

# Competing phases in dipolar quantum gas

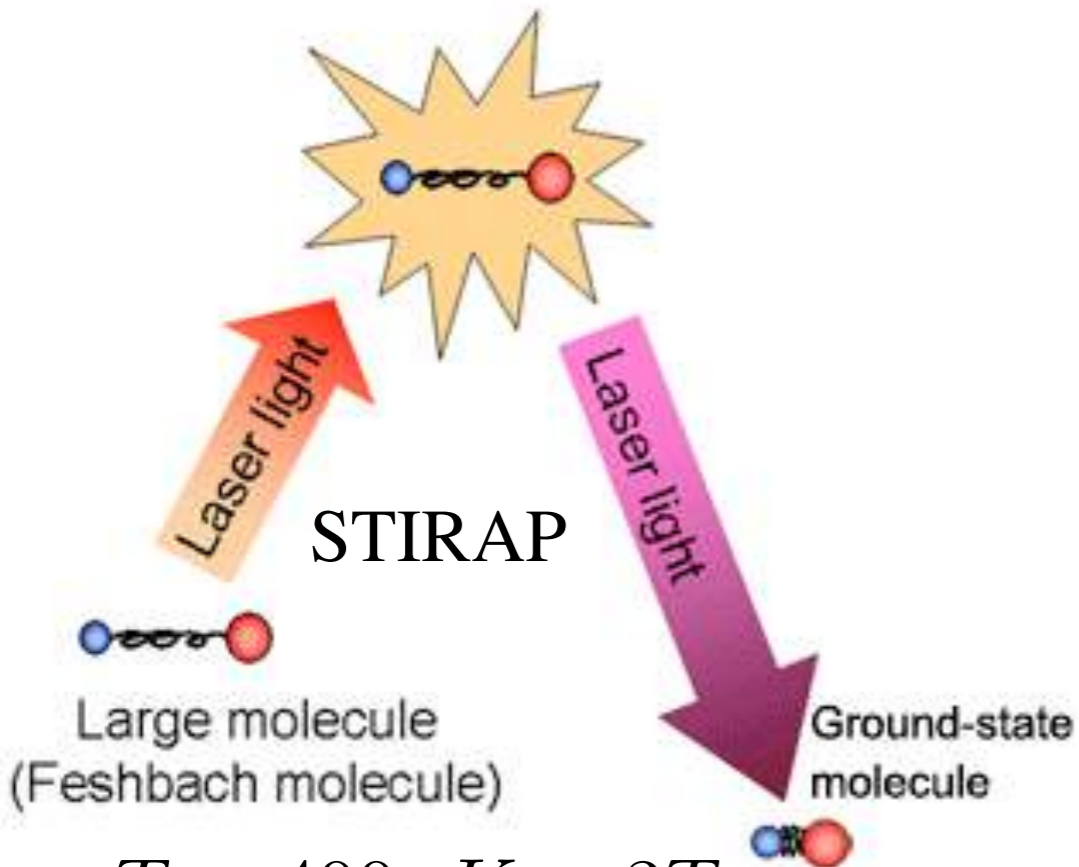
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George Mason University



# Fermi gas of polar molecules: KRb, NaK

## Quantum gas of $^{40}\text{K}^{87}\text{Rb}$



$$T \sim 400\text{nK} \sim 3T_F$$

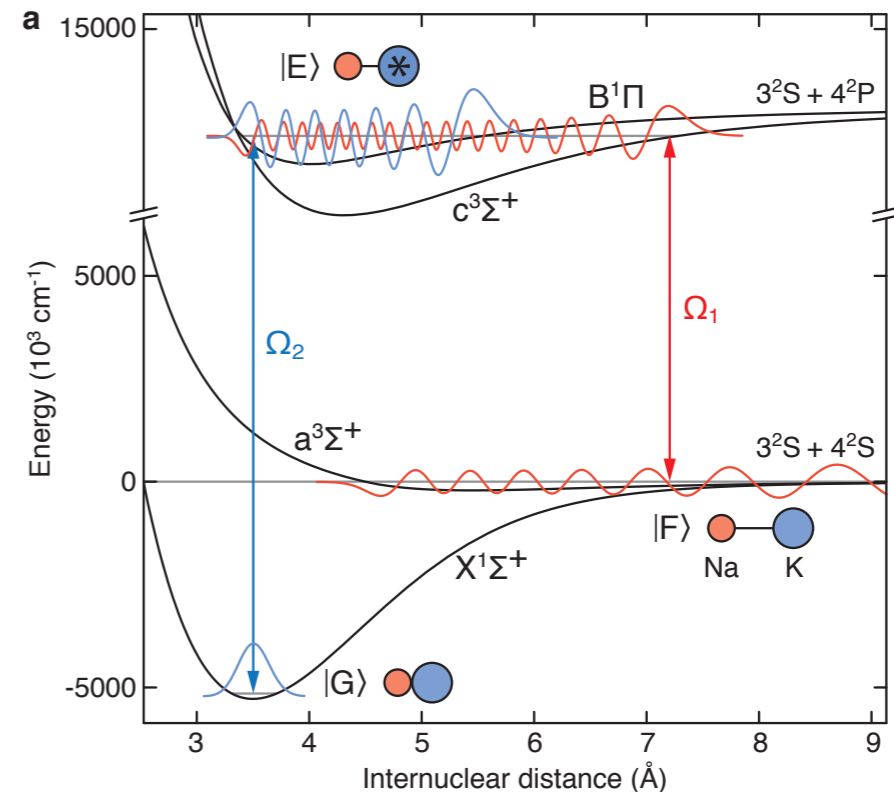
$$d \sim 0.5 \text{ Debye}$$

Ni et al, Science 322, 231-235 (2008)

D. S. Jin and J. Ye, Physics Today 64, 5(2011)

Chotia et al, PRL 108, 080405 (2012)

## Ground state $^{23}\text{Na}^{40}\text{K}$ molecules



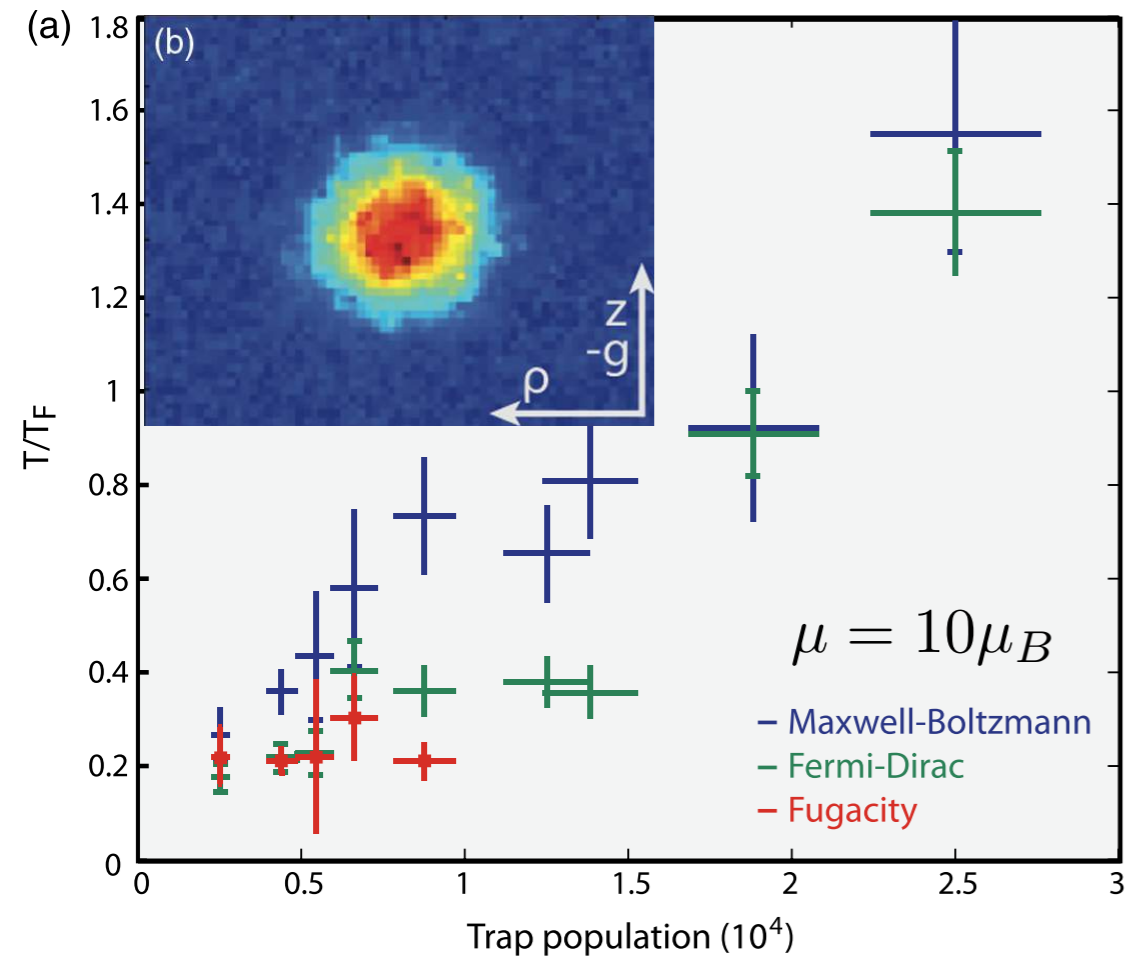
Chemically stable.  $d \sim 0.8$  Debye.  
Life time  $> 2.5\text{s}$ ;  $T \sim 500\text{nK} \sim 2T_F$

Wu et al, PRL 109, 085301 (2012)

Park, Will, Zwierlein, arxiv:1505.00473 (2015)

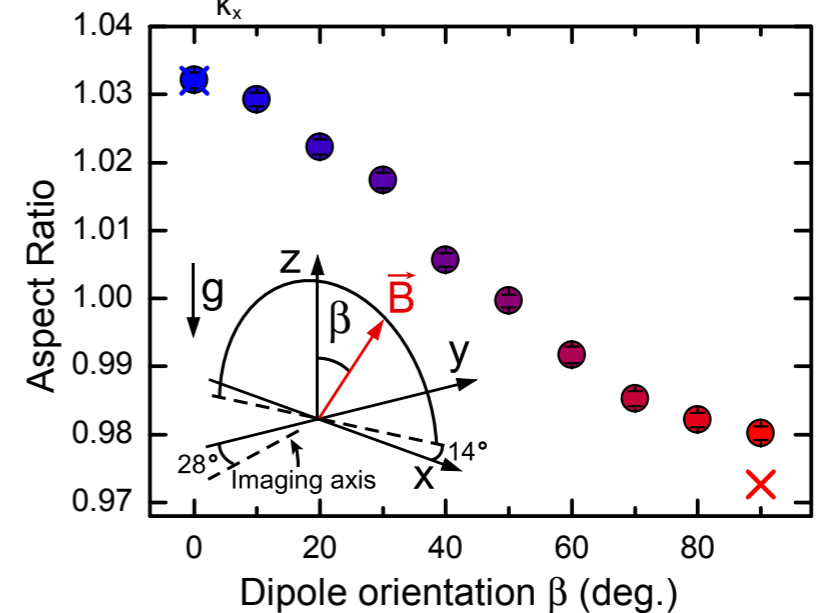
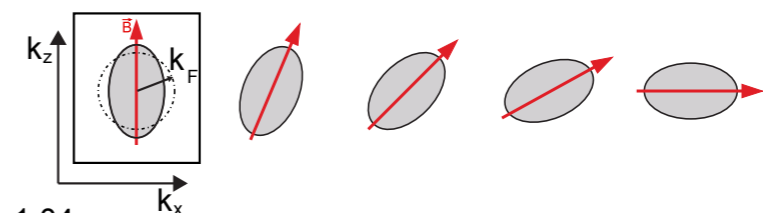
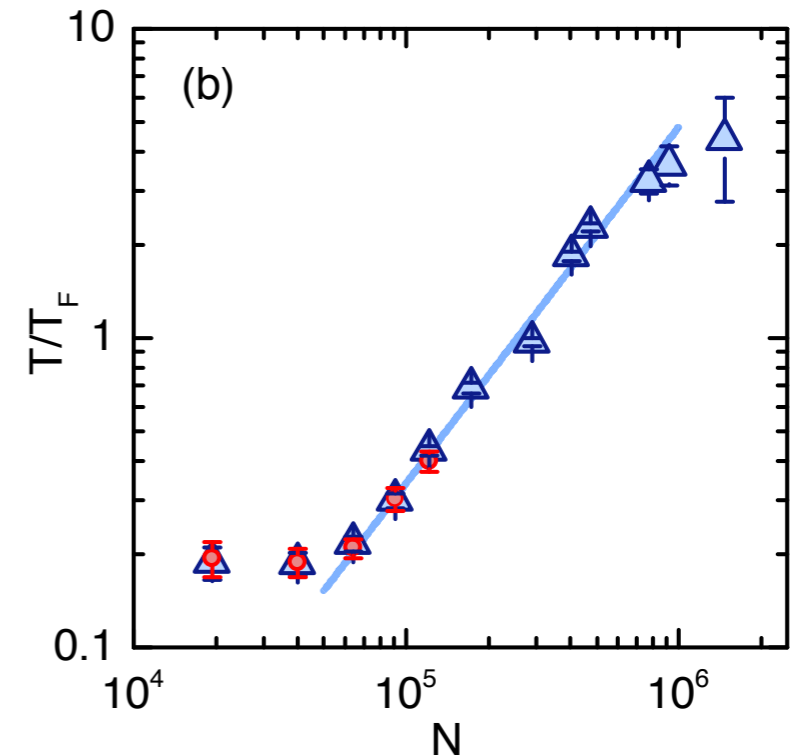
# Degenerate Fermi gas of magnetic atoms: $^{161}\text{Dy}$ , $^{167}\text{Er}$

Sympathetic cooling of  $^{161}\text{Dy}$  with bosonic  $^{162}\text{Dy}$



$$T/T_F = 0.2 \quad T_F = 300 \text{ nK}$$

Lu, Burdick, Lev, PRL 108, 215301 (2012)

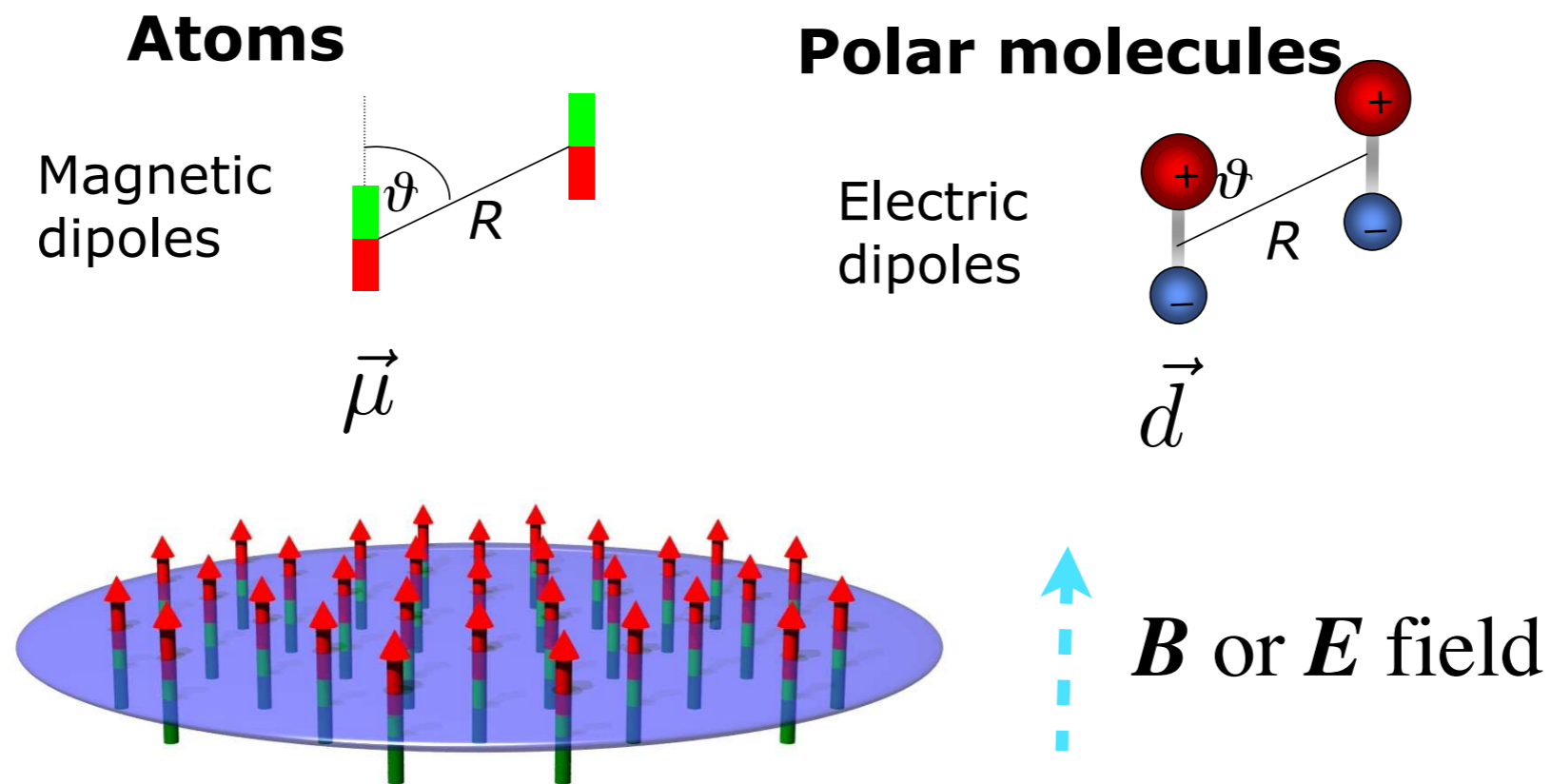


Aikawa et al, PRL 112, 010404 (2014)  
Science 345, 1484 (2014)

# Quantum phases of dipolar fermi gases

**Q:** What are the many-body phases of fermions with dipole-dipole interaction?

Are they all “boring,” i.e., known and understood in condensed matter physics?



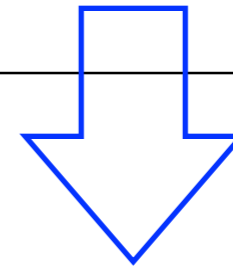
For dipoles pointing in the same direction:

$$V_{dd} = \frac{d^2}{4\pi\epsilon_0} \frac{1 - 3\cos^2\theta}{r^3}$$

—————→  $P_2(\cos\theta)$  *anisotropic*  
—————→ *long-ranged*

# Comparing to other Fermi systems

Fermi System	Interaction	Typical Phases
2D electron gas	Coulomb	Fermi liquid, Wigner crystal
Fermi-Hubbard model	onsite, repulsive	antiferromagnet, <i>d</i> -wave superfluid(?)
2-component Fermi gas	contact, attractive	<i>s</i> -wave superfluid (BCS-BEC crossover)
dipolar Fermi gas	dipole-dipole	



Candidate phases of dipolar fermions:

- ★ anisotropic Fermi liquid
- ★ charge density waves (CDW)
- ★ *p*-wave superfluid
- ★ stripes, quantum liquid crystals?
- ★ supersolid? ...

Baranov et al, Chemical Reviews 112, 5012 (2012); Physics Reports, 464, 71 (2008). Lahaye et al, Rep. Prog. Phys. 72, 126401 (2009), etc.

## Outline of this talk

1. Dipolar Fermi gas on square lattice @ half filling:  
phase diagram from functional renormalization group
2. Continuum gas of dipolar fermions:  
trying to go beyond Hartree-Fock and RPA
3. Frustrated magnetism of localized (deeply trapped) dipoles:  
hints from exact diagonalization on a small lattice

The common theme of the 3 problems is competing order.

Wish: treat (all) orders on the same footing, without a priori bias.

# 1. Dipolar fermions on lattice

*Collaborators:*

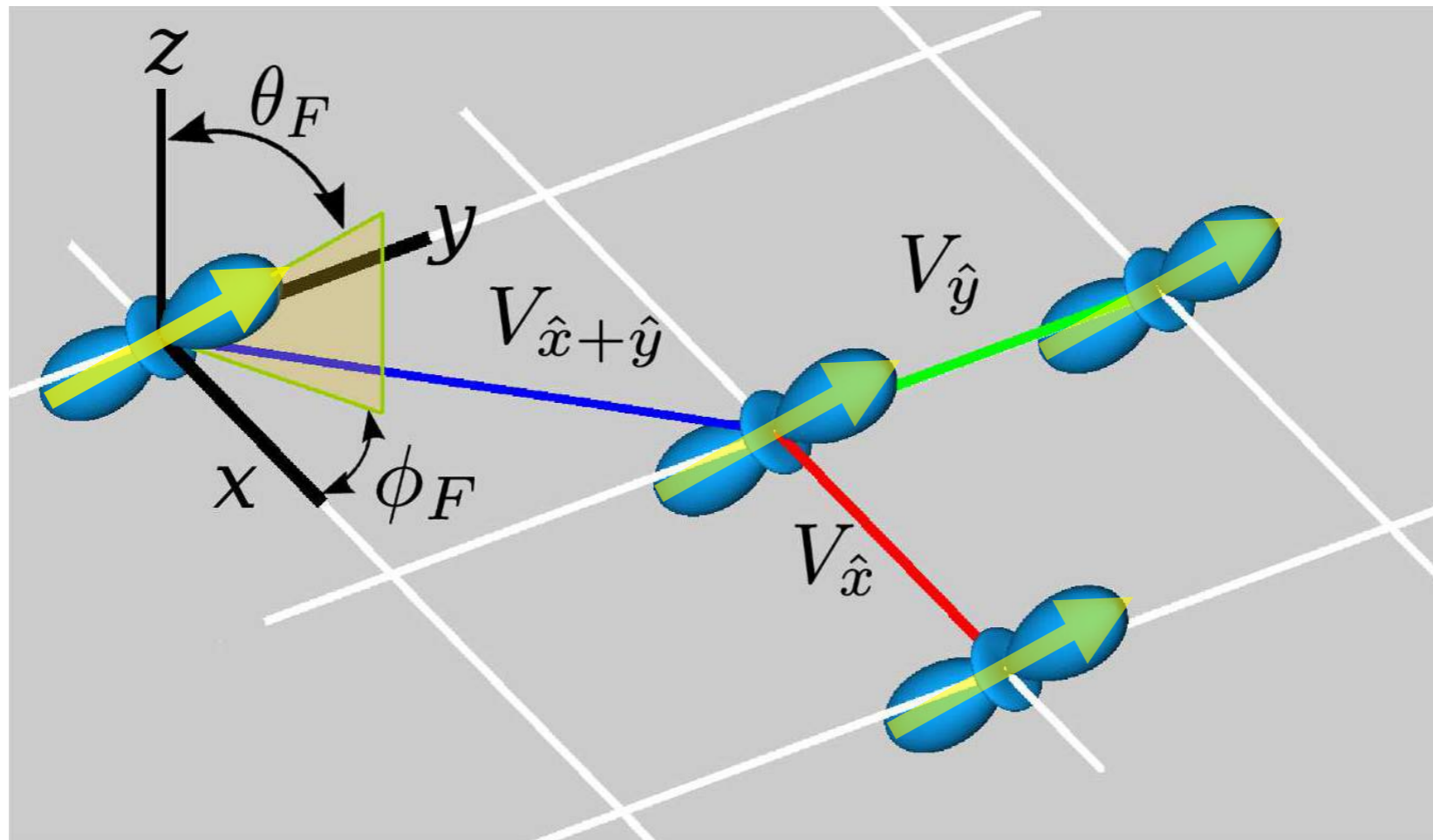
Satyan Bhongale (GMU)

Ludwig Mathey (Hamburg)

Shan-Wen Tsai (UC Riverside)

Charles Clark (NIST/JQI)

# Dipolar fermions on square lattice: model Hamiltonian



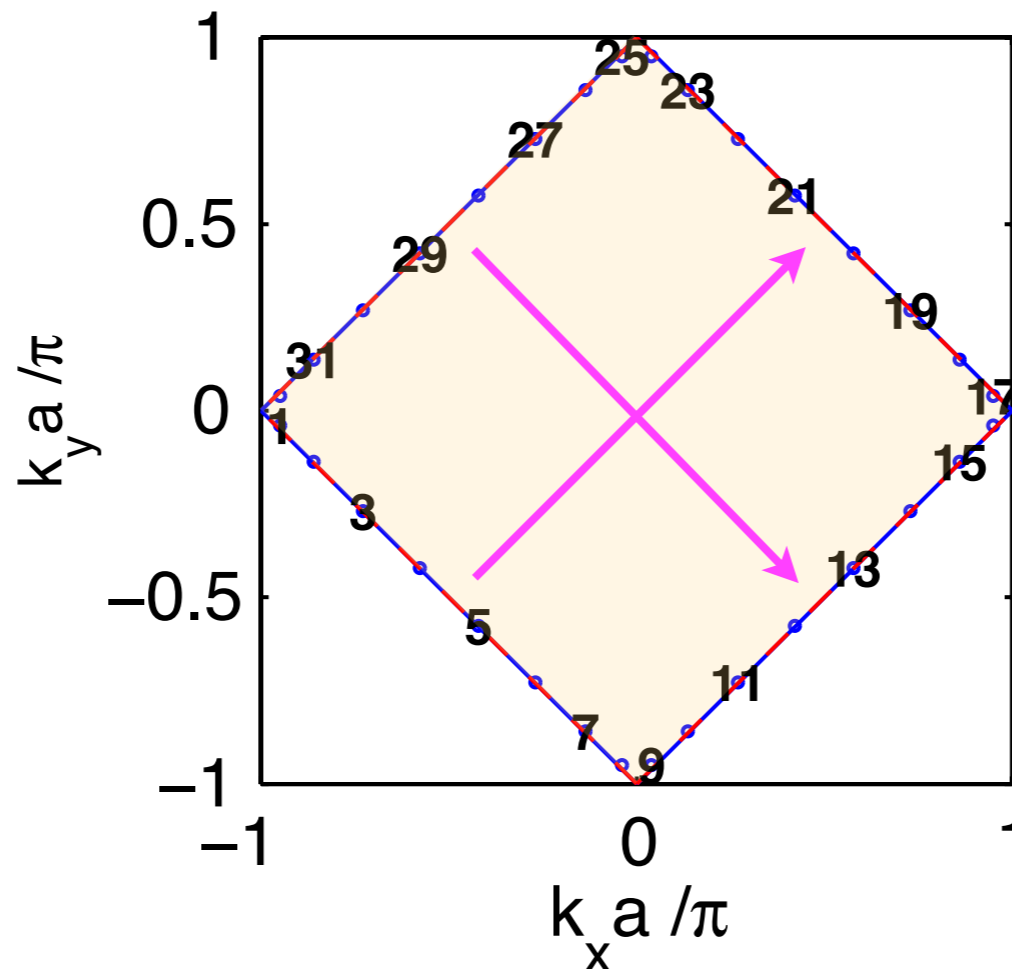
$$H = -t \sum_{\langle ij \rangle} a_i^\dagger a_j + \frac{1}{2} \sum_{i \neq j} V_{dd}(\mathbf{r}_{ij}) n_i n_j,$$

- ★ Half filling: on average, one fermion every two sites.
- ★ Zero temperature; Neglect collapse instability.



# The Fermi surface is just a square (half filling)

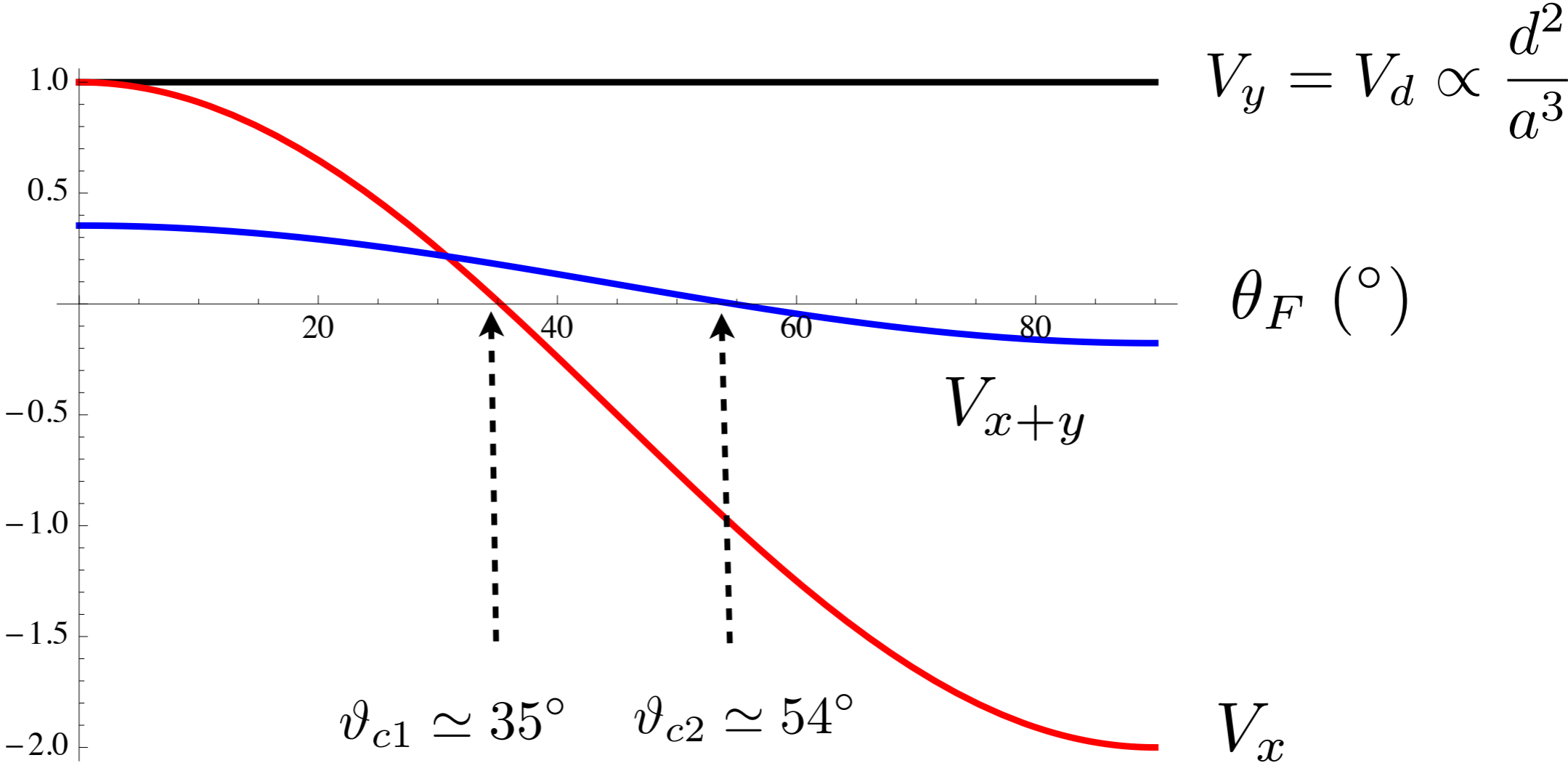
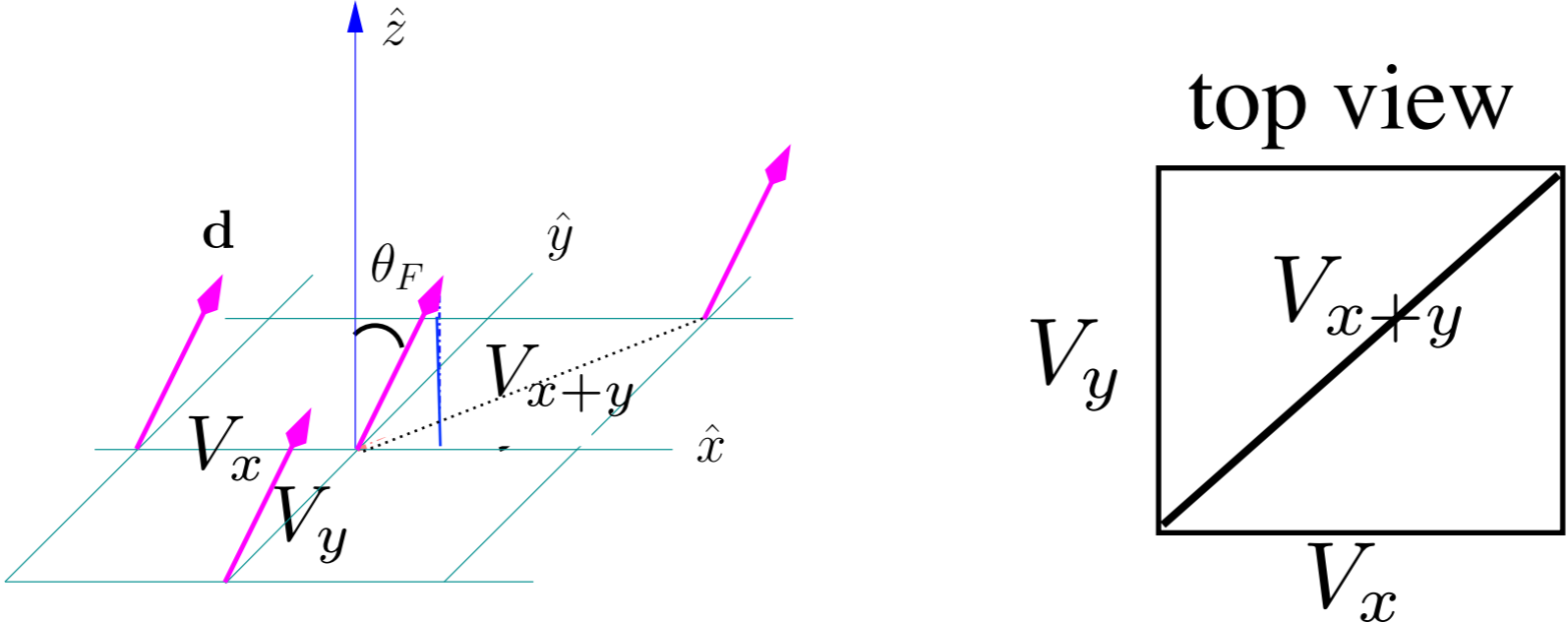
In the absence of dipole-dipole interaction:



$$\mathbf{Q} = (\pi, \pm\pi)$$
$$(a = 1)$$

- ★ Perfect Nesting:  $\mathbf{Q}$  couple  $\mathbf{k}$  points on the opposite sides of the FS.
- ★ We will discretize the Fermi surface into  $N$  patches.
- ★ The Fermi surface may become unstable when  $V_{dd}$  is turned on.

# Interactions for dipoles tilting in the x direction



# Two limits easy to understand

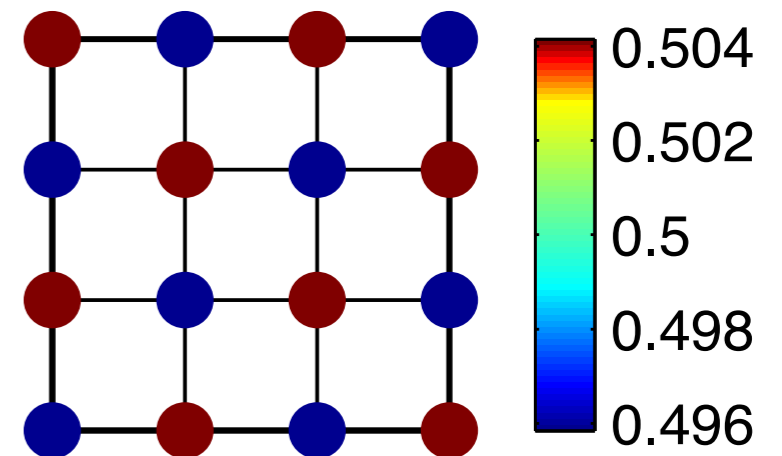
1. Small tilting angle ( $\theta_F < \vartheta_{c1}$ ): all interactions are repulsive.

## Density wave (CDW):

Periodic modulation of on-site density.

$$\langle a_i^\dagger a_i \rangle$$

In  $\mathbf{k}$  space, this is an instability of FS in the particle-hole channel with  $\mathbf{Q}$ .



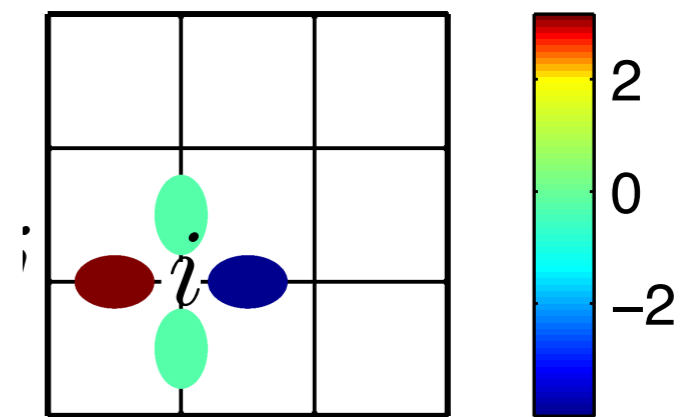
2. Large tilting angle ( $\theta_F > \vartheta_{c2}$ ):  $V_x$  and  $V_{x+y}$  attractive, but  $V_y$  repulsive.

## Anisotropic p-wave pairing (BCS):

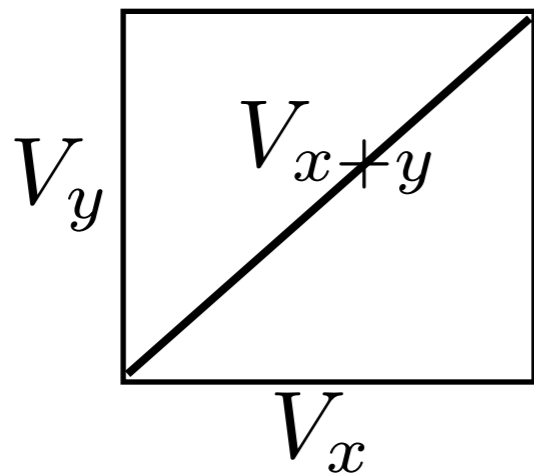
The pairing order parameter

$$\langle a_i a_{i+\hat{x}} \rangle = -\langle a_i a_{i-\hat{x}} \rangle \quad \langle a_i a_{i\pm\hat{y}} \rangle = 0$$

In  $\mathbf{k}$  space, this is an instability of FS in the particle-particle channel.

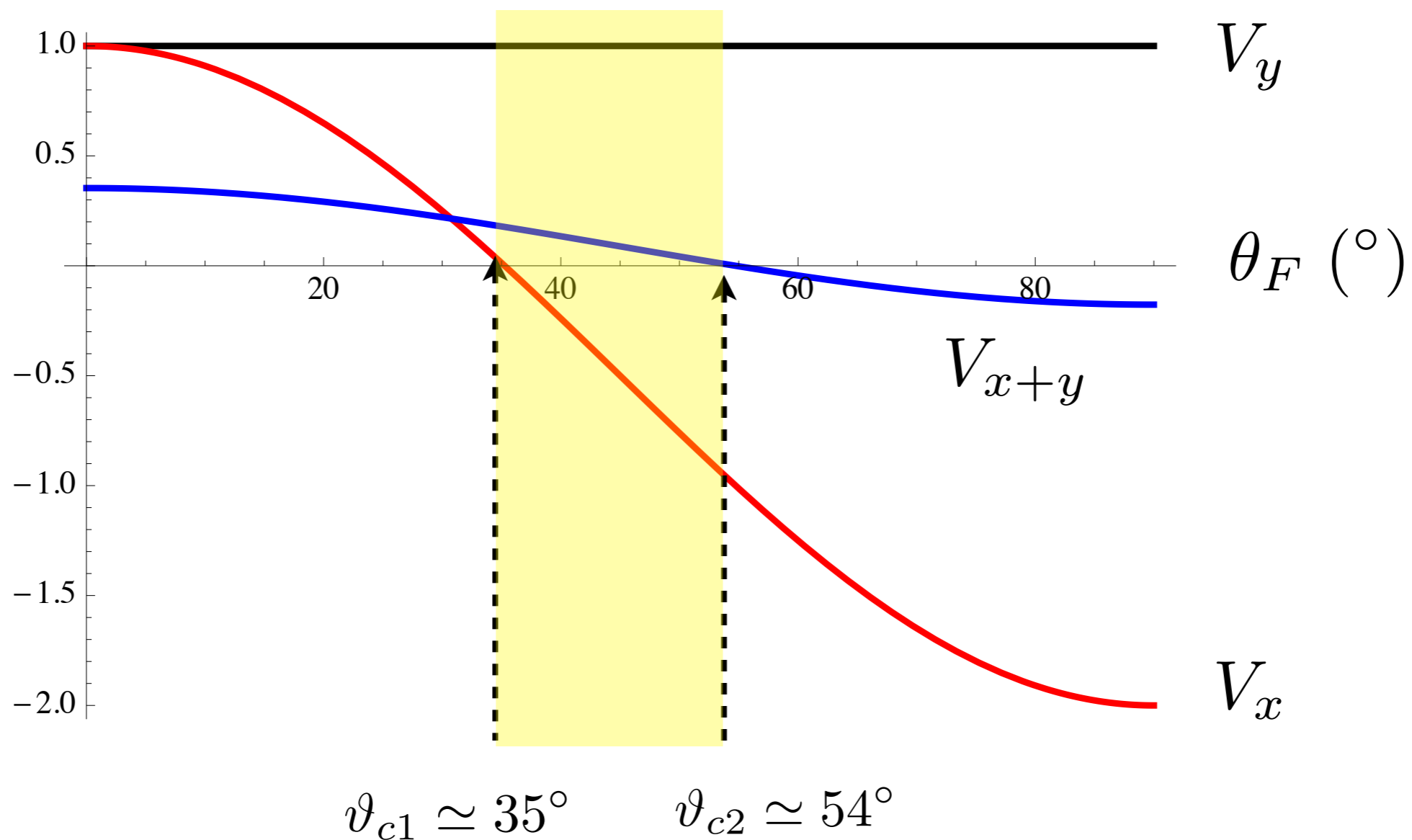


# How about the intermediate tilting angle



$V_x$  and  $V_y$  opposite in sign and comparable in magnitude. What do the fermions do?

Settle to BCS or CDW? Neither? Both?



# Competing orders in interacting dipolar fermions

Three possible scenarios:

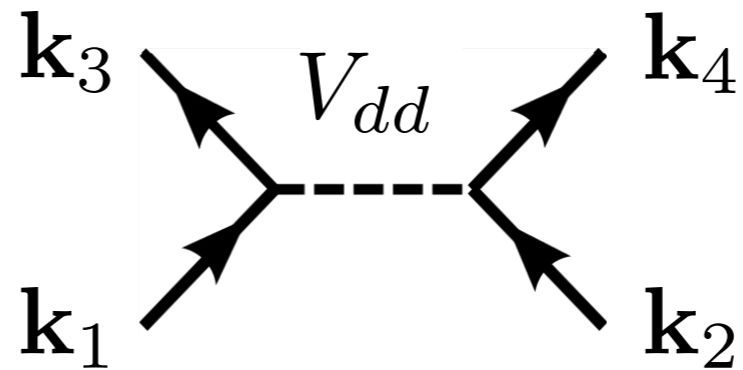
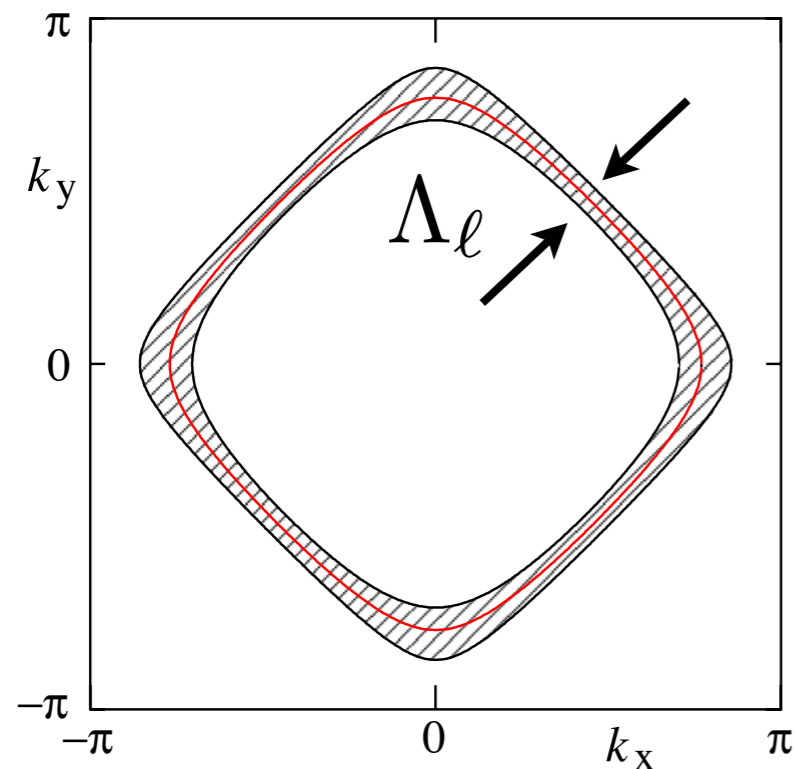
- ★ Direct (1st order) transition from CDW to p-wave BCS superfluid.
- ★ Coexistence: density modulation + pairing = supersolid.
- ★ Or, some other completely different animal.

The problem of competing order is at the heart of the many-body physics of dipolar fermions.

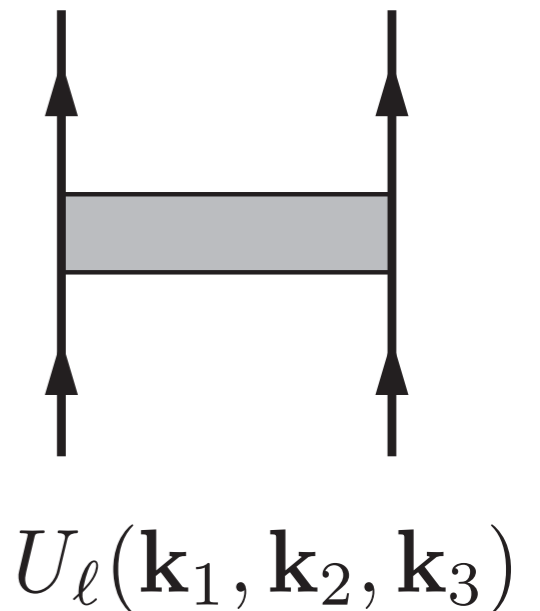
Simple mean field theories or perturbation theories, such as single-channel Renormalization Group or Random Phase Approximation, are insufficient/unreliable to treat competing orders in the regime of intermediate tilting angle.

We need a theory that can **treat all ordering instabilities on equal footing, without any a priori assumptions about dominant orders.**

# Functional Renormalization Group (FRG)



$$\mathbf{k}_4 = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3$$

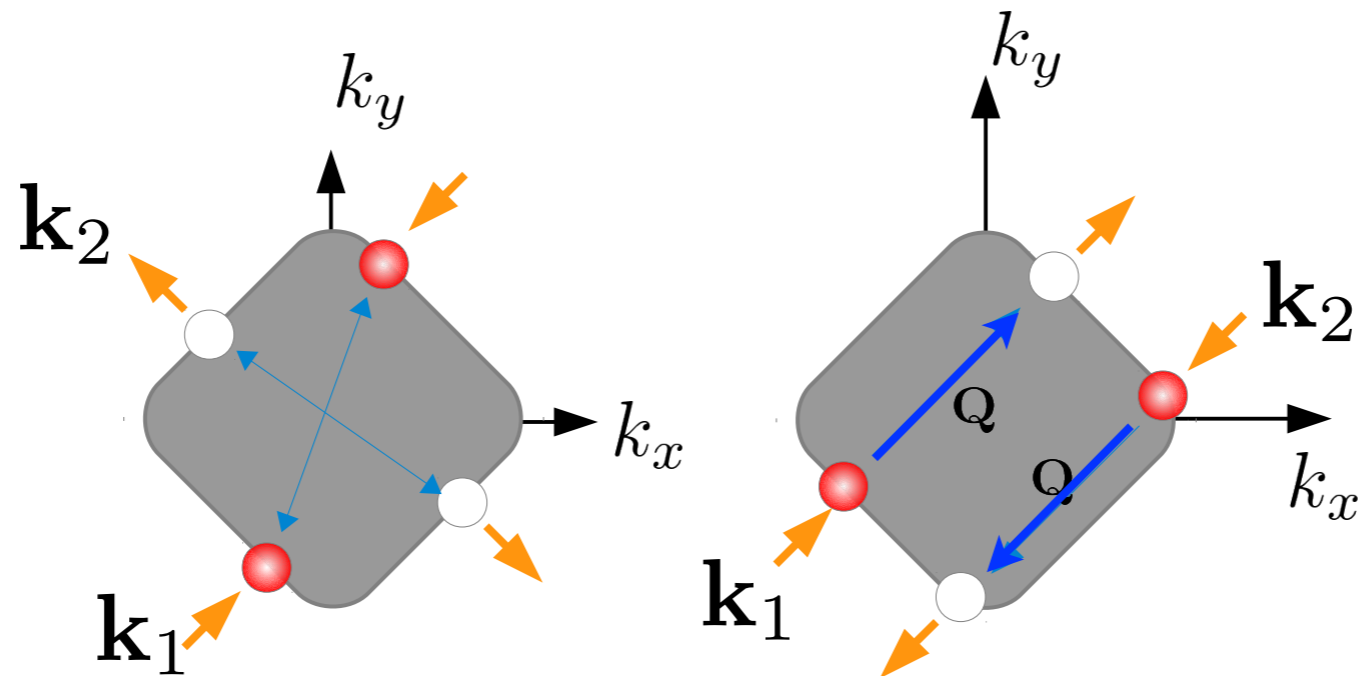


$$U_\ell(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$$

$$\Lambda_\ell = \Lambda_0 e^{-\ell}$$

- ★ Separate the low-energy modes and high energy modes with scale  $\Lambda$ .
- ★ At each scale  $\Lambda$ , there is an effective theory description, including the effective interaction (vertex function)  $U$  between the low energy modes.
- ★ As  $\Lambda$  is reduced, the evolution of  $U$  obeys the exact “flow equation.”
- ★ For weak coupling, the infinite hierarchy of flow eqns can be truncated and solved numerically by discretizing  $\mathbf{k}$ .

# FRG applied to interacting dipolar fermions



$$U_\ell(\mathbf{k}_1, -\mathbf{k}_1, \mathbf{k}_2),$$

BCS Channel

$$U_\ell(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_1 + \mathbf{Q}),$$

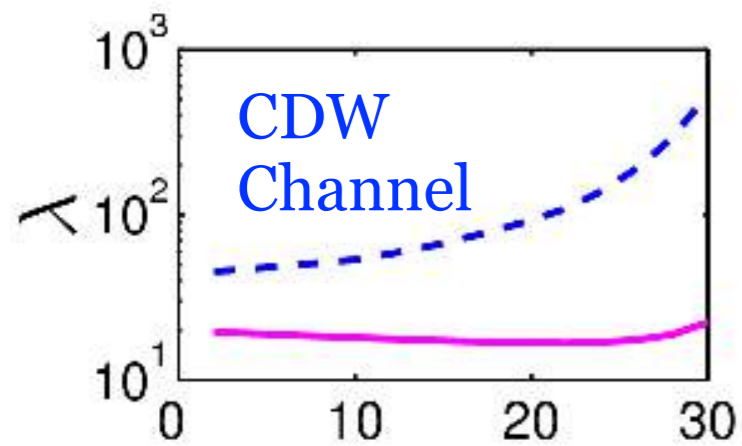
CDW Channel

FRG keeps track of all effective interactions as the high energy modes are traced out, including the p-p and p-h channel, as well as their subtle interplay. Especially, we are interested in the BCS and the CDW channel.

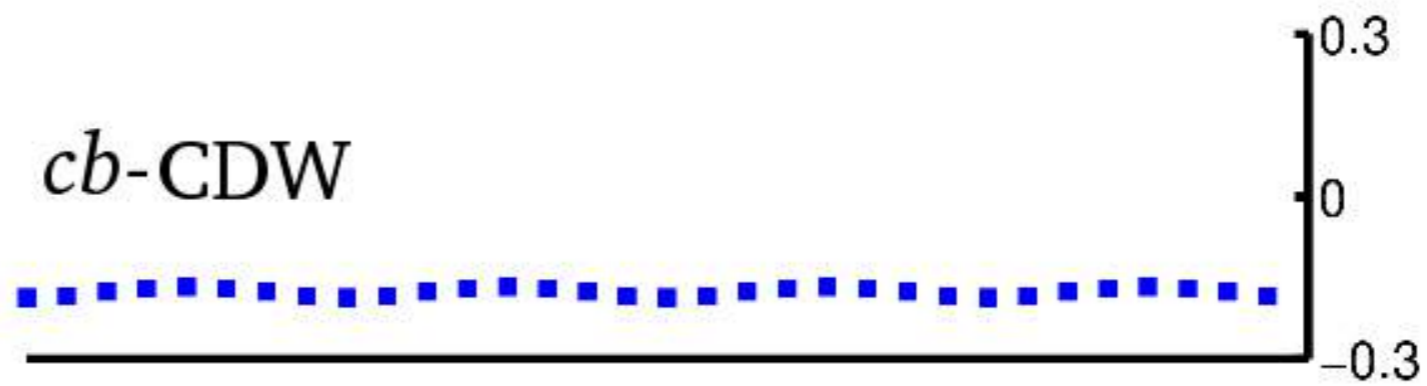
The most dominant instability can be inferred from the most diverging eigenvalue of  $U$ , which is a matrix of  $\mathbf{k}_1$  and  $\mathbf{k}_2$ . The corresponding eigenvector indicates the symmetry of the incipient order.

# Instability analysis within FRG

Eigenvalue

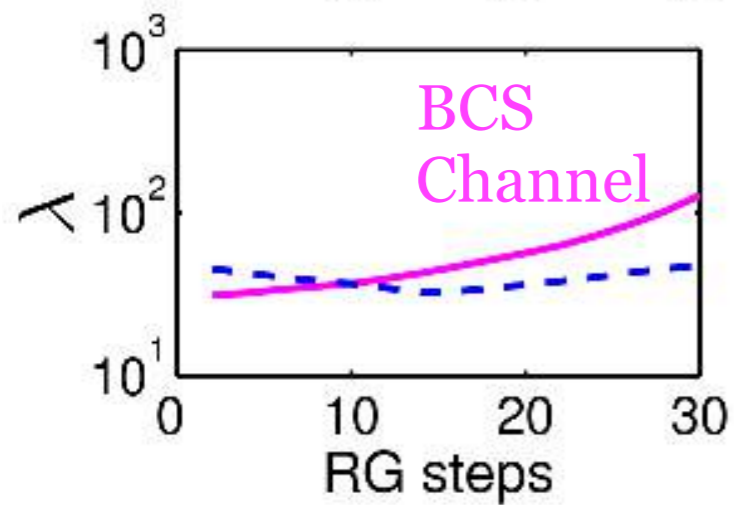


Eigenvector

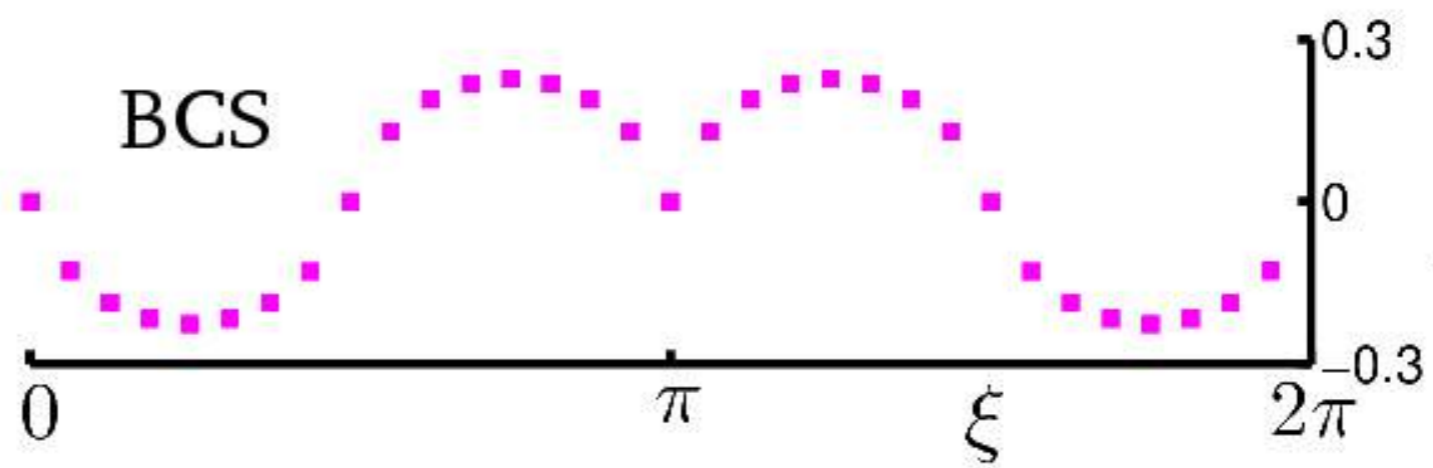


$$\theta_F = 30^\circ$$

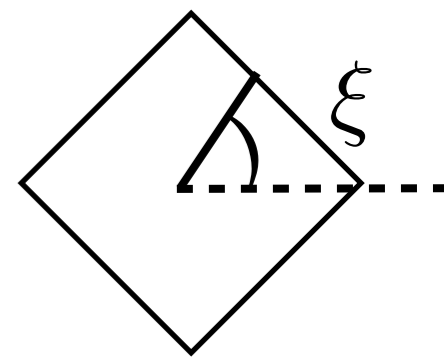
BCS Channel



BCS



$$\theta_F = 70^\circ$$





# Bond order solid (BOS)

Such p-wave instability in the CDW channel corresponds to a spatial modulation of “bonds”, more precisely, the average of hopping

$$\langle a_i^\dagger a_{i+y} \rangle$$

How can such bond order save energy?

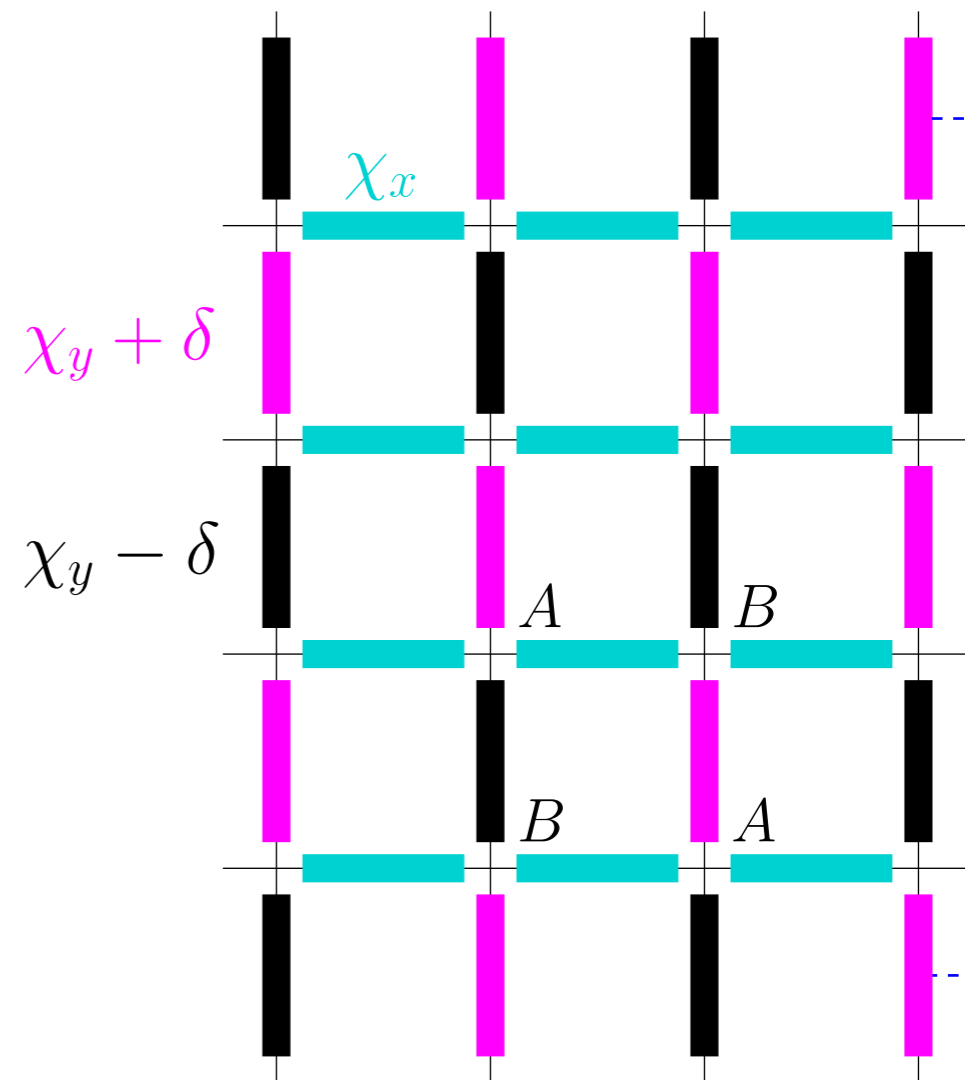
A mean field perspective:

$$n_i n_j = -\boxed{a_i^\dagger a_j a_j^\dagger a_i} + n_i$$

$$\rightarrow a_i^\dagger a_j \rho_{ji} + \rho_{ij} a_j^\dagger a_i - |\rho_{ij}|^2.$$

with  $\rho_{ij} = \langle a_i^\dagger a_j \rangle$

$$\rho_{i, i \pm \hat{x}} = \chi_x, \rho_{i, i \pm \hat{y}} = \chi_y \pm \delta$$

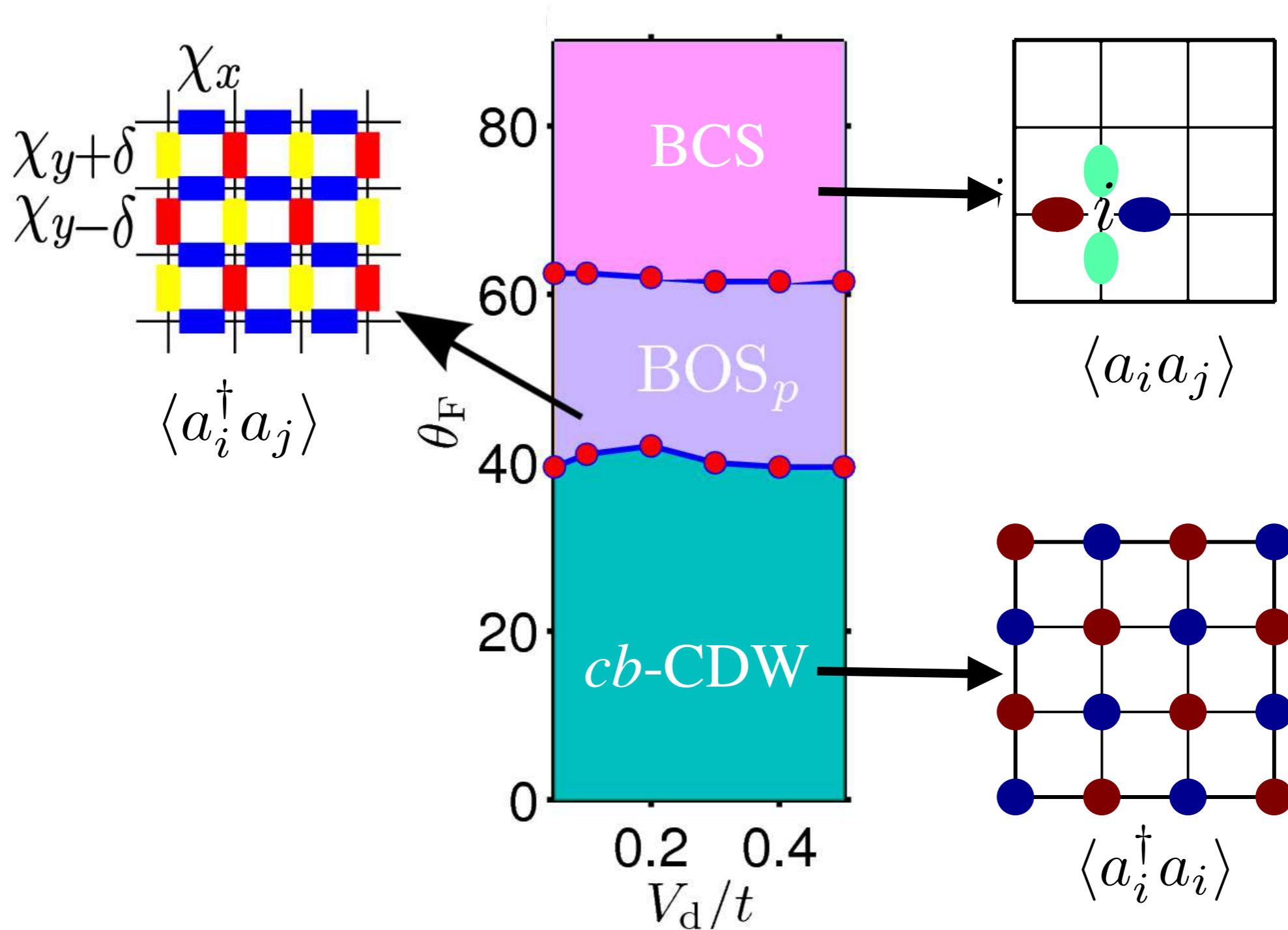


★ Opening up a gap at the Fermi surface.

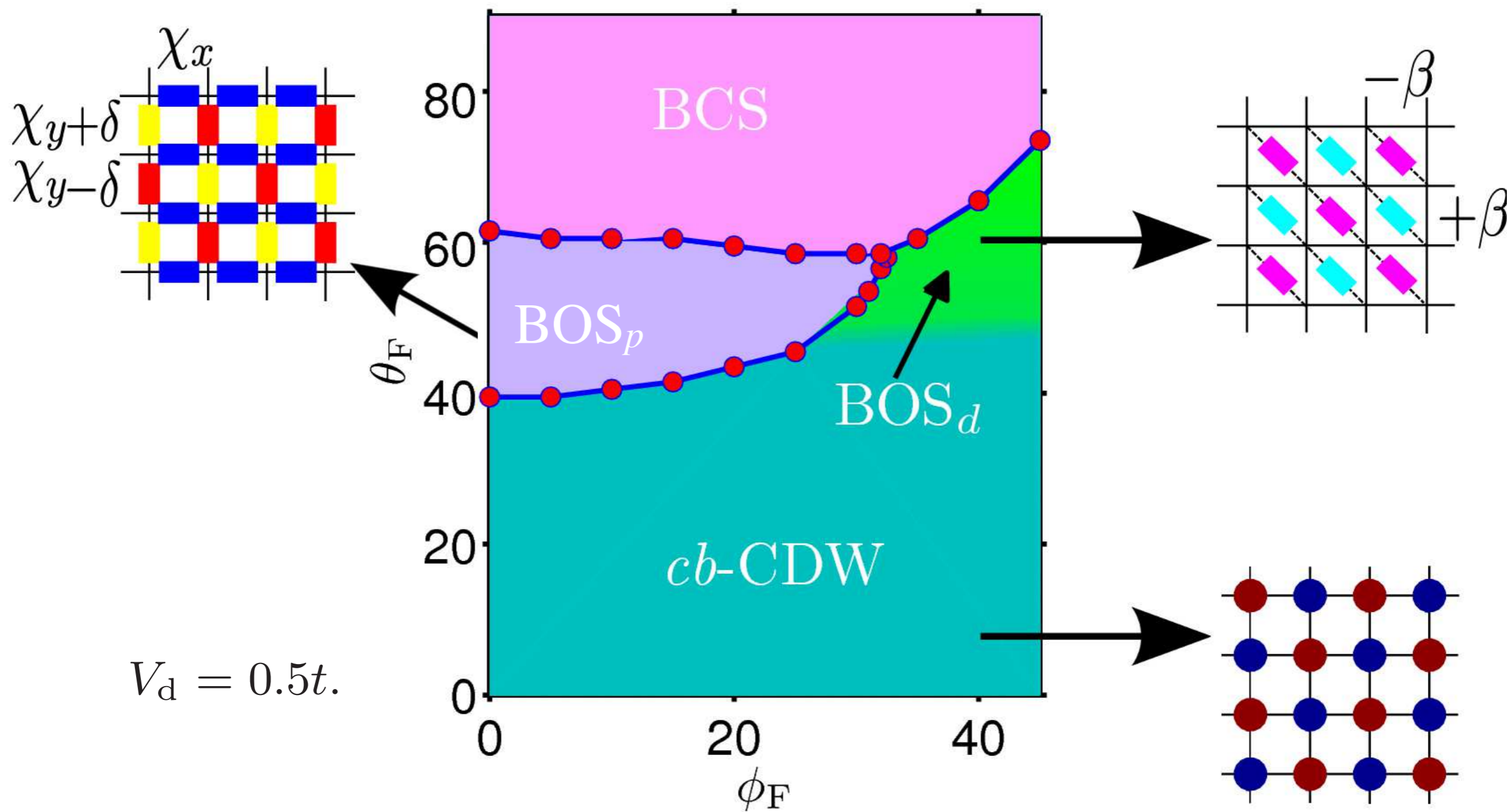
★ Ground state energy:  $E_{\text{GS}} = -2(\chi_x + \chi_y)(t + V_x + V_y) - 2V_y \delta^2$

finite bond modulation  $\delta$  is energetically favored

# Phase diagram ( $T=0$ , half-filling, $\phi_F=0$ )



# Phase diagram for general dipole tilting



# Classification of density waves

Superconductors (condensate of Cooper pairs):

$$\langle f_\alpha(\mathbf{k}) f_\beta(-\mathbf{k}) \rangle = \begin{cases} \Delta(\mathbf{k}) \cdot (i\sigma_y)_{\alpha\beta} & \text{spin singlet, } l=0,2,.. \\ \mathbf{\Delta}(\mathbf{k}) \cdot (\boldsymbol{\sigma} i\sigma_y)_{\alpha\beta} & \text{spin triplet, } l=1,3,.. \end{cases}$$

s-wave superconductor,  $l=0$

p-wave superconductors,  $l=1$

d-wave superconductors,  $l=2$

.....

Density waves (condensate of particle-hole pairs):

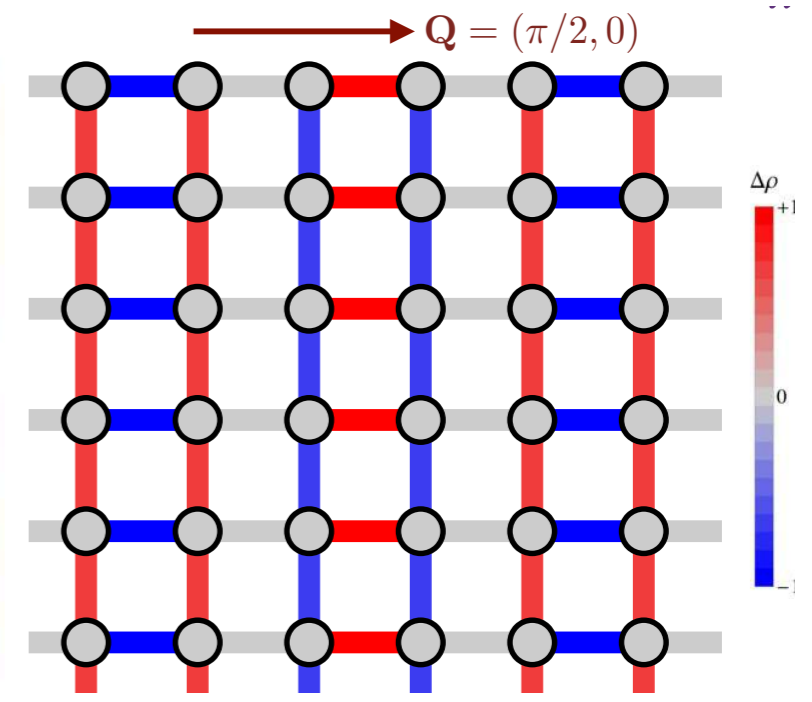
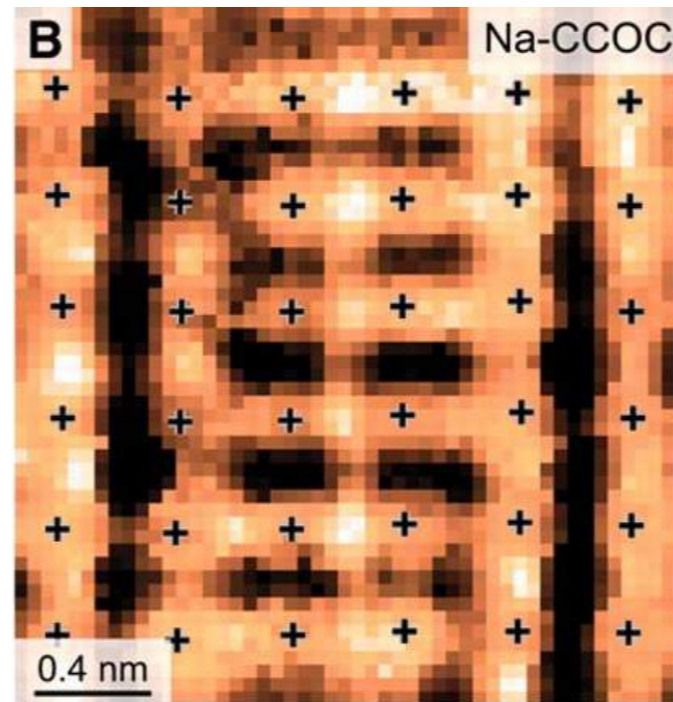
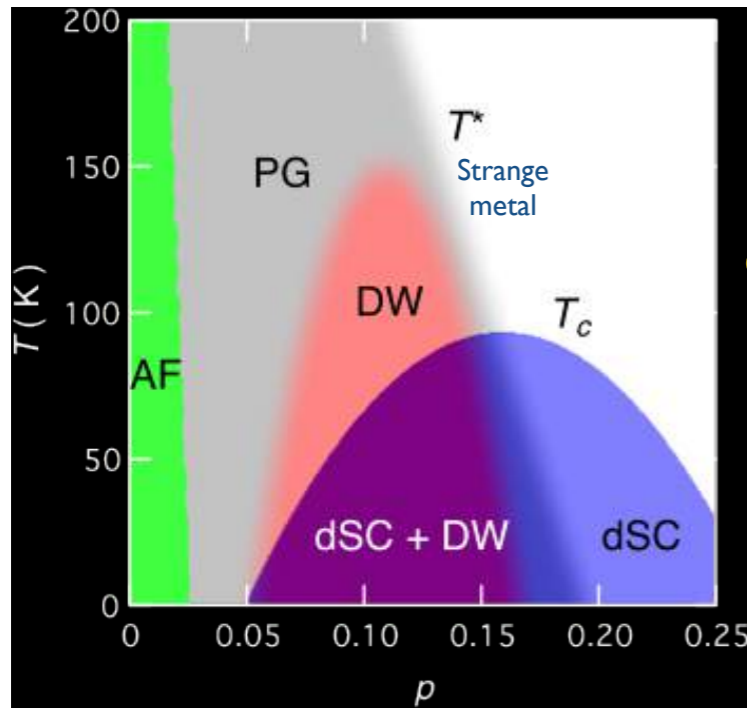
$$\langle f_\alpha^\dagger(\mathbf{k} + \mathbf{Q}) f_\beta(+\mathbf{k}) \rangle = \Phi(\mathbf{k}) \delta_{\alpha\beta} \begin{cases} \text{s-wave CDW (checkerboard)} \\ \text{p-wave CDW} \\ \text{d-wave CDW (DDW) ...} \end{cases}$$

$$\langle f_\alpha^\dagger(\mathbf{k} + \mathbf{Q}) f_\beta(+\mathbf{k}) \rangle = \Phi(\mathbf{k}) \cdot \boldsymbol{\sigma}_{\alpha\beta} \begin{cases} \text{s-wave SDW (~Neel order)} \\ \text{p-wave SDW...} \end{cases}$$

Density-wave states of nonzero angular momentum,  
Chetan Nayak, Phys. Rev. B 62, 4880 (2000)

They show up in dipolar  
Fermi gas!

# Observation of d-wave density waves?



## Observation of d-form factor density waves (in BSCCO and Na-CCOC)

Experiments: Kohsaka et al, Science 315, 1380 (2007). Fujita et al, PNAS 111, E3026 (2014).

Theory: Metlitski & Sachdev, PRB 82, 075128 (2010); PRL 111, 027202 (2013); etc.

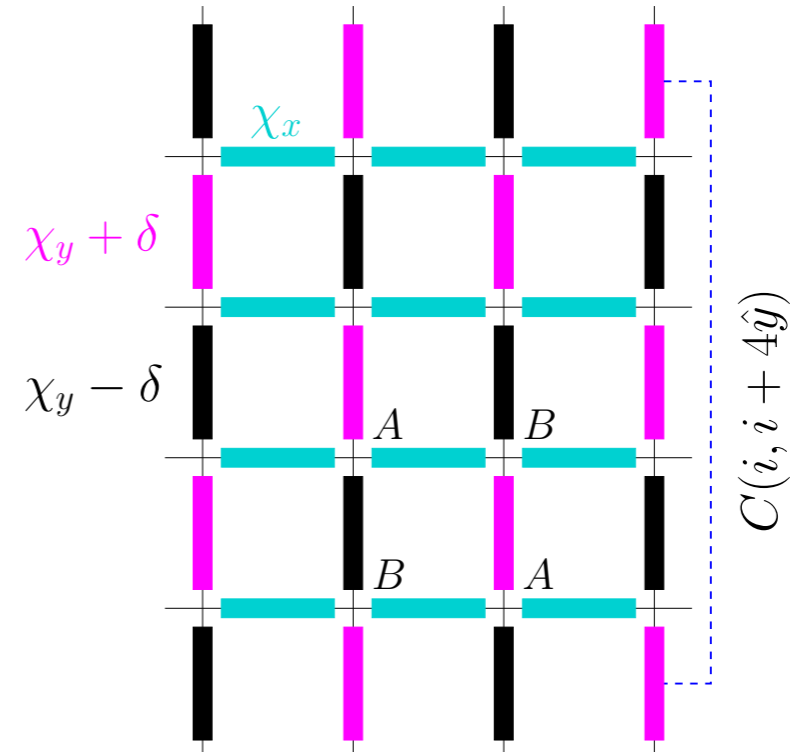
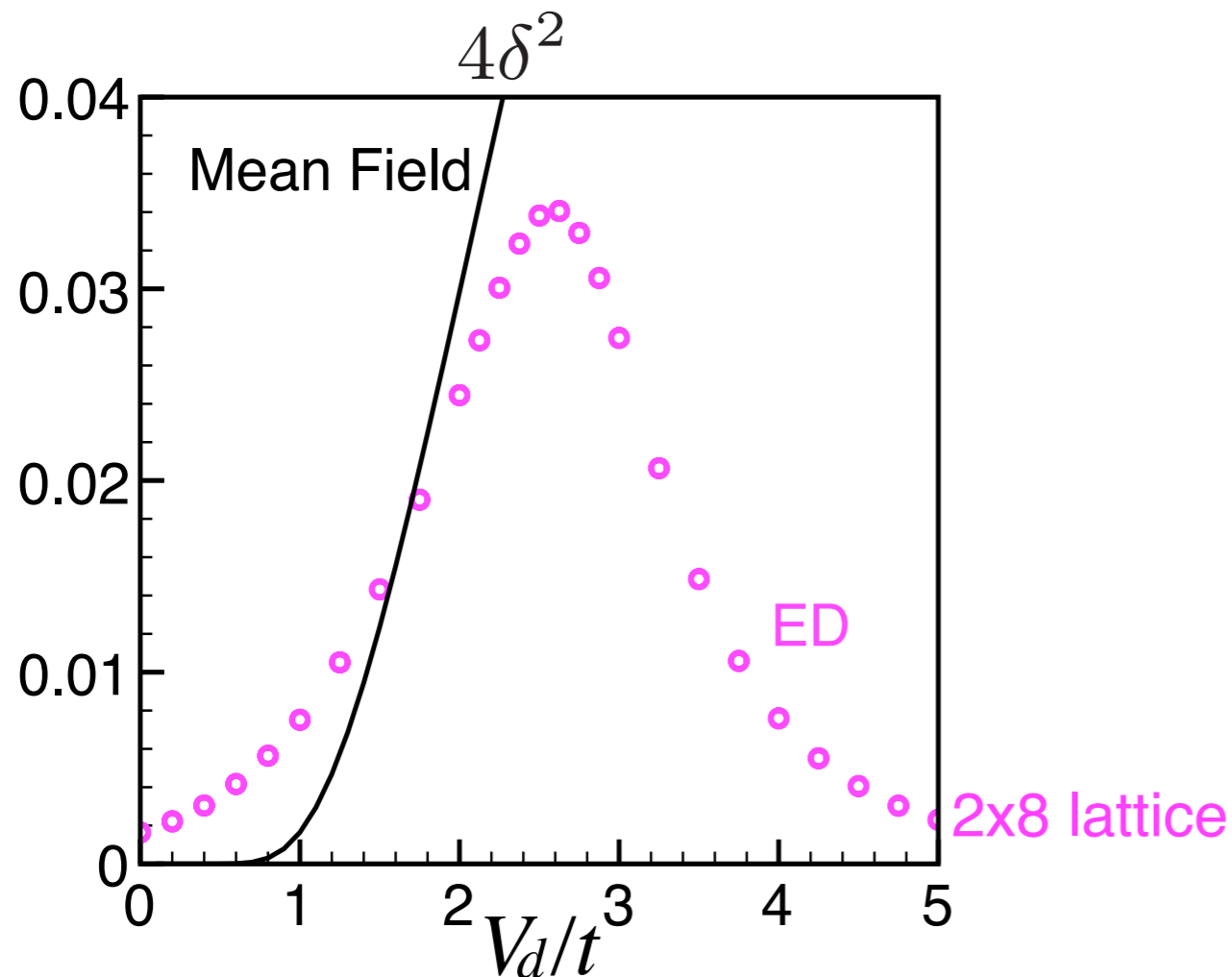
$$P_{ij} = \langle c_{i\alpha}^\dagger c_{j\alpha} \rangle \text{ for } i = j, \text{ and } i, j \text{ nearest neighbors.}$$

$$P_{ij} = \left[ \int_{\mathbf{k}} \mathcal{P}(\mathbf{k}) e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right] e^{i\mathbf{Q} \cdot (\mathbf{r}_i + \mathbf{r}_j)/2} + \text{c.c.}$$

$$\mathcal{P}(\mathbf{k}) = e^{i\phi} [\cos(k_x) - \cos(k_y)] \quad \text{and} \quad \mathbf{Q} = 2\pi(1/4, 0)$$

# Beyond weak coupling

Bond order is most robust for intermediate interaction,  $V_d \sim 2.5t$ , where the mean field gap is  $0.23t$ , or  $0.05 E_F$ .

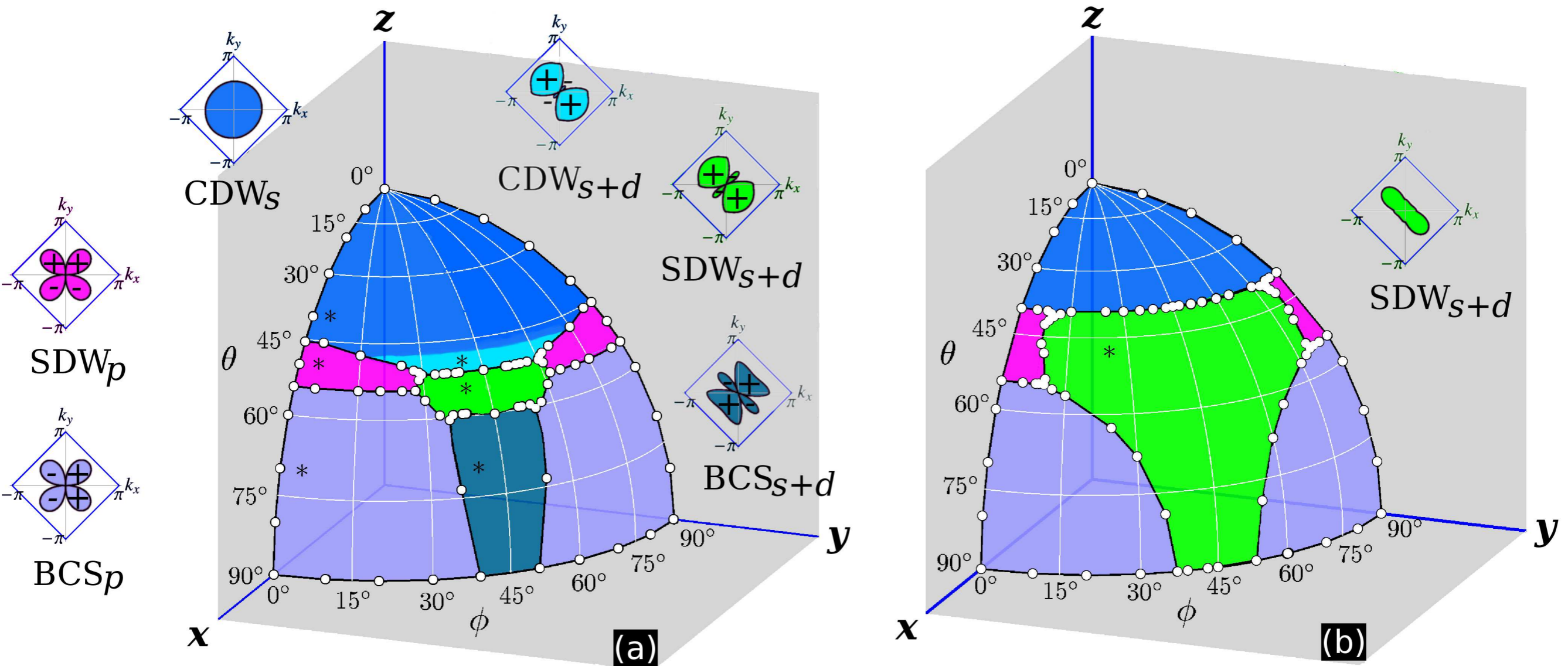


Exact diagonalization (ED) yields the hopping correlation function

$$C(i, j) = \langle K_{i, i+y} K_{j, j+y} \rangle - \langle K_{i, i+y} \rangle \langle K_{j, j+y} \rangle \quad K_{i, j} \equiv (a_i^\dagger a_j + h.c.)$$

It approaches  $4\delta^2$  in the limit of large  $|i-j|$ .

# Spin half dipolar Fermi gas

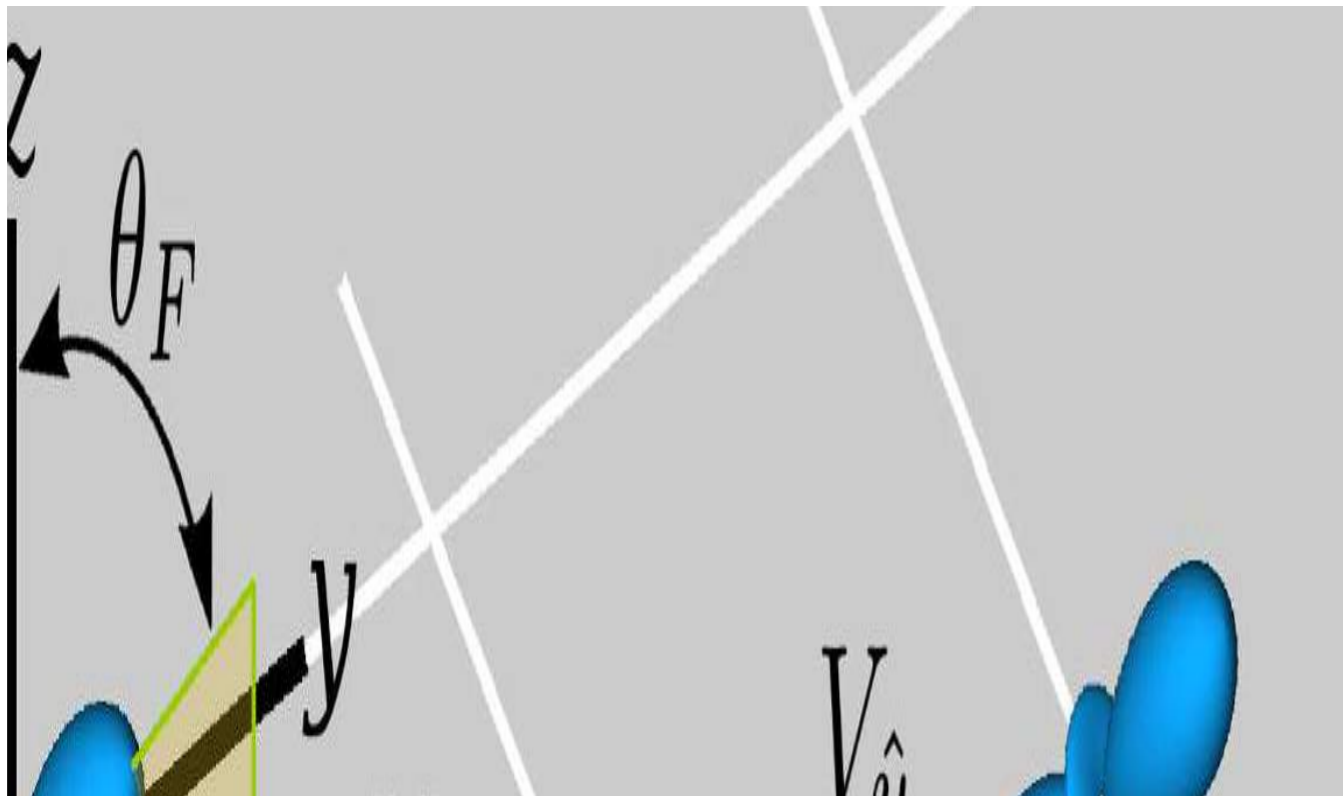


$$V_d = 0.5, U = 0.1$$

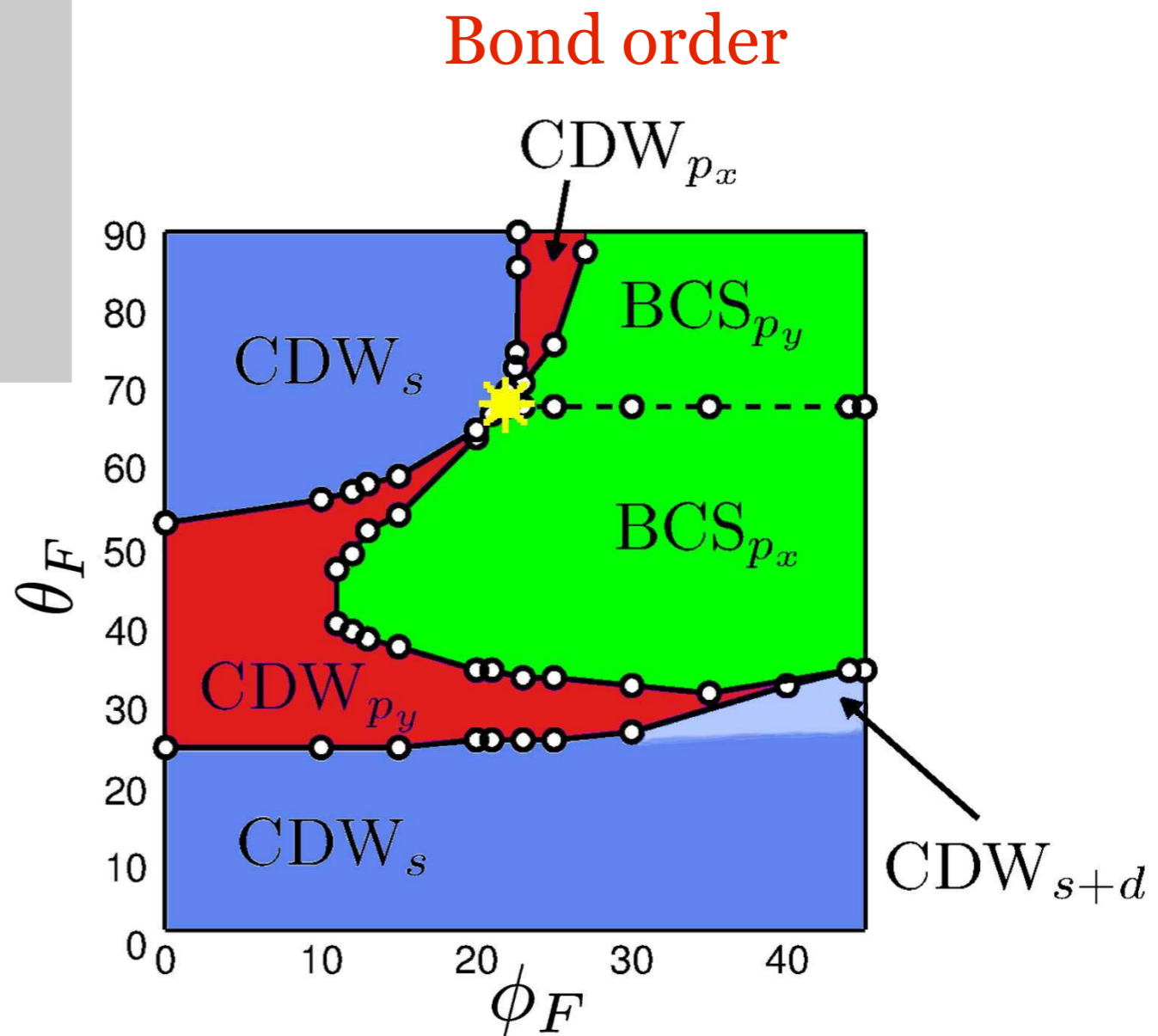
$$V_d = 0.5, U = 0.5$$

The p-wave spin density wave phase is sandwiched between the CDW and BCS superfluid phases. Its phase boundary depends on  $U$ .

# Quadrupolar Fermi gas



$$V^{qq} = V(3 - 30 \cos^2 \theta + 35 \cos^4 \theta) / r^5$$



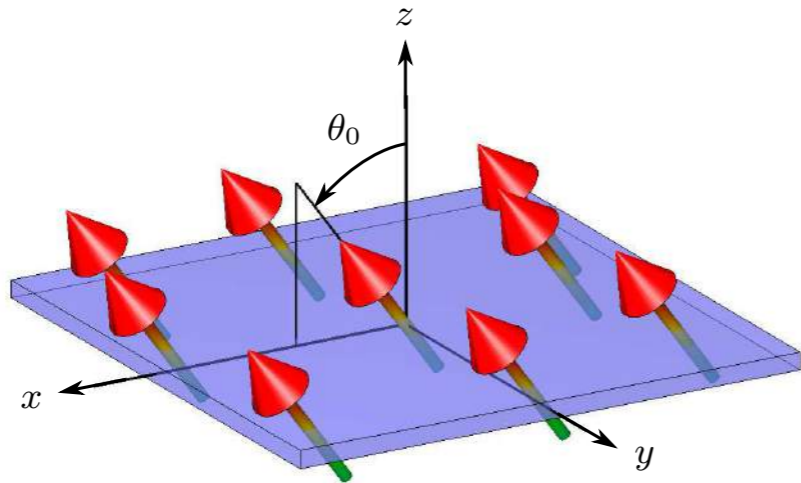


## 2. Functional renormalization group analysis of continuum dipolar gas in 2D

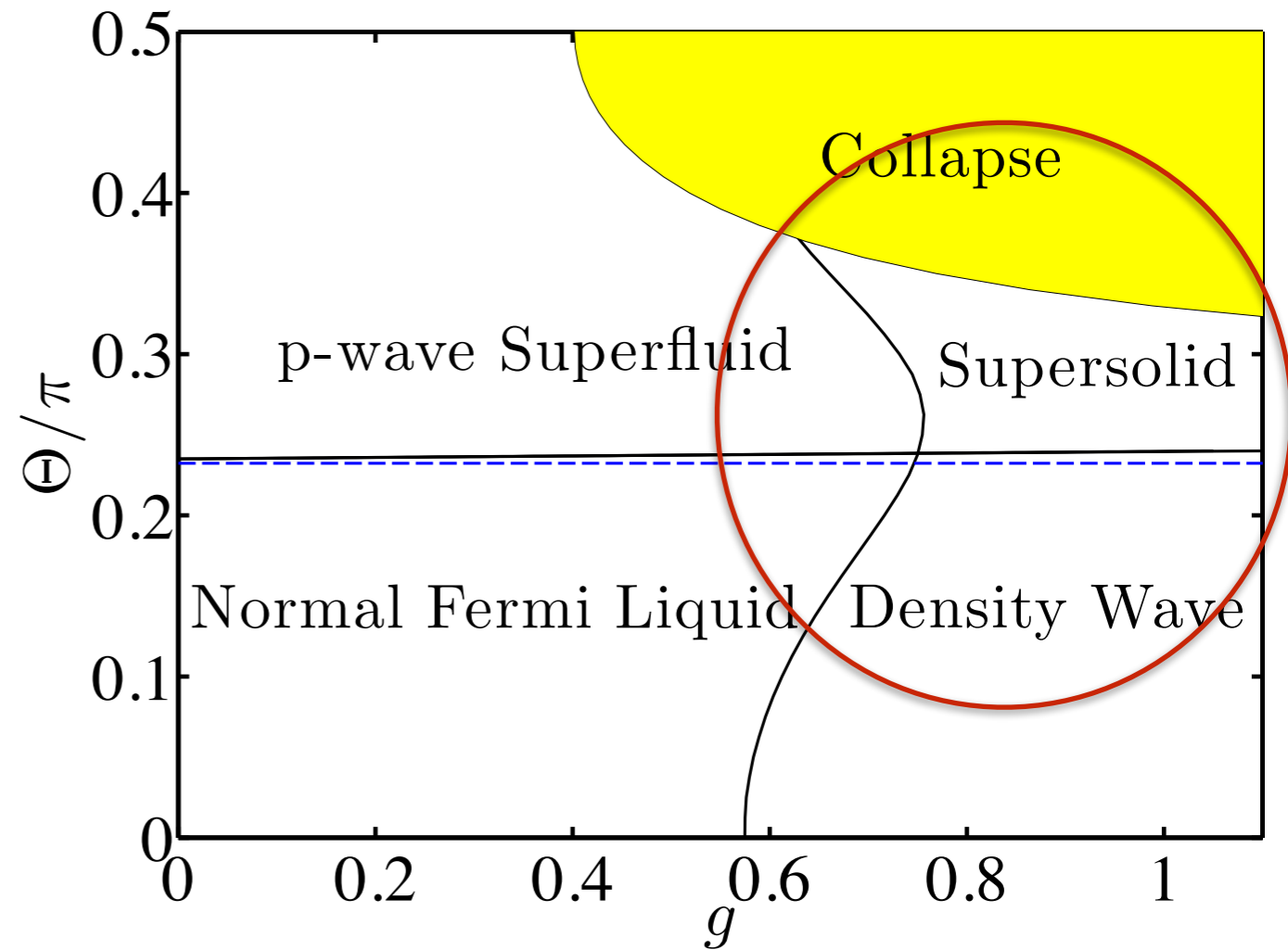
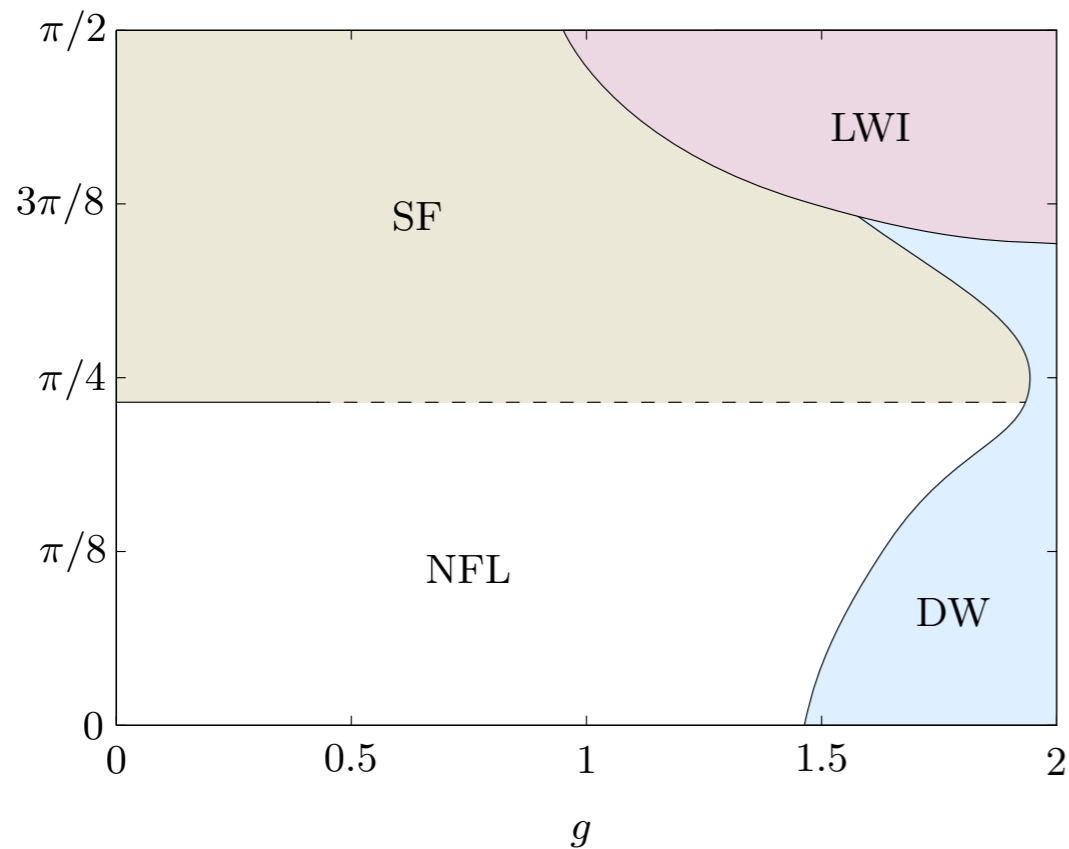
Collaborator:

Ahmet Keles (Pitt and GMU)

# 2D dipolar Fermi gas, mean field and RPA predictions



Tightly confined in z direction



Sieberer and Baranov, PRA 84, 063633 (2011)  
 See also: Babadi & Demler, PRB 2011;  
 Zhao et al (Pu's group) PRA, 2010;  
 Bruun and Taylor PRL 2008; and many others.

Wu, Block, Bruun, arXiv:1412.2783 (2014)

# Technical slide 1: Flow of effective action

Add infrared regulator  $R_k$  to the action  $S$ ,  $k$  being the sliding momentum scale, e.g.,

$$R_k(\mathbf{p}) = \left[ \frac{k^2}{2m} \text{sgn}(\xi(\mathbf{p})) - \xi(\mathbf{p}) \right] \theta\left(\frac{k^2}{2m} - |\xi(\mathbf{p})|\right)$$

Wetterich's flow equation:

$$\partial_k \Gamma_k = -\frac{1}{2} \tilde{\partial}_k \text{Tr} \ln [\Gamma^{(2)} + R_k]$$

C. Wetterich, Phys. Lett. B, 301(1), 90–94 (1993).

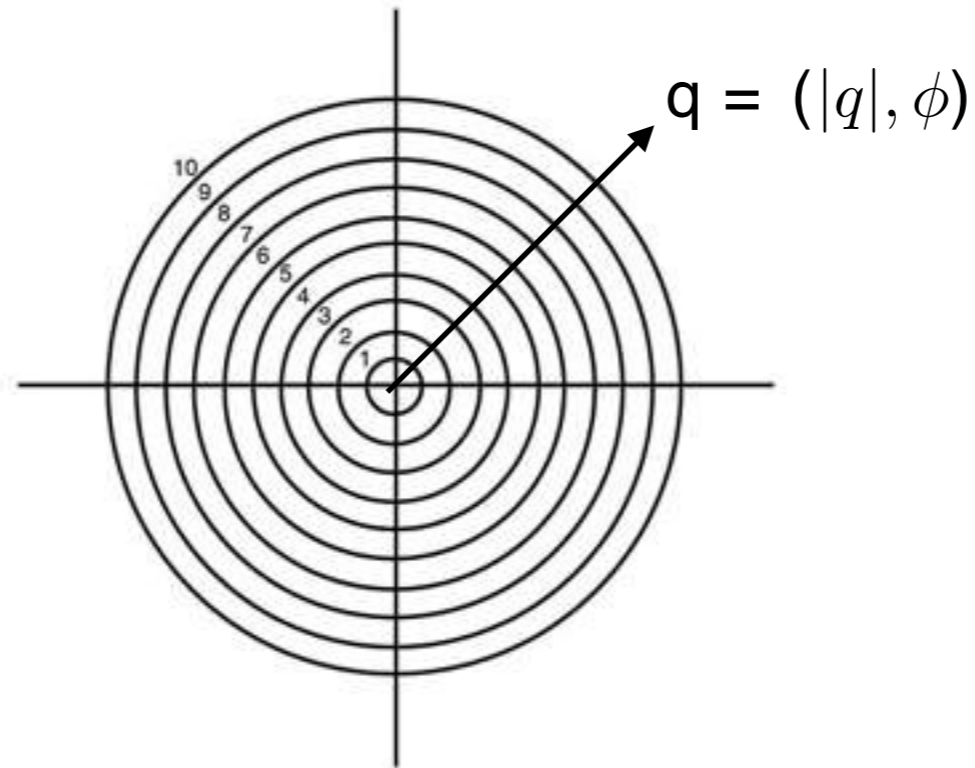
T. R. Morris, Inter. J. of Mod. Phys. A, 9(14), 2411–2450 (1994).

Expand  $\Gamma$  to quartic order,  $\Gamma_k = \bar{\psi}_1 [G_0^{-1} - \Sigma_k + R_k] \psi_2 + \Gamma^{(4)} \bar{\psi}_1 \bar{\psi}_2 \psi_3 \psi_4 + \dots$

Truncate the flow equation,

The diagram shows the flow equation for the self-energy. On the left, the derivative  $\partial_k$  acts on a self-energy diagram represented as a square with four external legs. The top-left and bottom-left legs have momenta  $\frac{p}{2} + q'$  and  $\frac{p}{2} + q$  respectively, while the top-right and bottom-right legs have momenta  $\frac{p}{2} - q'$  and  $\frac{p}{2} - q$ . On the right, the derivative  $\tilde{\partial}_k$  acts on a self-energy diagram with a loop (a square with a loop on top) and a sum over diagrams with two loops (two squares connected by a loop). The loop diagram has a loop with momentum  $l$  and external legs with momenta  $\frac{p}{2} + q'$ ,  $\frac{p}{2} - q'$ ,  $\frac{p}{2} + q$ , and  $\frac{p}{2} - q$ . The two-loop diagrams have external legs with momenta  $\frac{p}{2} + q'$ ,  $\frac{p}{2} + q$ ,  $\frac{p}{2} - q$ , and  $\frac{p}{2} - q'$ , and a loop with momentum  $l$ .

## Technical slide 2: parametrize the flow



Discretize  $|q|$  and decompose  $\Gamma$  into angular momentum channels  $\{m\}$ .

$$\Gamma_k(p; q, q') = \sum_m \Gamma_m(p; |q|, |q'|) e^{im(\phi - \phi')}$$

In the limit of large  $k \gg k_F$ ,  $\Gamma$  is the bare interaction.

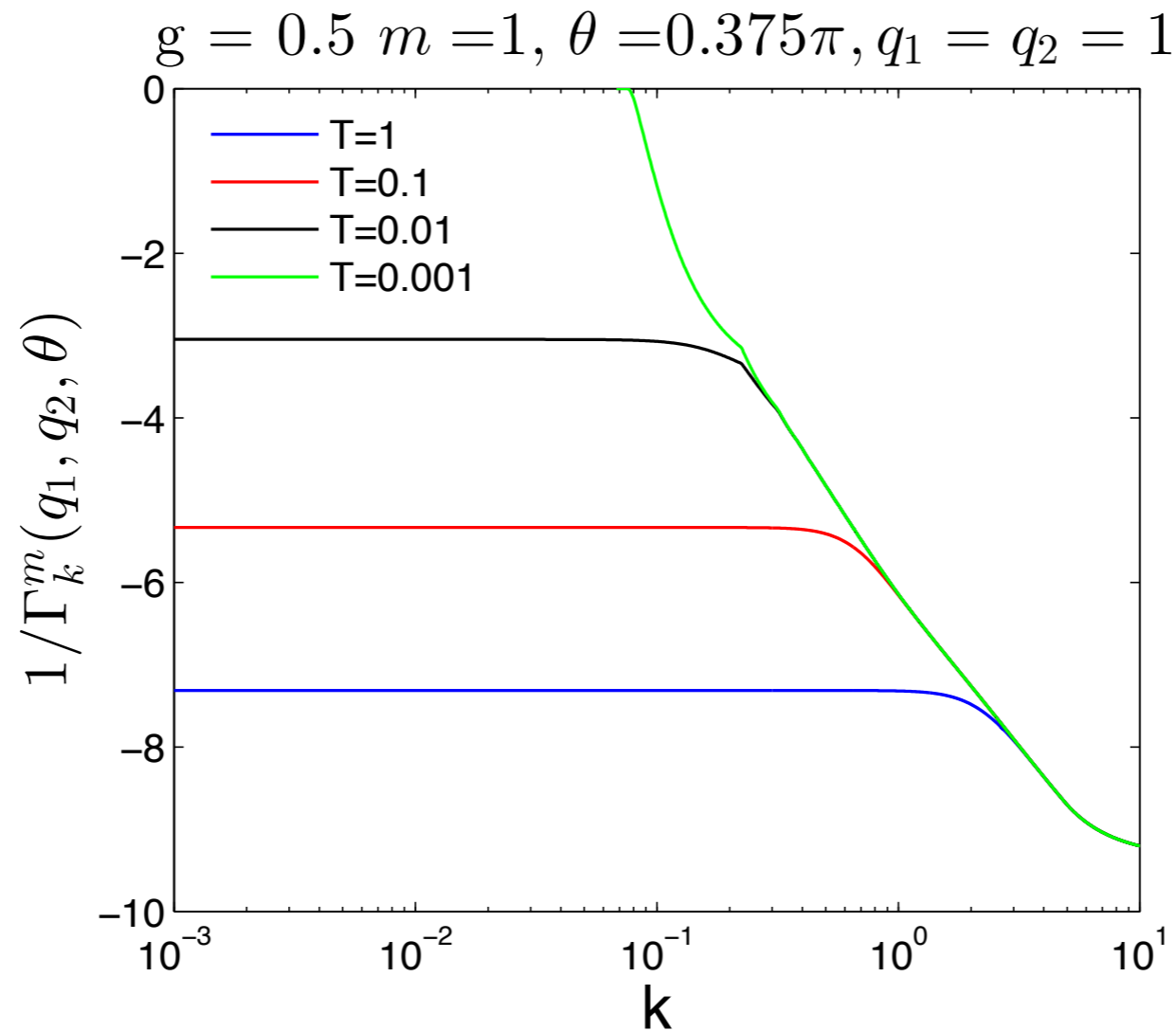
$$\Gamma_{k \rightarrow \Lambda}(q, q') = V(\mathbf{q} - \mathbf{q}') \quad V(\mathbf{p}) = 2\pi p [\cos^2 \phi \sin^2 \theta - \cos^2 \theta] d^2$$

$\Gamma_k$  at the end of the flow  $k \rightarrow 0$  contains information about the instability and  $T_c$ .

# Flow in the particle-particle channel: p-wave superfluidity

Divergence of  $\Gamma$  (i.e. zero of  $1/\Gamma$ ) signals the transition to superfluid.

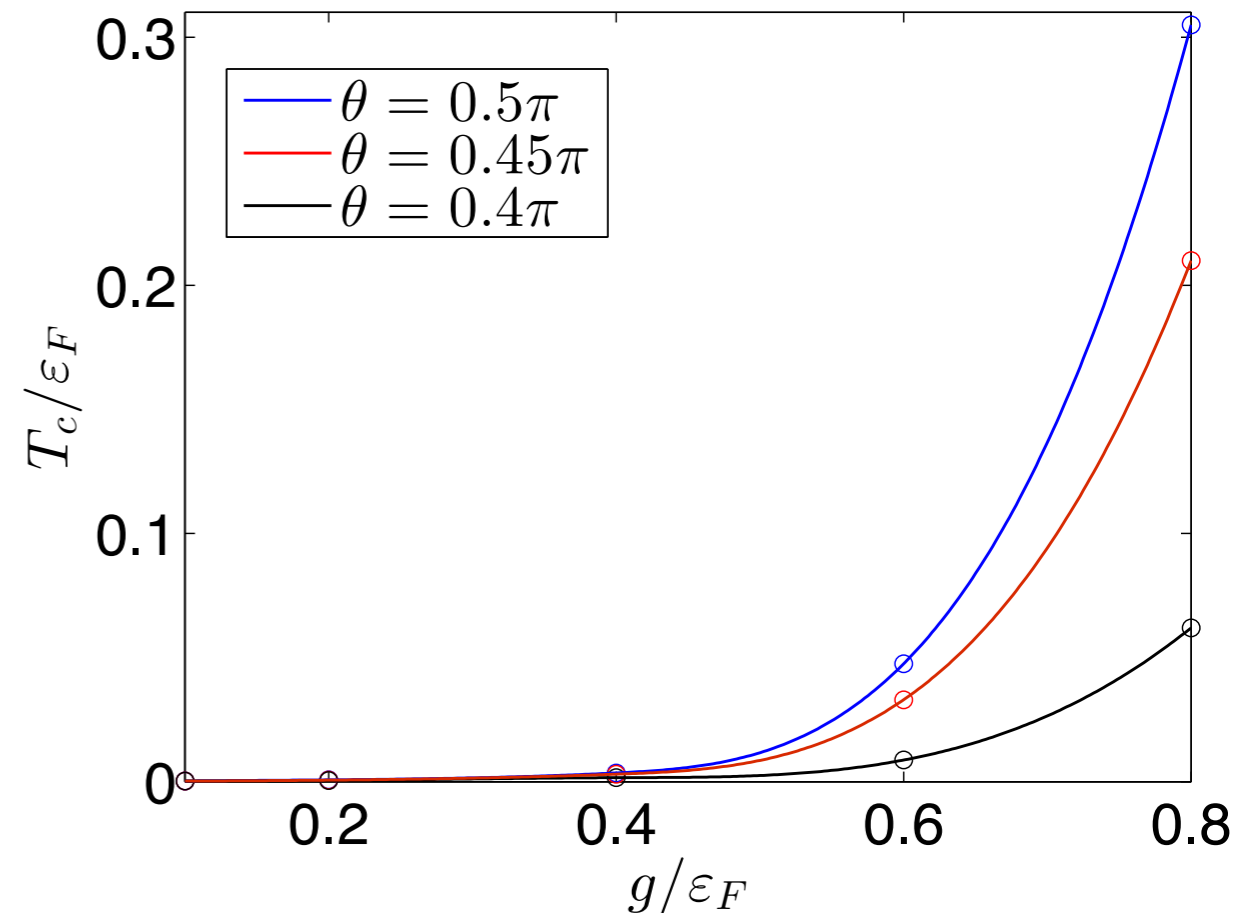
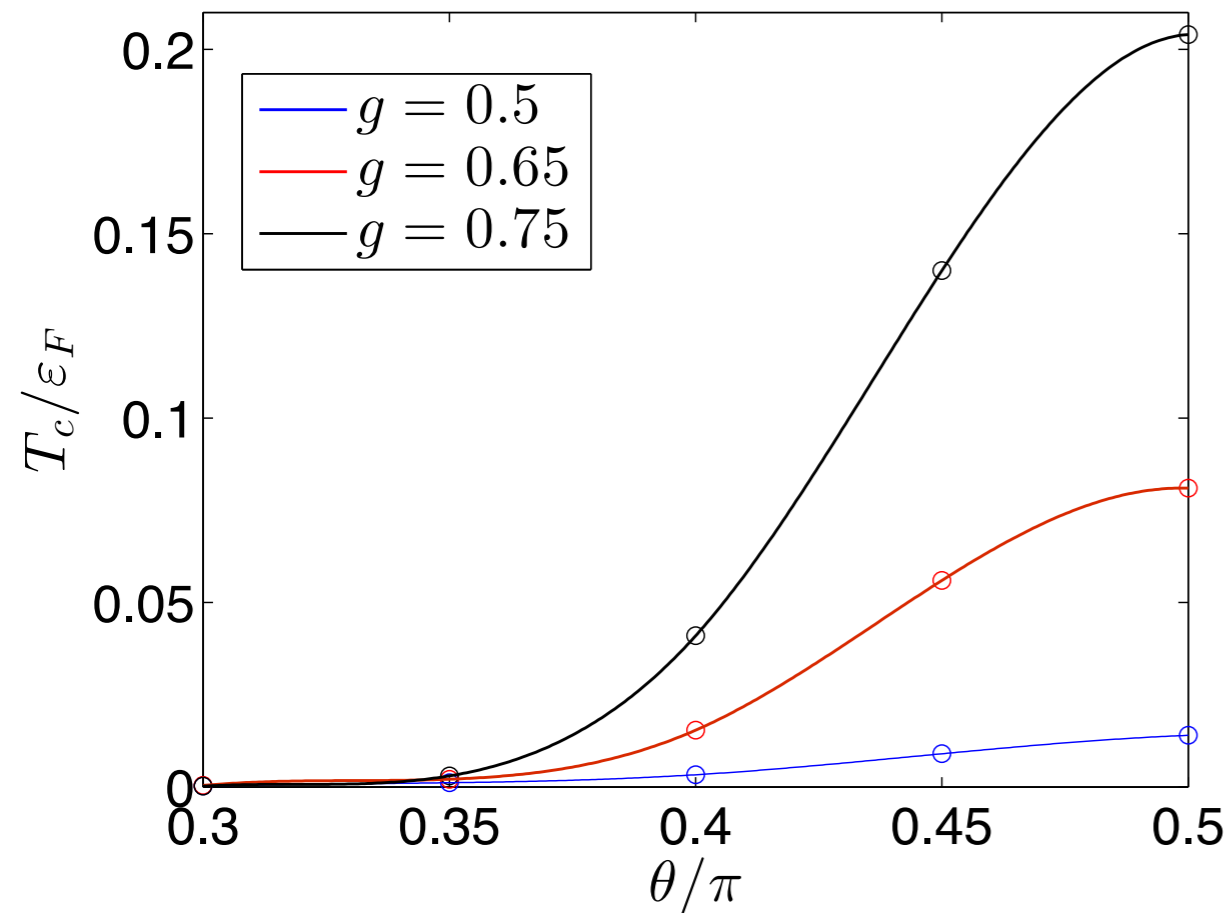
$$\left[ \Gamma_{\mathbf{k}=0}^{(4)}(\mathbf{p} = 0) \right]^{-1} = 0 \text{ at } T = T_c.$$



$q_1, q_2$  and  $k$  are in units of  $p_F$

- Neglected the self energy correction;
- Neglected the particle-hole channel.

# The superfluid transition temperature



Remaining questions:

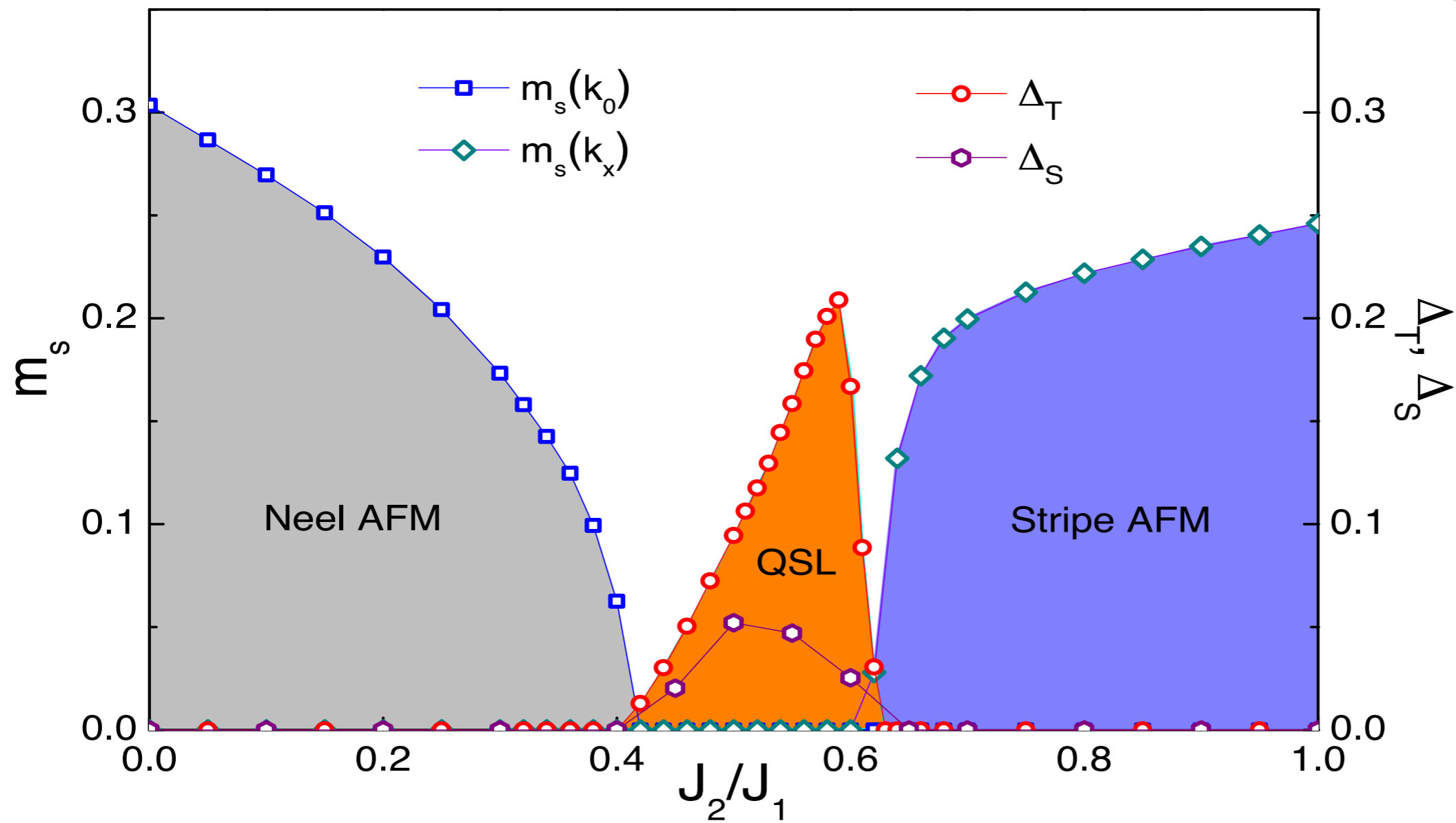
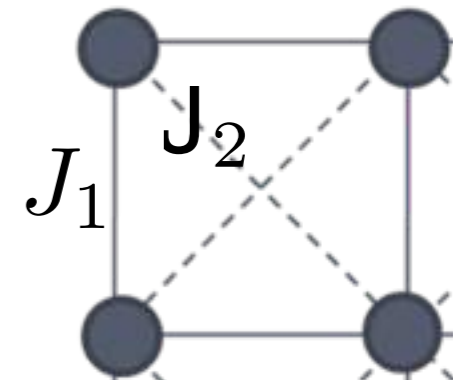
1. How about the particle-hole channel?
2. Self energy corrections (Fermi surface distortion, nematic phase...).
3. Solving the full flow equation numerically.

### 3. Magnetism of confined dipoles on lattice (preliminary results, very speculative)

Collaborator:  
Zhenyu Zhou (Pitt and GMU)

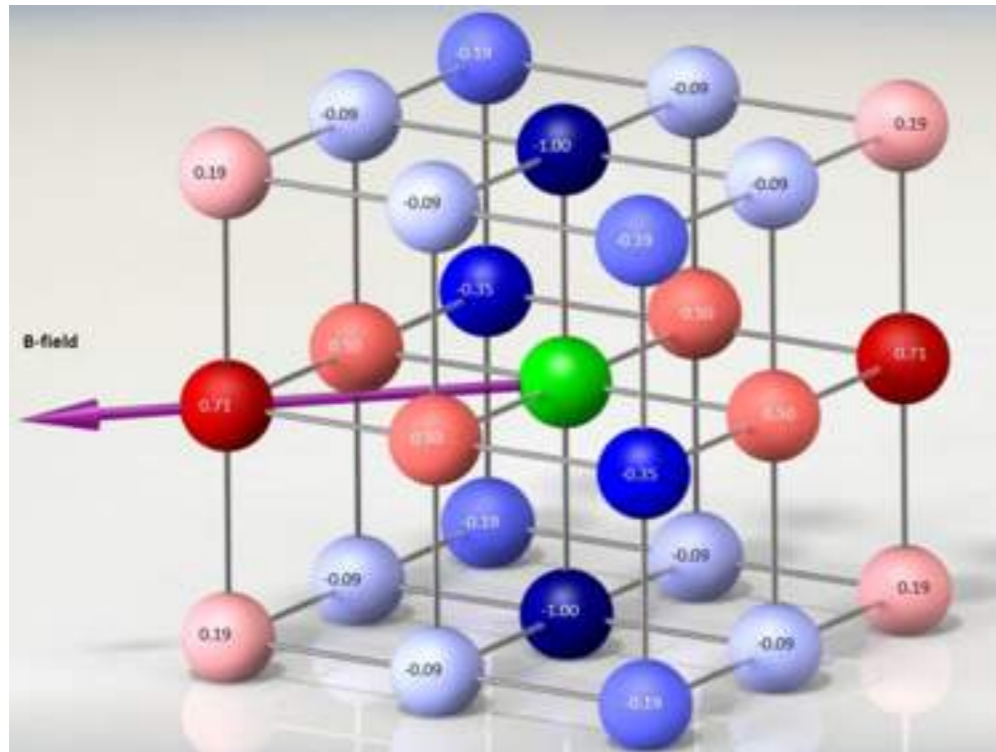
# Quantum spin liquid in frustrated spin model: J1-J2 model

$$H = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$





# Experiments

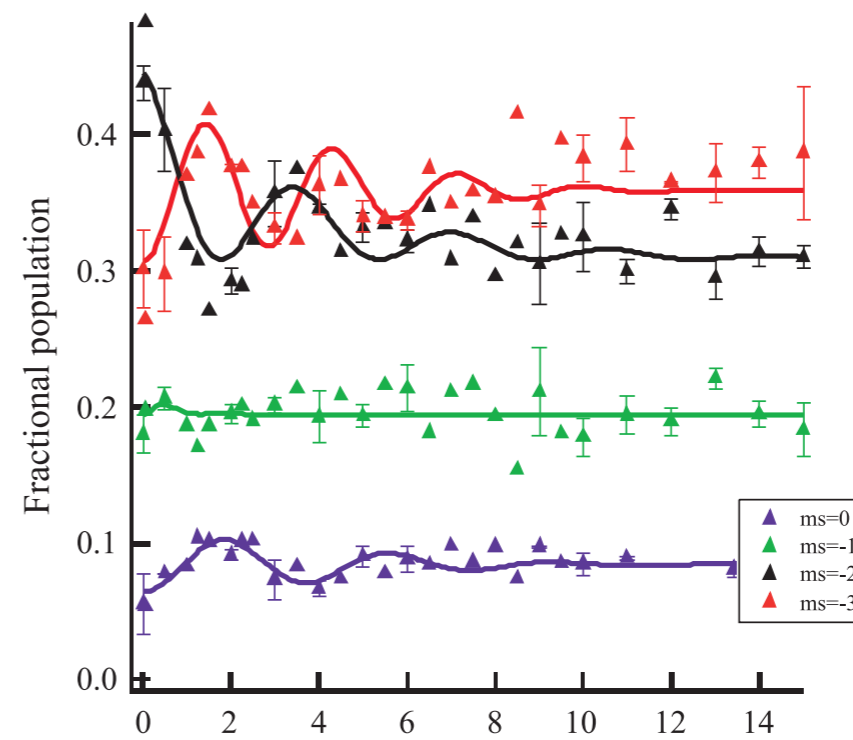
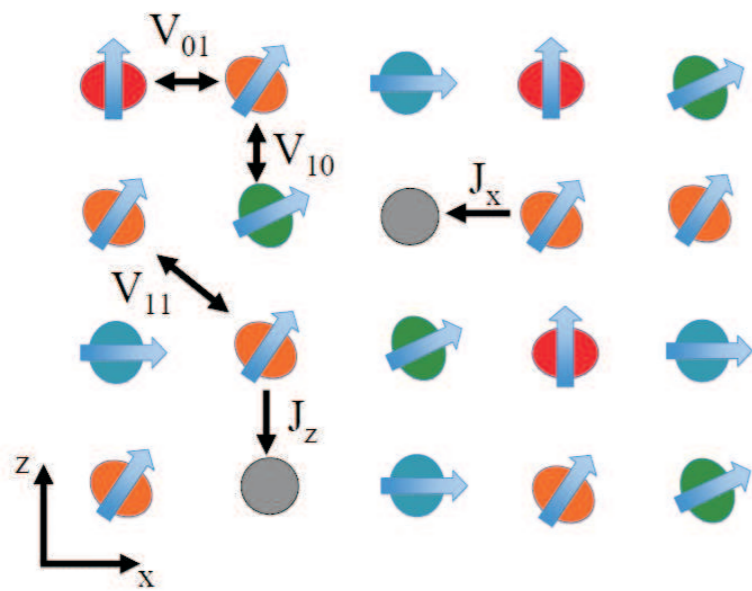


Observation of dipolar spin-exchange interactions with lattice-confined polar molecules,

B. Yan, S. A. Moses, B. Gadway, J. P. Covey, K. R. A. Hazzard, A. M. Rey, D. S. Jin & J. Ye,  
*Nature* 501, 521–525 (2013).

Nonequilibrium quantum magnetism in a dipolar lattice gas.

A. de Paz, A. Sharma, A. Chotia, E. Maréchal, J. H. Huckans, P. Pedri, L. Santos, O. Gorceix, L. Vernac, and B. Laburthe-Tolra,  
*Phys. Rev. Lett.* 111, 185305 (2013)

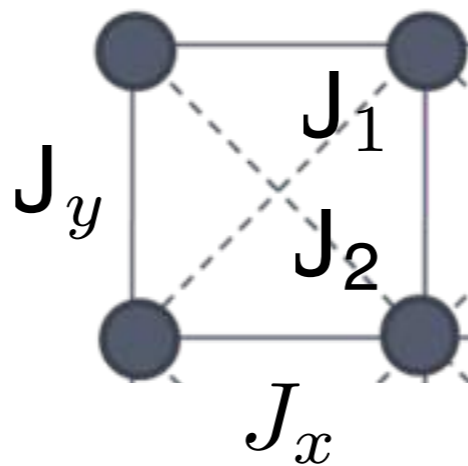


## Lattice spin model: 2d, square lattice

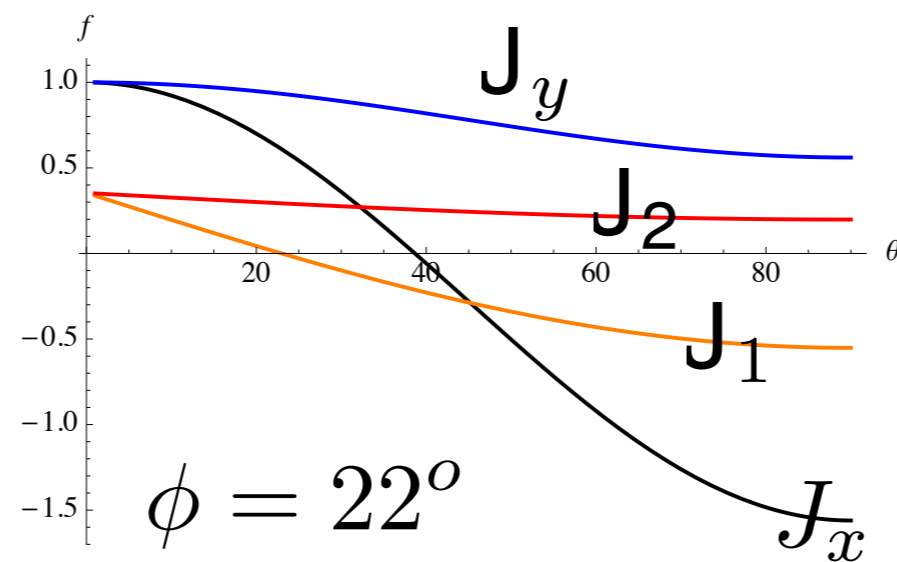
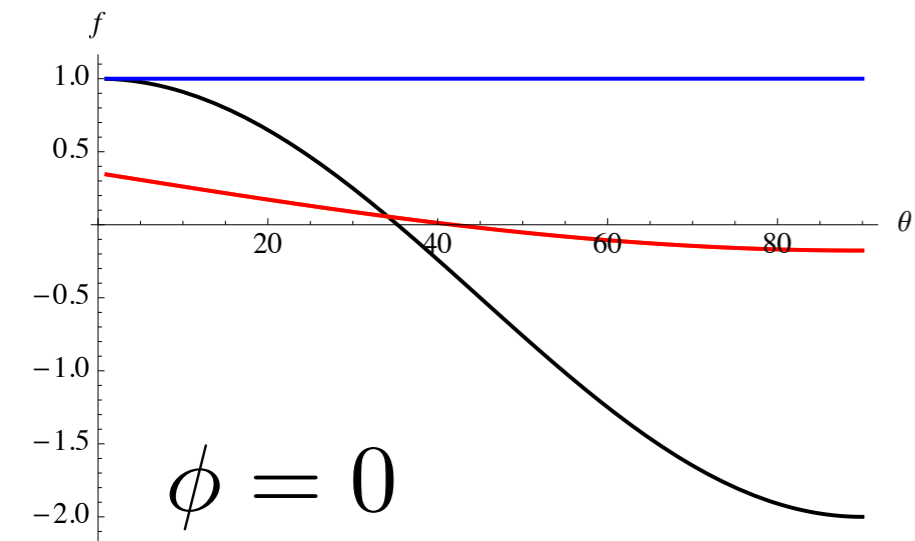
$$H_d = \frac{J}{2} \sum_{i \neq j} f(\mathbf{r}_i - \mathbf{r}_j) (s_i^x s_j^x + s_i^y s_j^y + \eta s_i^z s_j^z).$$

Here  $\mathbf{s}_i = (s_i^x, s_i^y, s_i^z)$  is the spin at site  $i$ ,  $\eta$  describes the anisotropy depending on the detailed implementation (e.g.,  $\eta = 0$  for the KRb experiment),  $f(r) = [1 - 3 \cos^2(\hat{\mathbf{r}} \cdot \hat{\mathbf{d}})](a/r)^3$  characterizes the long range, anisotropic spin exchange due to dipolar interaction, and  $a$  is the lattice constant.

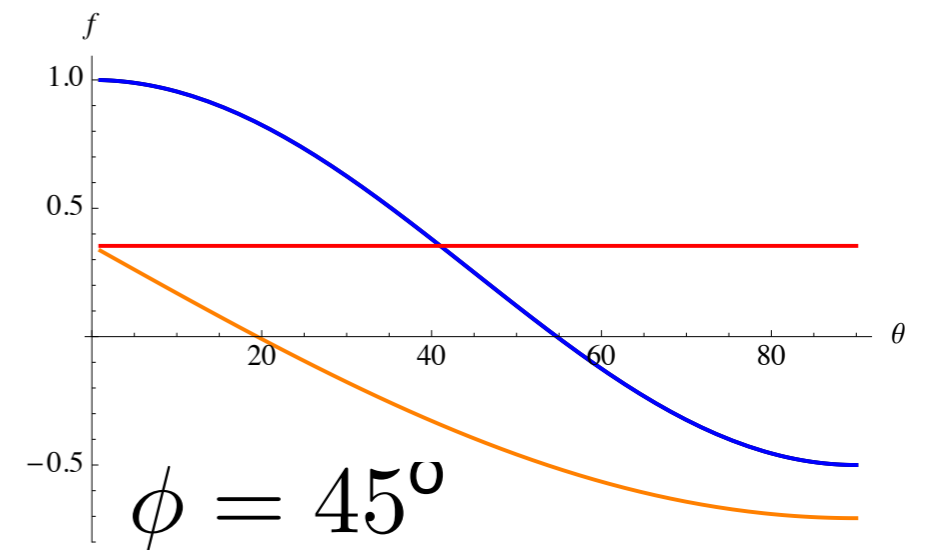
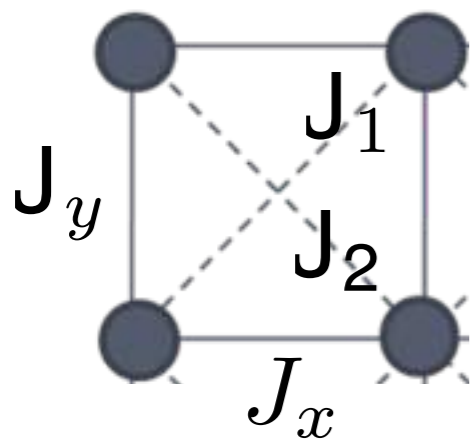
Consider  $S=1/2$ ,  $\eta=1$ , and [truncate](#) exchange interactions to next nearest neighbor.



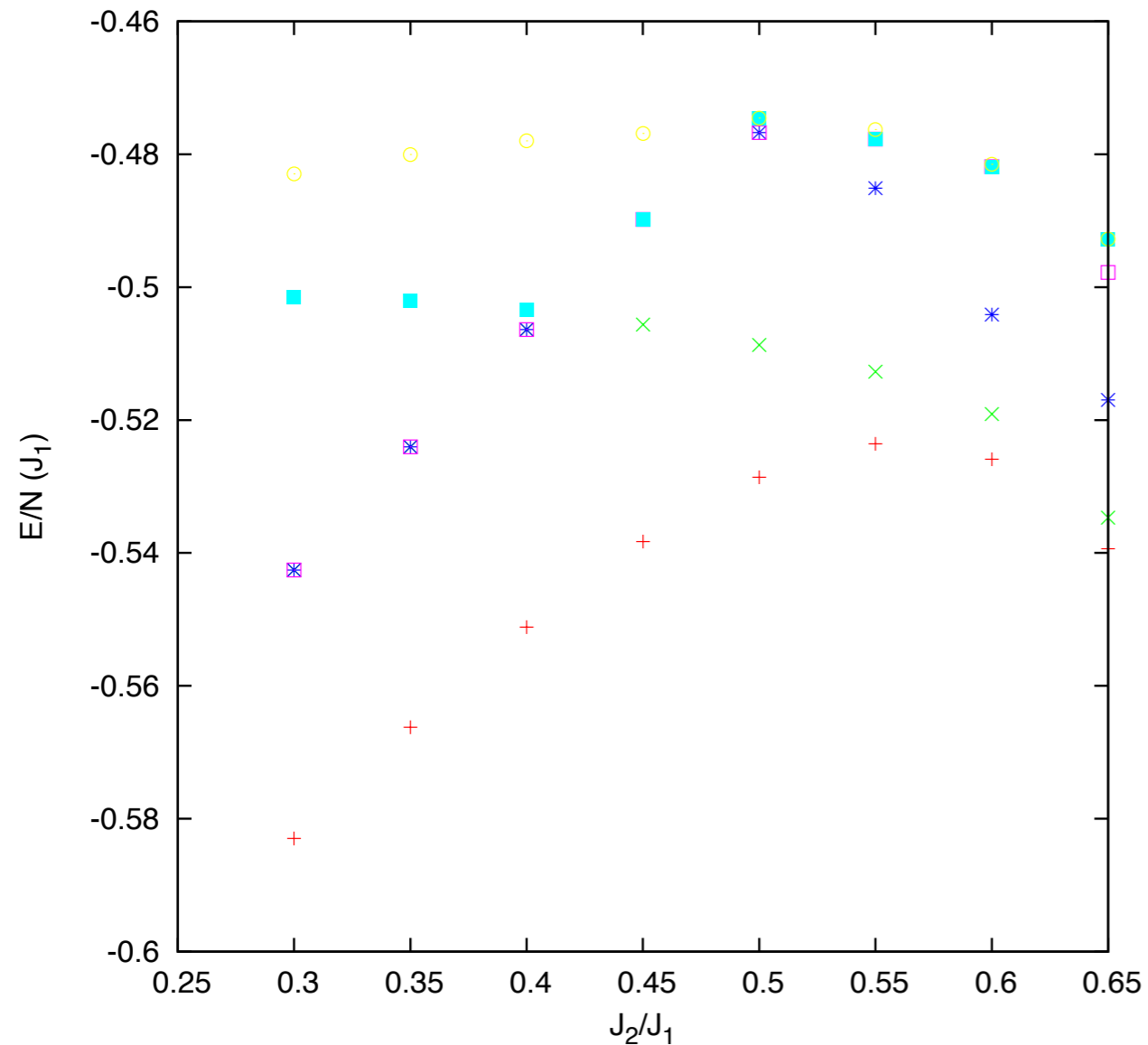
# Competing exchange interaction



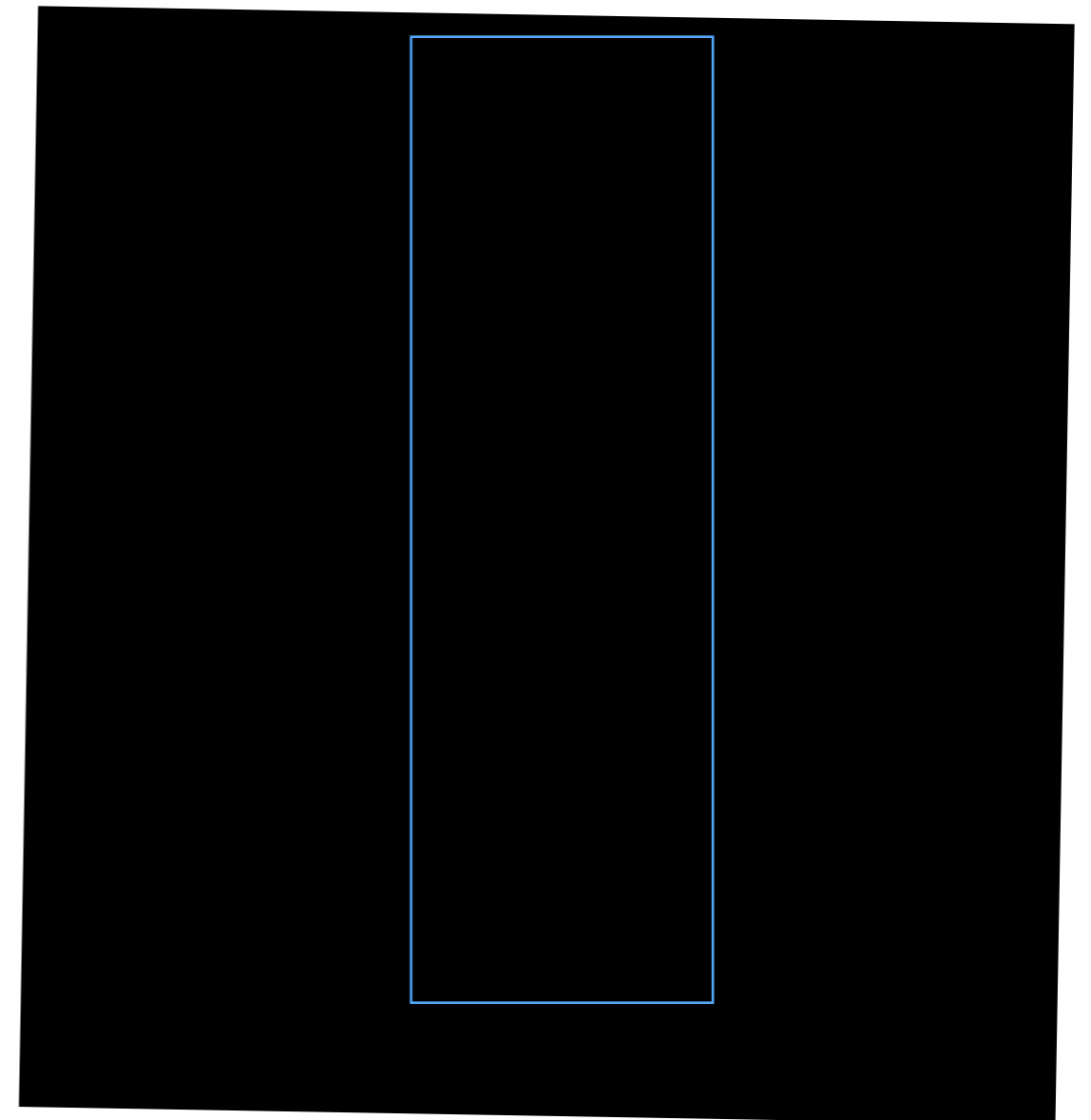
Sweet spots?  
 $J_x \sim J_y$   
 $\sim 2J_1 \sim 2J_2$



# Benchmarking the exact diagonalization: J1-J2 model



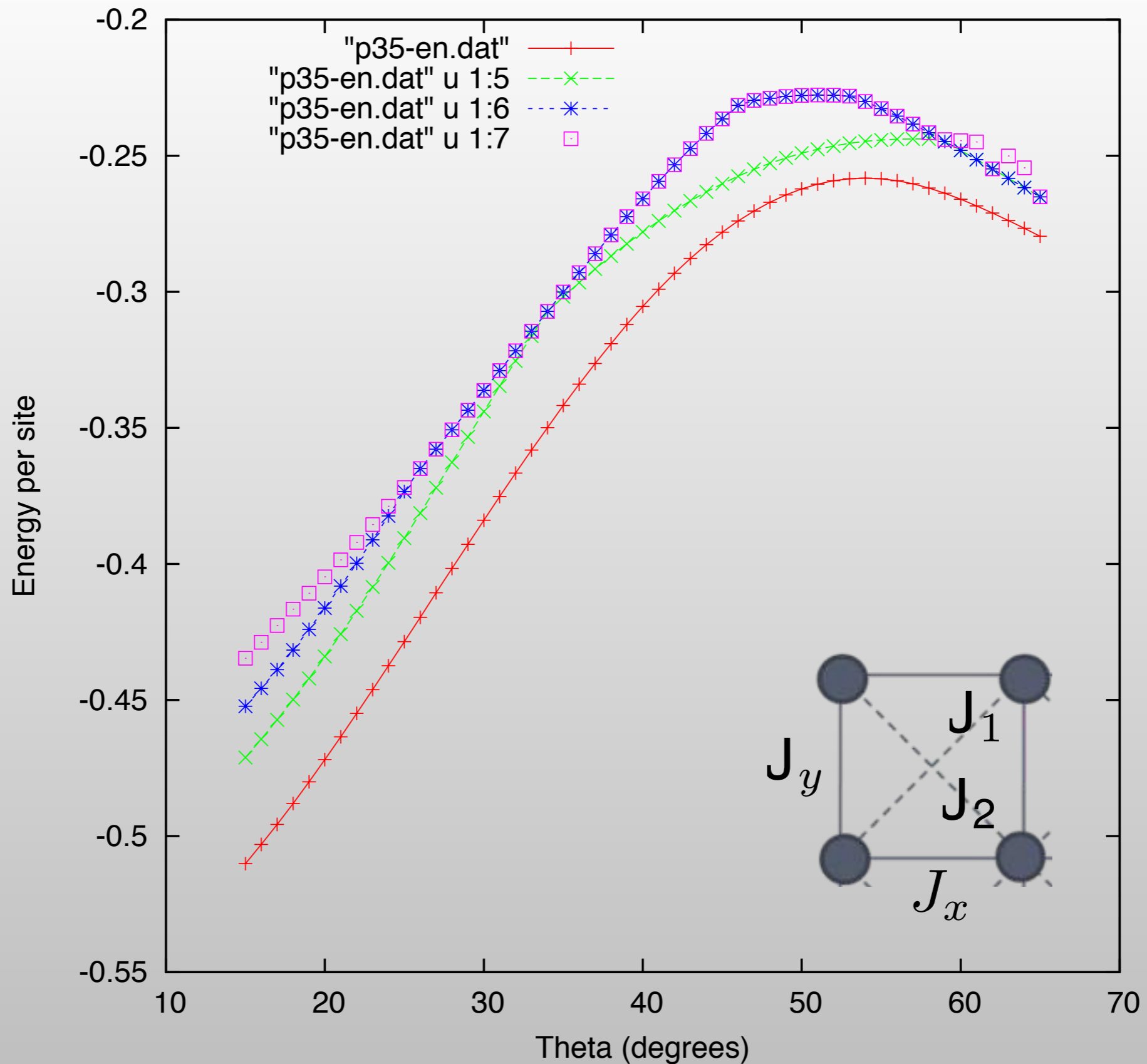
16 sites, our calculation.



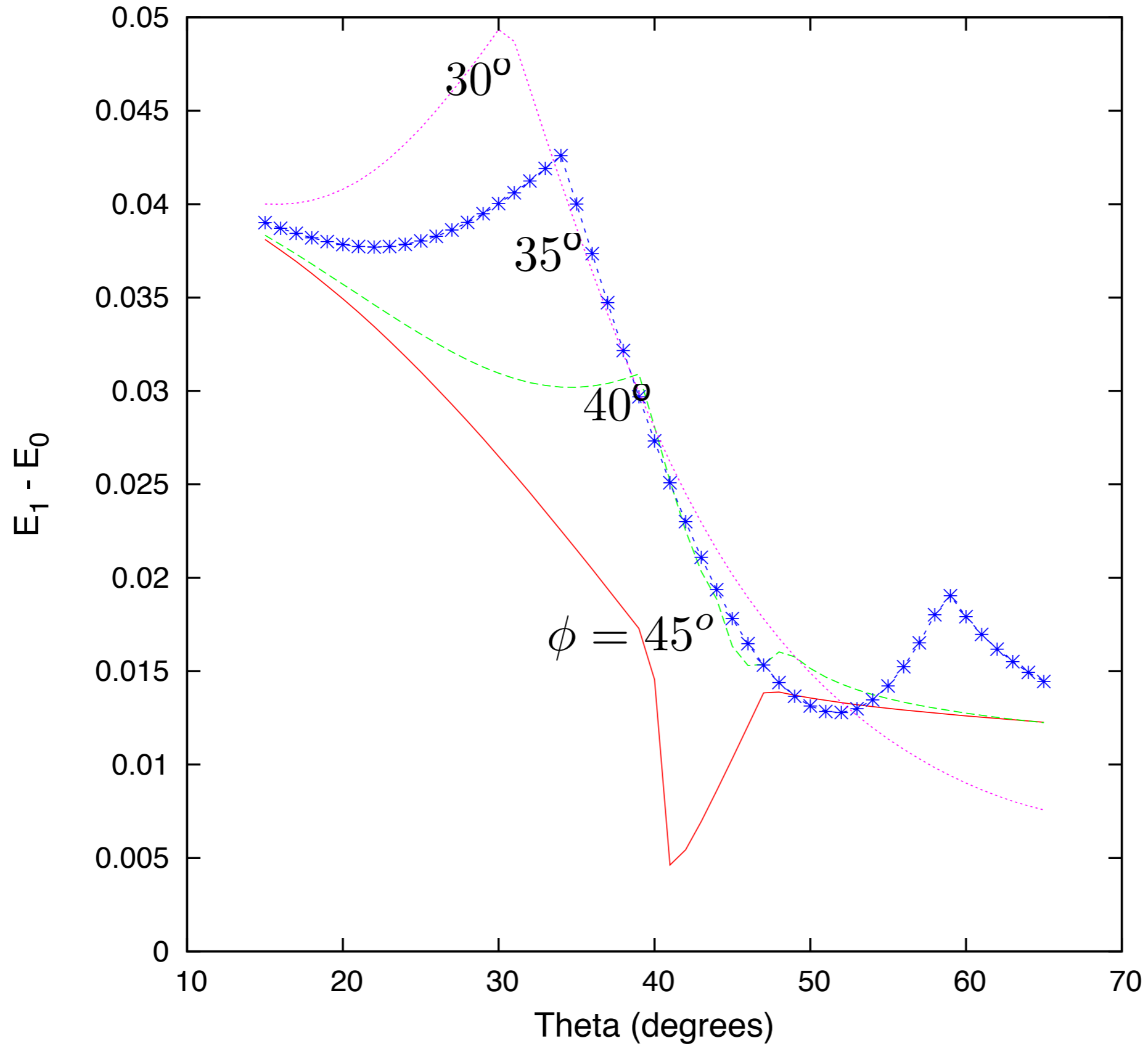
16 sites, with  $J_1=2$ .  
Dagotto and Moreo, PRL 1989

State of the art: 40 sites, # of basis: 430 909 650  
J. Richter and J. Schulenburg, Eur. Phys. J. B 73, 117–124 (2010)

An example of the energy spectrum  $\phi = 35^\circ$

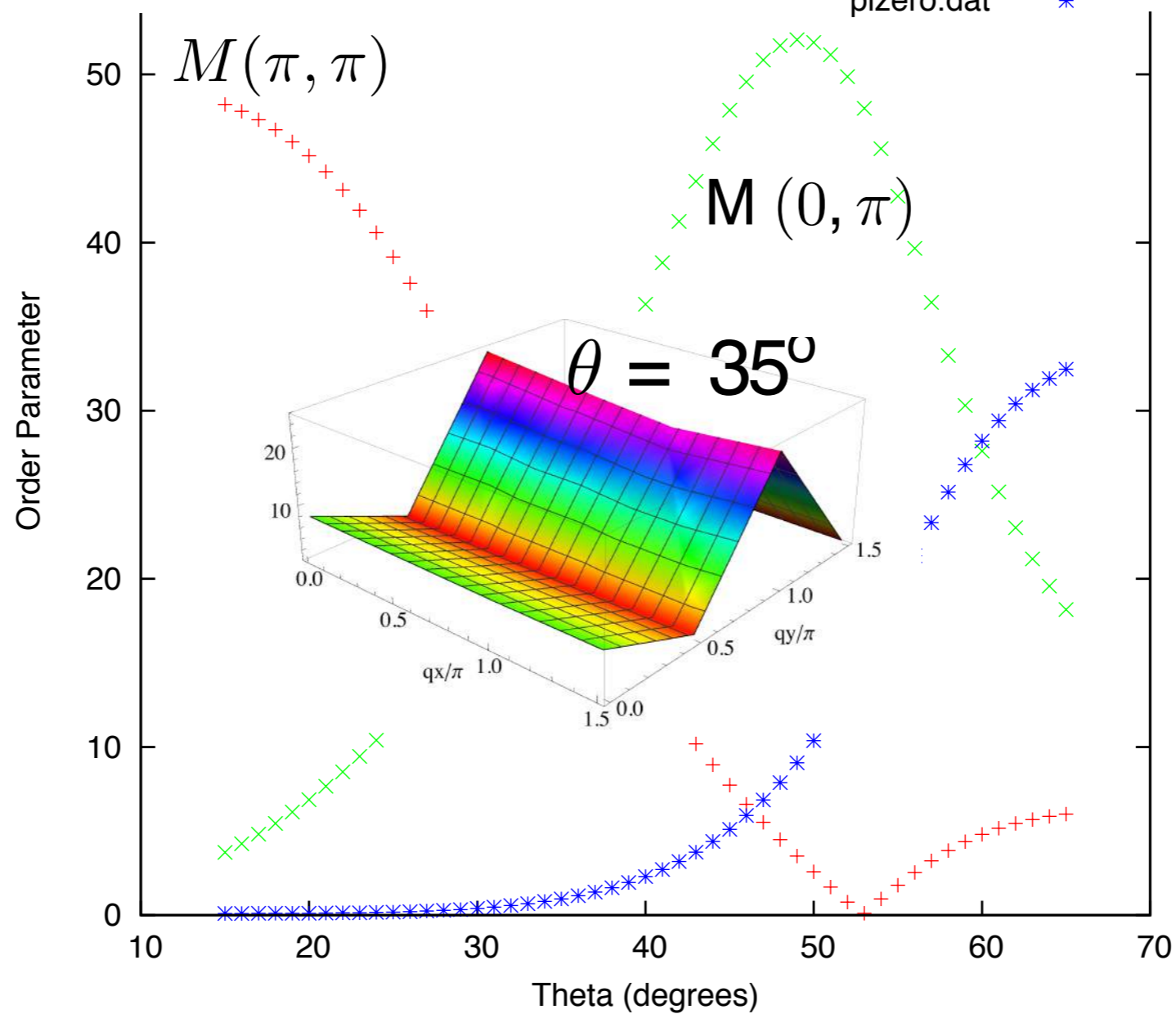
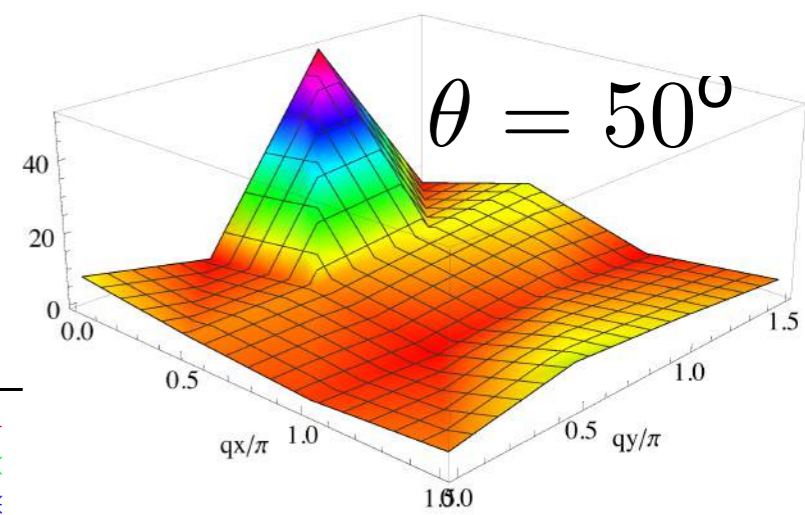
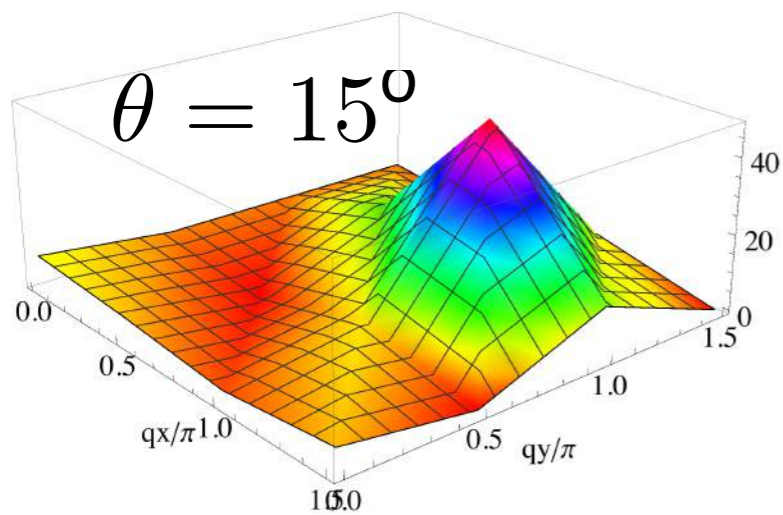


# Excitation (spin) gap

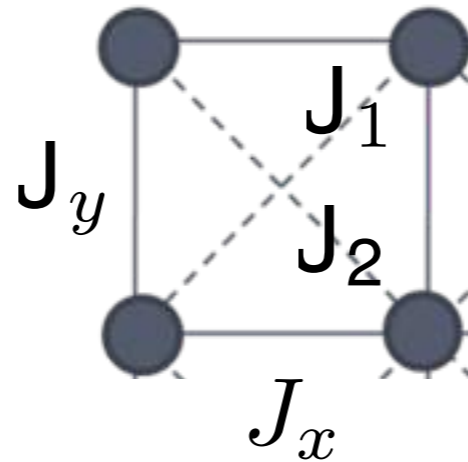


# "Order Parameter"

$$M(\mathbf{Q}) = \sum_{i,j} \langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle e^{i\mathbf{Q} \cdot (\mathbf{r}_i - \mathbf{r}_j)}$$



# Speculations



- This model can be highly, even maximally, frustrated;
- It is closely related to J1-J2 model; but the physics is even richer;
- Our numerical study (for small lattice) suggests a gaped quantum paramagnetic phase between the Neel and collinear ordered phase;
- Numerics on larger size systems is required to resolve the phase diagram.