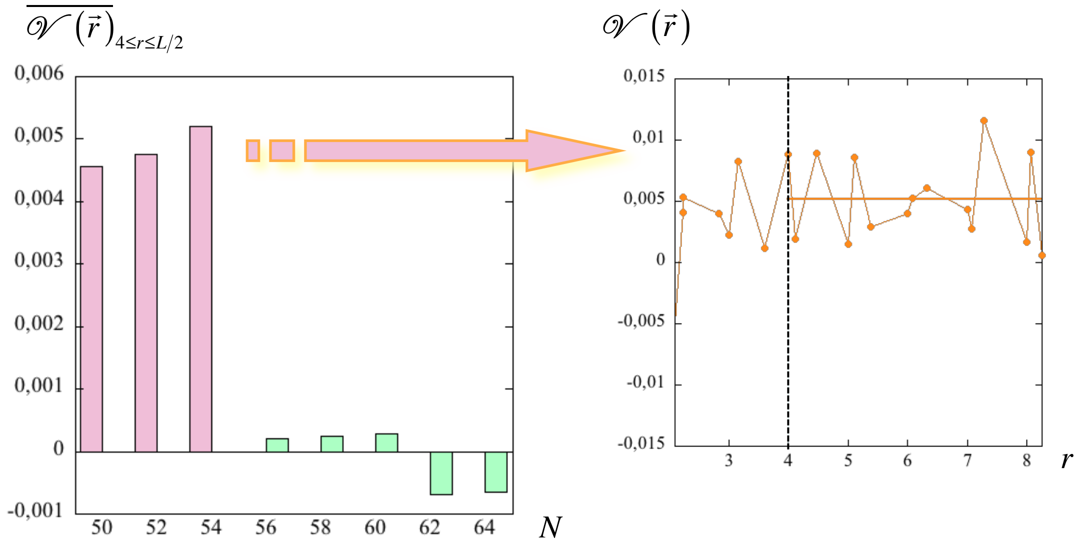
Spiral with wavevector $\vec{q}_S$



$$S(\vec{q}) \propto \delta_{\vec{q},\vec{q}_S} \text{ and } \overline{\mathscr{V}(\vec{r})}_{r\to\infty} > 0$$

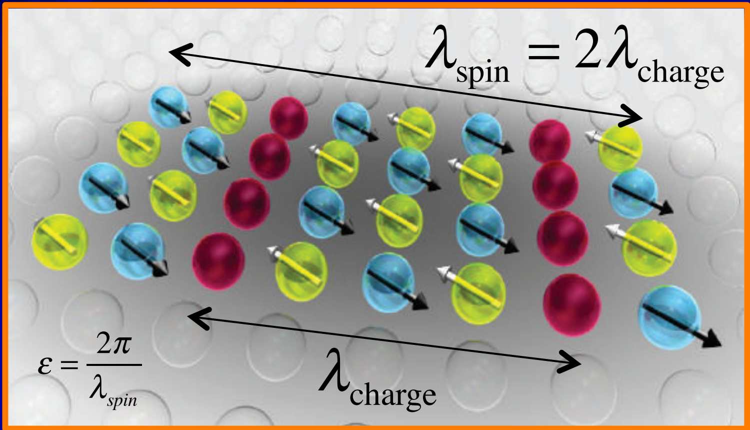
Dependence of magnetic correlations on hole doping at U=8t

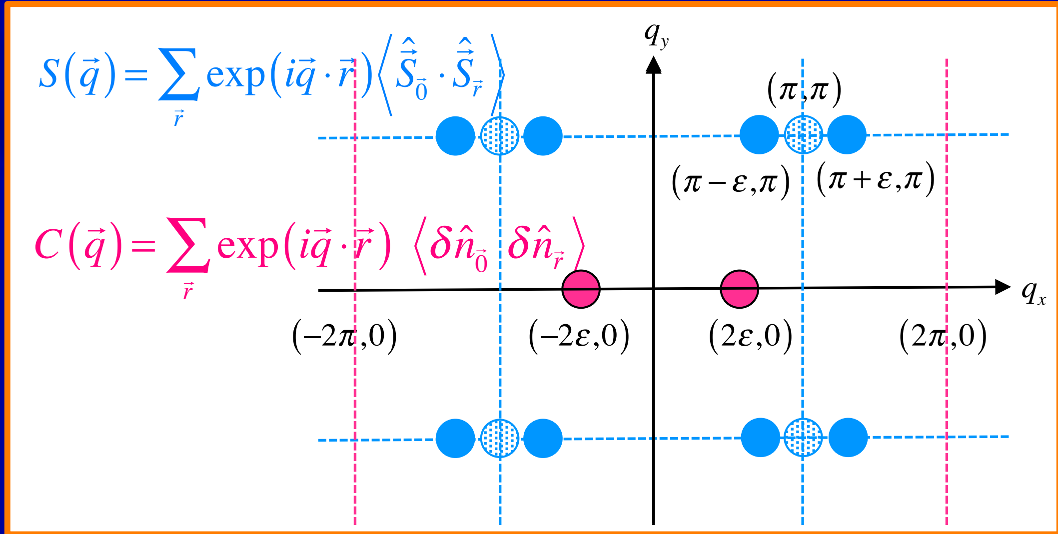




Signatures of stripe ordering

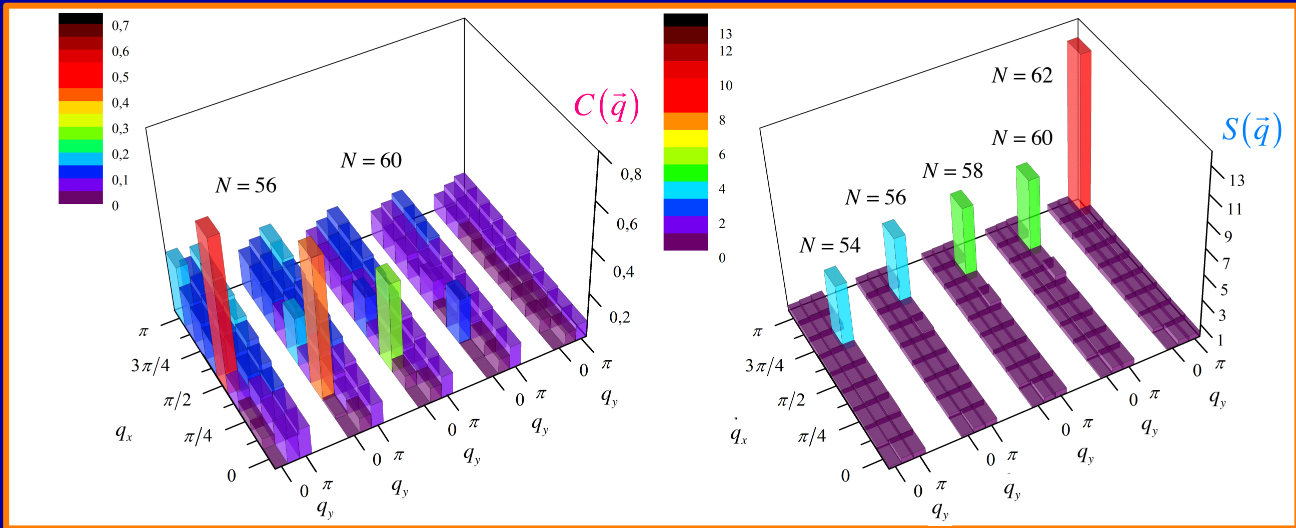
Related peaks in the Fourier transform of the spin-spin and density-density correlation functions





Dependence of magnetic and charge correlations on hole doping

$$U = 12t$$

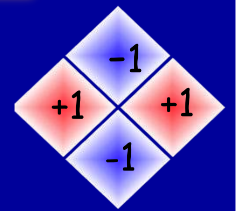


Signature of d-wave superconductivity

Long-ranged pair correlations : $\mathscr{D}\left(\vec{R}\right)=\frac{1}{2}\left\langle \hat{D}_{\vec{0}}^{+}\hat{D}_{\vec{R}}+\hat{D}_{\vec{0}}\hat{D}_{\vec{R}}^{+}\right\rangle \xrightarrow[R\to\infty]{} Cte$

Singlet d-wave pair field

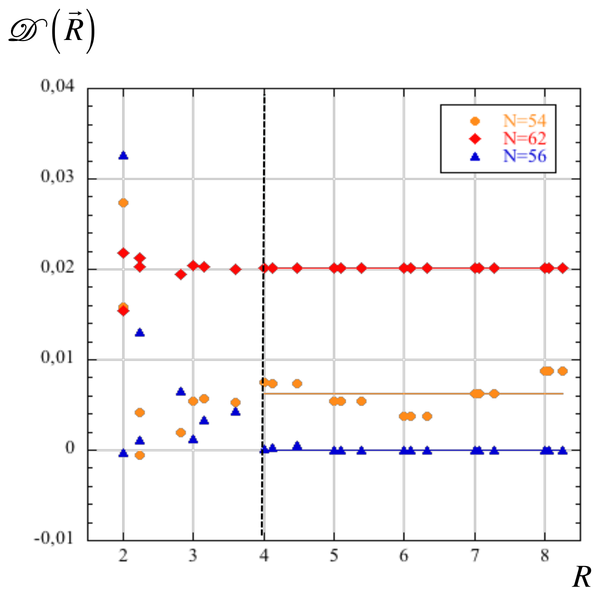
$$\sum_{\vec{r}\in\left\{\pm\vec{u}_x,\pm\vec{u}_y\right\}} f\left(\vec{r}\right)\frac{1}{\sqrt{2}}\left(\hat{c}_{\vec{R}\uparrow}^{+}\hat{c}_{\vec{R}+\vec{r}\downarrow}^{+}-\hat{c}_{\vec{R}\downarrow}^{+}\hat{c}_{\vec{R}+\vec{r}\uparrow}^{+}\right) \text{ with } f\left(\vec{r}\right)=$$

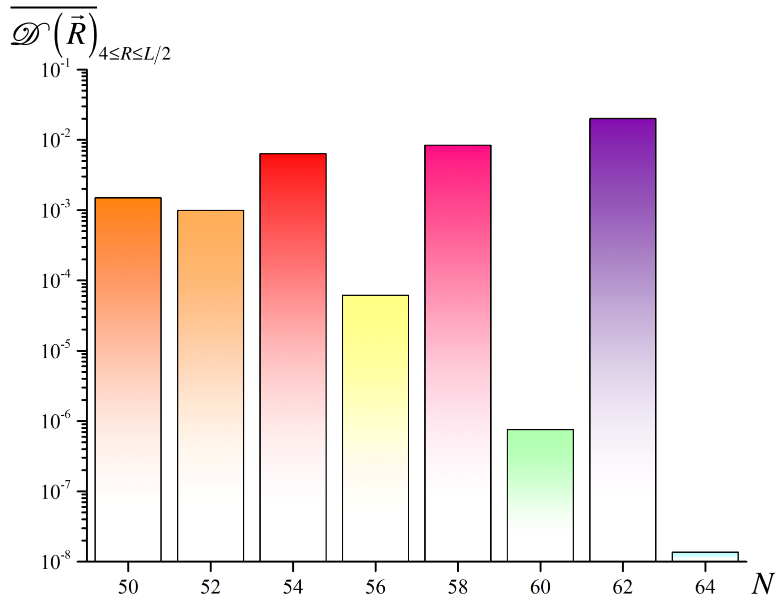


$$\left\langle \hat{c}_i^{+}\hat{c}_j^{+}\hat{c}_k\hat{c}_l\right\rangle \to \left\langle \hat{c}_i^{+}\hat{c}_j^{+}\hat{c}_k\hat{c}_l\right\rangle - \left(\left\langle \hat{c}_i^{+}\hat{c}_l\right\rangle\left\langle \hat{c}_j^{+}\hat{c}_k\right\rangle - \left\langle \hat{c}_i^{+}\hat{c}_k\right\rangle\left\langle \hat{c}_j^{+}\hat{c}_l\right\rangle\right) \Rightarrow \mathscr{D}\left(\vec{R}\right)=0 \text{ for non-interacting electrons}$$

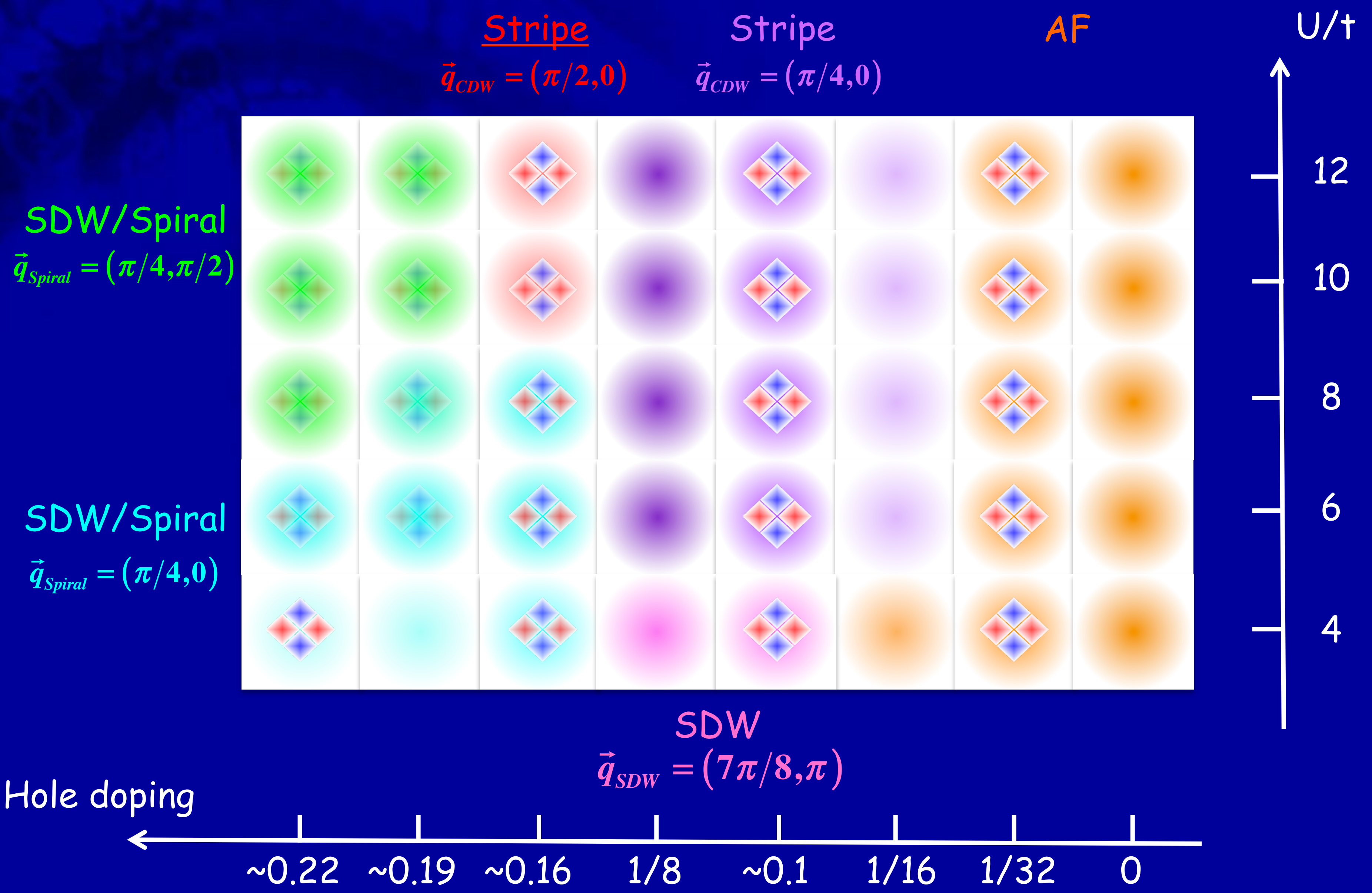
Dependence of superconductivity on hole doping

$U=12t$





Phase diagram from symmetry-projected HF/BCS wavefunctions



Reliability of the symmetry projected HF/BCS scheme

Comparison with exact results at half-filling

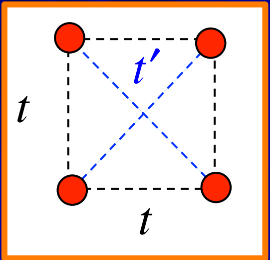
$\hat{P}^{(\Gamma)} \left|\Phi_{HF}\right\rangle$ is the exact ground-state at any coupling for the 2x2 cluster

A. Leprévost, O. Juillet & R. Frésard, Ann. der Phys. (2014)

		$Energy/t$	$S(\pi,\pi)$	$C(\pi,\pi)$
$4\times4-U=4t-t'=0$	$Ex.\,Diag.$	-13.6224	2.73	0.385
	$HF-BCS\ (S=0)$	-13.618	2.743	0.386
$6\times6-U=4t-t'=0$	QMC	$-30.87(2)$	$4.365(3)$	$0.418(2)$
	$HF-BCS\ (S=0)$	-30.724	4.562	0.411

Reliability of the symmetry projected HF/BCS scheme

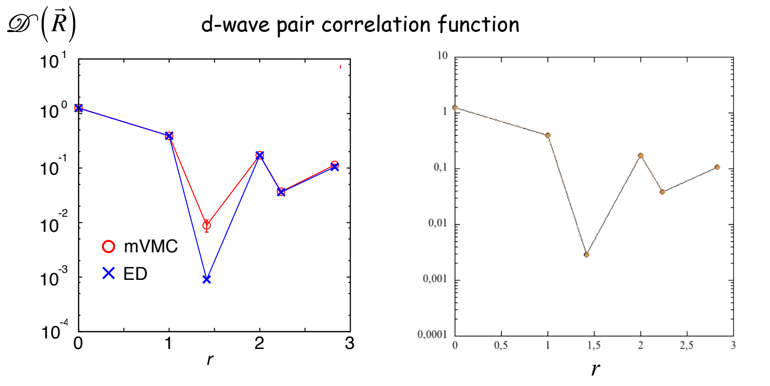
Comparison with exact results on doped small clusters



		$Energy/t$	$S(\pi,\pi)$	$C(\pi,\pi)$
$4\times4-N=14$ $U=8t-t'=-0.3t$	$Ex.Diag.$	-12.503	0.724	0.279
	$HF-BCS\ (S=0)$	-12.439	0.727	0.288

$4\times4-N=10-U=10t-t'=0$

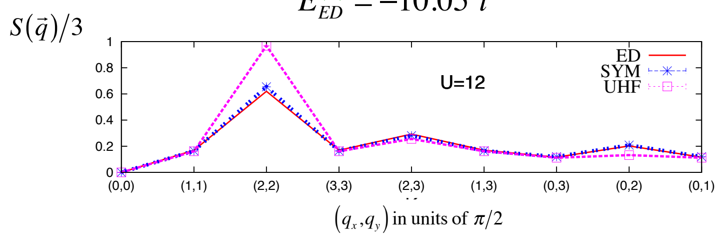
$E_{ED}^{(\Gamma)}=-16.902\ t$ $\qquad$ $\left\langle \hat{H}\right\rangle_{HF-BCS\ (S=0)}^{(\Gamma)}=-16.876\ t$



T. Misawa, M. Imada, arxiv/cond-mat (2013)

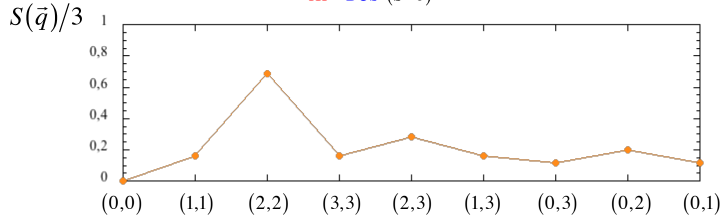
$4\times4-N=14-U=12t-t'=0$

$E_{ED}^{(\Gamma)}=-10.05\ t$



H. Shi, S. Zhang, Phys. Rev B (2013)

$\left\langle \hat{H}\right\rangle_{HF-BCS\ (S=0)}^{(\Gamma)}=-9.957\ t$



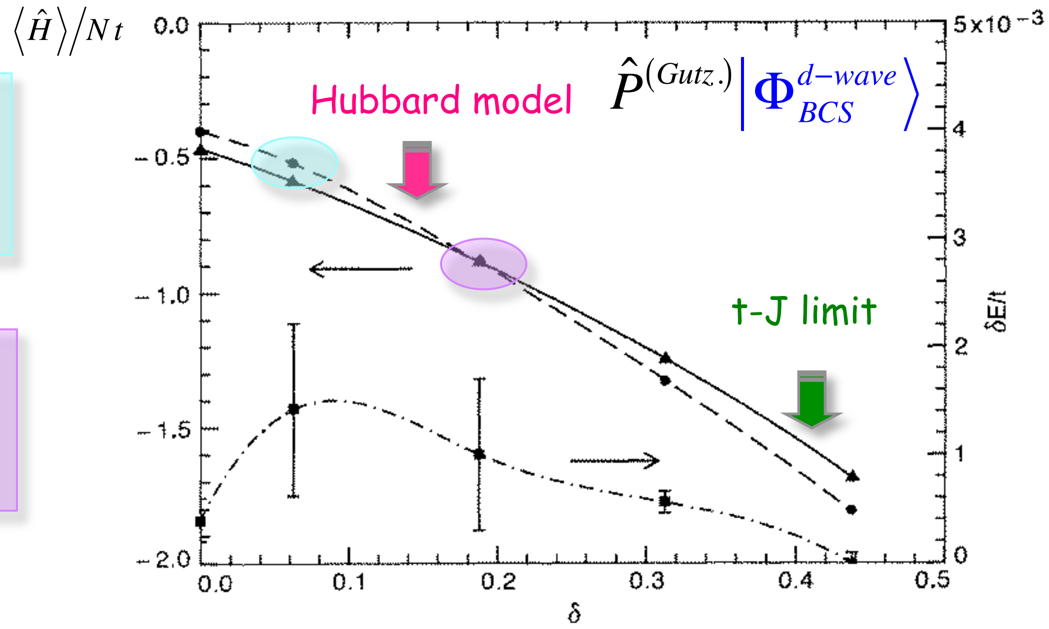
Reliability of the symmetry projected HF/BCS scheme

Comparison with the Gutzwiller wavefunction

8x8 lattice – U=10t

$$\left\langle \hat{H} \right\rangle^{(\Gamma)}_{HF-BCS} \Big/ N \sim \begin{cases} -0.525 \\ -0.536 \;\; (S=0) \end{cases}$$

$$\left\langle \hat{H} \right\rangle^{(\Gamma)}_{HF-BCS} \Big/ N \sim \begin{cases} -0.826 \\ -0.829 \;\; (S=0) \end{cases}$$



T. Giamarchi & C. Lhuillier, Phys. Rev. B. (1991)

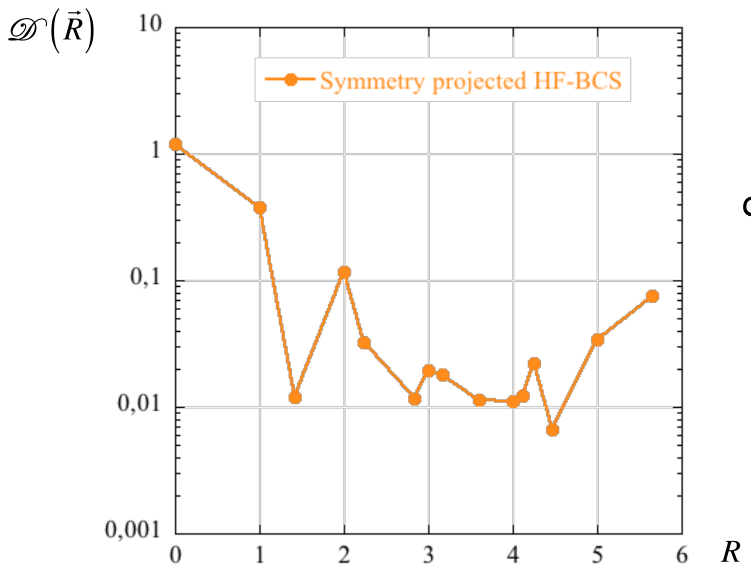
Reliability of the symmetry projected HF/BCS scheme

Comparison with quantum number projection on QMC and Gutzwiller wavefunctions

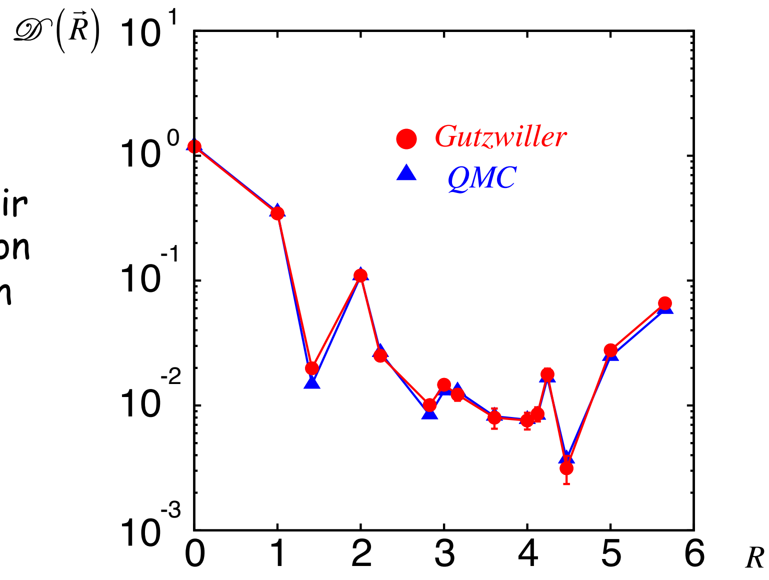
8x8 lattice - U=4t - N=50 electrons

$$\left\langle \hat{H} \right\rangle^{(\Gamma)}_{HF-BCS} \sim \begin{cases} -69.87\ t \\ -70.13\ t\ \left(S=0\right) \end{cases}$$

$$\left\langle \hat{H} \right\rangle^{(\Gamma)}_{Gutzwiller} = -71.4t, \quad \left\langle \hat{H} \right\rangle^{(\Gamma)}_{QMC} = -72.5t$$



d-wave pair correlation function



T. Misawa, M. Imada, arxiv/cond-mat (2013)

Energy improvements on the symmetry projected HF/BCS scheme

$$\left|\Psi_0^{(\Gamma)}\right\rangle \to \left|\Phi_{HF-BCS}^{(\Gamma)}\right\rangle = \hat{P}^{(\Gamma)} \left(\sum_{i=1}^{\mathcal{N}_{HF}} c_{HF}^{(i)} \left|\Phi_{HF}^{(i)}\right\rangle + \sum_{i=1}^{\mathcal{N}_{BCS}} c_{BCS}^{(i)} \left|\Phi_{BCS}^{(i)}\right\rangle \right)$$

- Full symmetry restoration during the optimization $\Gamma = \left(N, \vec{K}, S, S_z, \cdots\right)$
- Mixture of unrestricted and restricted HF/BCS wave functions

States with good quantum number S_z

$$\begin{cases} \left|\Phi_{HF}\right\rangle = \left|\Phi\right\rangle_{\uparrow} \left|\Phi\right\rangle_{\downarrow} \\ \left|\Phi_{BCS}\right\rangle \propto \exp\left(\sum_{\vec{r},\vec{r}'} A_{\vec{r},\vec{r}'} \hat{c}^{+}_{\vec{r}\uparrow} \hat{c}^{+}_{\vec{r}'\downarrow} \right) \left| \, \right\rangle \end{cases}$$

- Sequential optimization

16x4 lattice – U=12t - N=56 electrons

$\mathcal{N}_{HF}$	$\mathcal{N}_{BCS}$	**Simultaneous optimization**	**S=0 projection during the energy minimization**	$\dfrac{\left\langle \hat{H} \right\rangle_{HF-BCS}^{(\Gamma)} - E_{HF}}{\left\| E_{HF} \right\|}$
1	1	YES	NO	~ -10.48 %
101	20	NO	YES	~ -17.13 %
40	0	NO	YES	~ -14.96 %

R. Rodríguez-Guzmán, C. Jiménez-Hoyos, G. Scuséria, arxiv/cond_mat (2014)

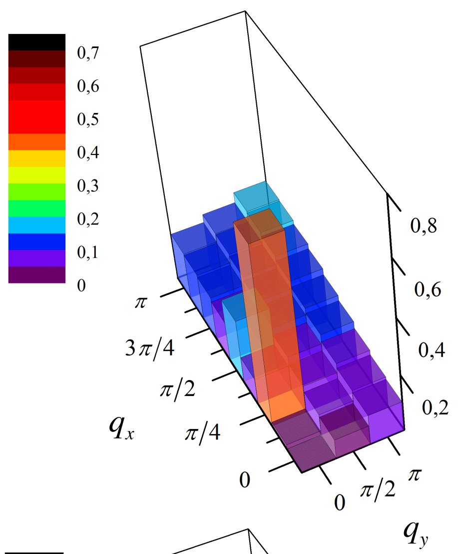
Energy improvements on the symmetry projected HF/BCS scheme

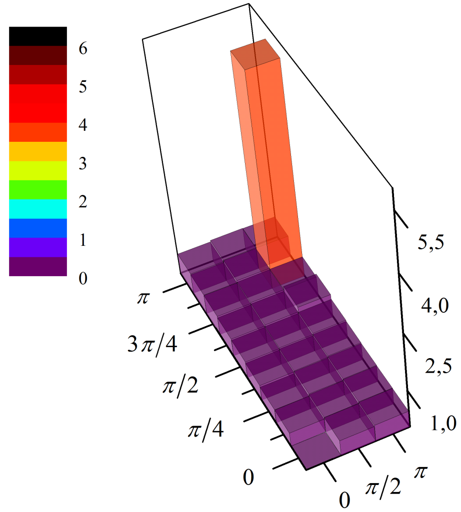
$$C(\vec{q})=\sum_{\vec{r}}\exp(i\vec{q}\cdot\vec{r})\,\langle\delta\hat{n}_{\vec{0}}\;\delta\hat{n}_{\vec{r}}\rangle$$

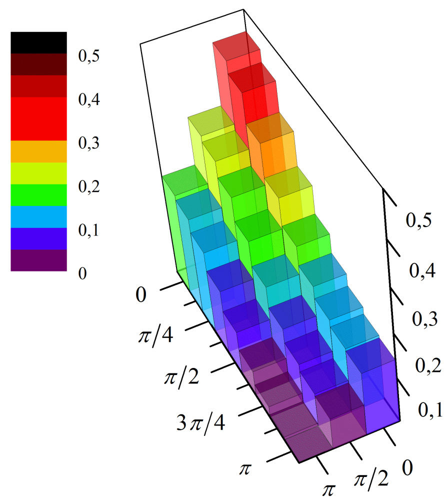
$$S(\vec{q})=\sum_{\vec{r}}\exp(i\vec{q}\cdot\vec{r})\langle\hat{\vec{S}}_{\vec{0}}\cdot\hat{\vec{S}}_{\vec{r}}\rangle$$

$$D(\vec{q})=\sum_{\vec{R}}\exp(i\vec{q}\cdot\vec{R})\;\mathscr{D}(\vec{R})$$

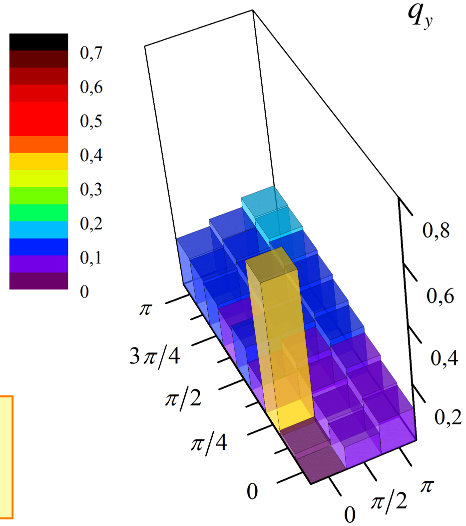
$\begin{cases}\mathscr{N}_{HF}=1\\ \mathscr{N}_{BCS}=1\end{cases}$

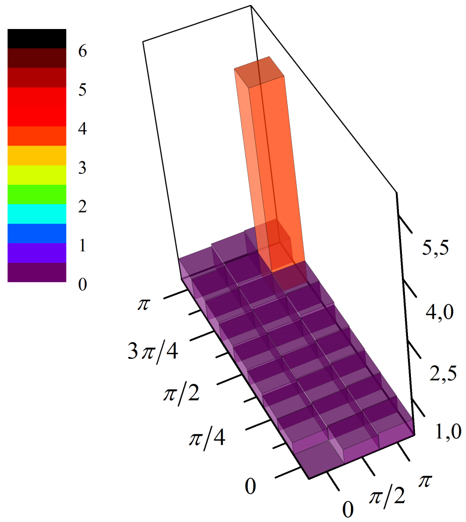


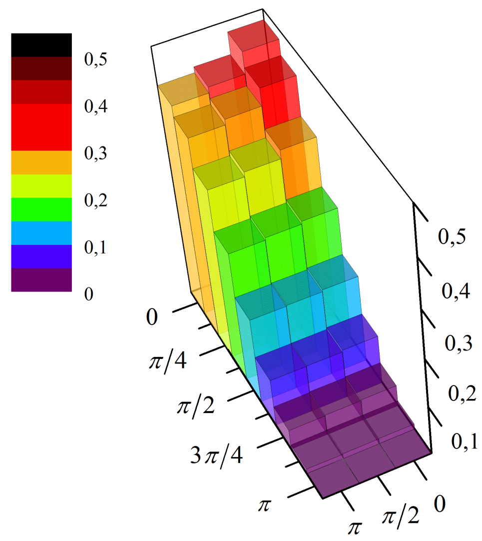




$\begin{cases}\mathscr{N}_{HF}=101\\ \mathscr{N}_{BCS}=20\end{cases}$





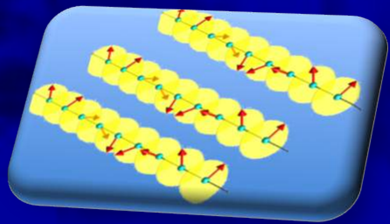


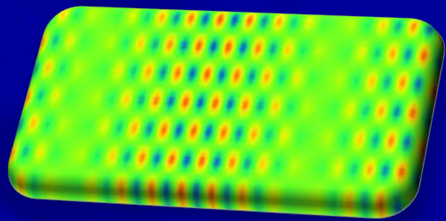
The symmetry projected HF/BCS scheme : new or not ?

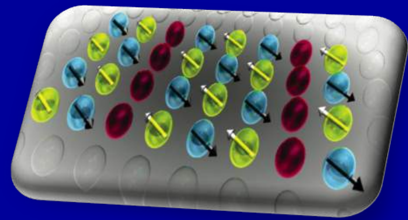
	$\left|\Psi_0^{(\Gamma)}\right\rangle \rightarrow \left|\Phi_{HF}^{(\Gamma)}\right\rangle = \hat{P}^{(\Gamma)} \left(\sum_{i=1}^{\mathcal{N}_{HF}} c_{HF}^{(i)} \left|\Phi_{HF}^{(i)}\right\rangle \right)$	$\left|\Psi_0^{(\Gamma)}\right\rangle \rightarrow \left|\Phi_{BCS}^{(\Gamma)}\right\rangle = \hat{P}^{(\Gamma)} \left(\sum_{i=1}^{\mathcal{N}_{HF}} c_{HF}^{(i)} \left|\Phi_{BCS}^{(i)}\right\rangle \right)$
	(*), (*) : Full symmetry restoration with totally unrestricted wavefunctions	
General features	➢ F. Fukutome, Prog. Theor. Phys. (1988)	➢ K.W. Schmid, F. Grümmer & A. Faessler, Phys. Rev. C (1984) ➢ H. Fukutome, Prog. Theor. Phys. (1991) ➢ J. A. Sheikh & P. Ring, Nucl. Phys. A (2000)
Nuclear shell model	➢ J. Bonnard & O. Juillet, Phys. Rev. Lett. (2013)	➢ K.W. Schmid, Prog. Part. Nucl. Phys. (2004) ➢ I. Maqbool *et al.*, J. Phys. G (2011)
Quantum chemistry	➢ C. Jiménez-Hoyos, R. Rodríguez-Guzmán & G. E. Scuseria, J. Chem. Phys. (2012), arxiv/physics.chem-ph (2014)	➢ G.E Scuseria *et al.*, J. Chem. Phys. (2011)
Hubbard model	<u>1D model</u> ➢ N. Tomita, Phys. Rev. B (2004) ➢ K.W. Schmid *et al.*, Phys. Rev. B (2005) ➢ R. Rodríguez-Guzmán et *al.*, Phys. Rev. B (2013) <u>2D model</u> ➢ N. Tomita & S. Watanabe, Phys. Rev. Lett. (2009) ➢ R. Rodríguez-Guzmán et *al.*, Phys. Rev. B (2012) ➢ O. Juillet & R. Frésard, Phys. Rev. B (2013) ➢ H. Shi *et al.* , Phys. Rev. B (2013 & 2014) ➢ A. Leprévost, O. Juillet & R. Frésard, Ann. der Phys. (2014) ➢ R. Rodríguez-Guzmán et *al.*, arxiv/cond-mat (2014)	

Present work

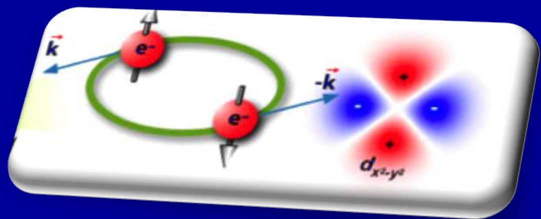
Summary







- Spiral, SDW, stripes find their place in the phase diagram of the 2D Hubbard model.
- They successively appear for decreasing doping at fixed U and for increasing U at fixed doping.



- Coexistence with d-wave superconductivity has been evidenced for long-ranged pairing correlations at strong coupling (U~10t) and up to a hole doping ~0.2, EXCEPT when the holes are totally trapped in stripes.
- These features are robust against extensions of the wavefunction.

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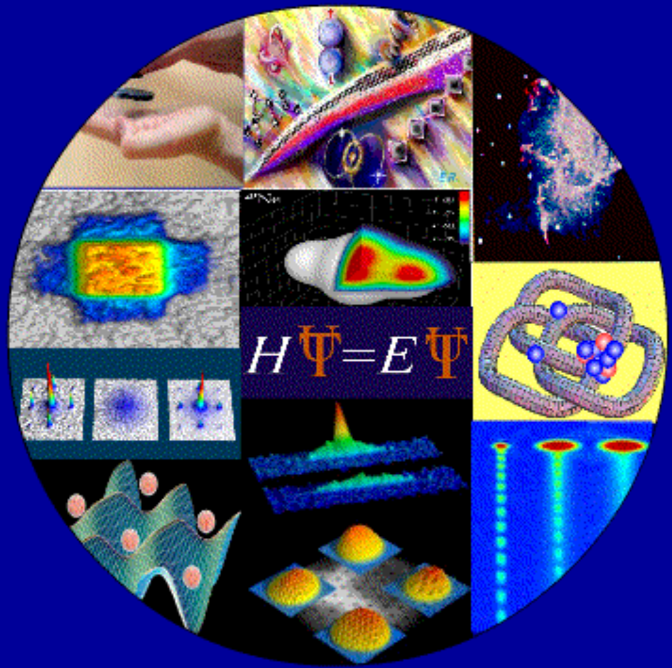
Nordita program - October 2014



Olivier Juillet, Alexandre Leprévost, Raymond Frésard

LPC Caen & CRISMAT