Feb. 25, 2013 KITP

Bond order of dipolar fermions on an optical lattice

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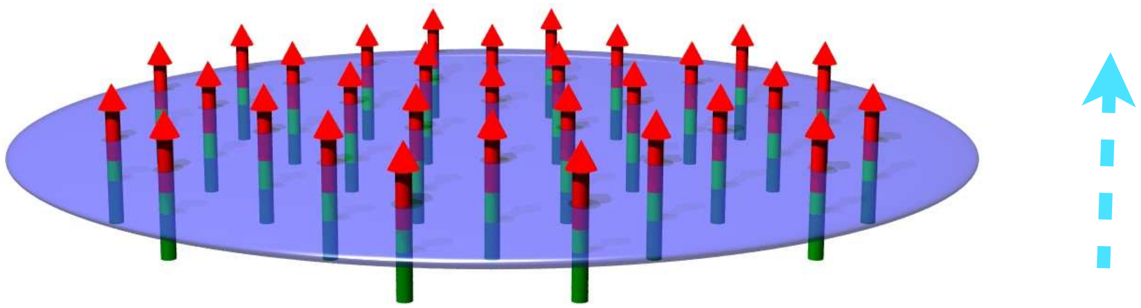
Question for many-body theorists

Suppose we can make quantum degenerate gases of fermionic polar molecules (or magnetic atoms), load them onto optical lattices, and cool the system to low temperatures.

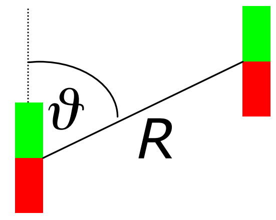
What kinds of many-body phases do we get?

Are they all "boring," i.e., known and studied in condensed matter physics?



Atoms

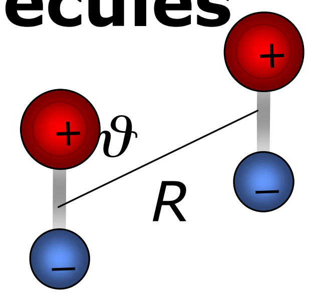
Magnetic dipoles



$\vec{\mu}$

Polar molecules

Electric dipoles



$\vec{d}$

Dipole-dipole interaction is special

$$V = \frac{1}{4\pi\epsilon_0}\frac{\vec{d}_1\cdot\vec{d}_2 - 3(\hat{r}\cdot\vec{d}_1)(\hat{r}\cdot\vec{d}_2)}{r^3}$$

$$\vec{r}_1 - \vec{r}_2 = r\hat{r}$$

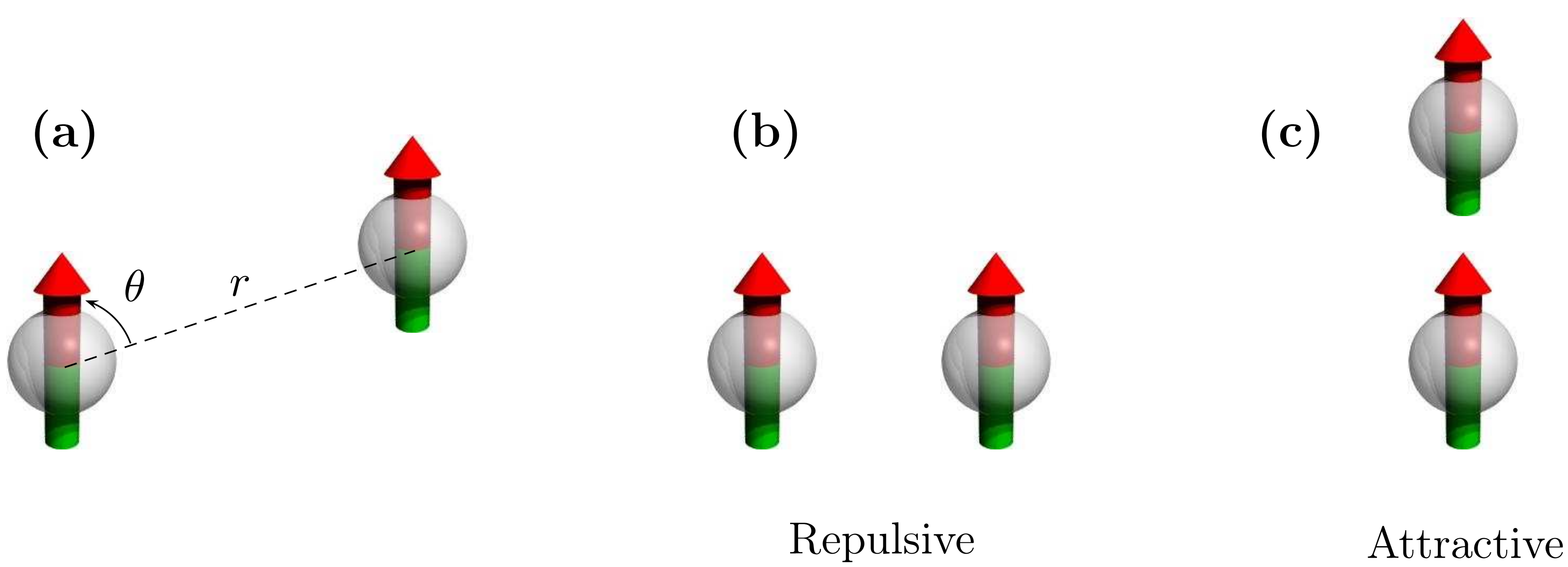
$$\vec{d} \to \vec{\mu},\ \frac{1}{\epsilon_0} \to \mu_0$$

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, d-wave superfluid(?)
2-component Fermi gas	contact, attractive	s-wave superfluid (BCS-BEC crossover)
dipolar Fermi gas	dipole-dipole	

Candidate phases of dipolar fermions:

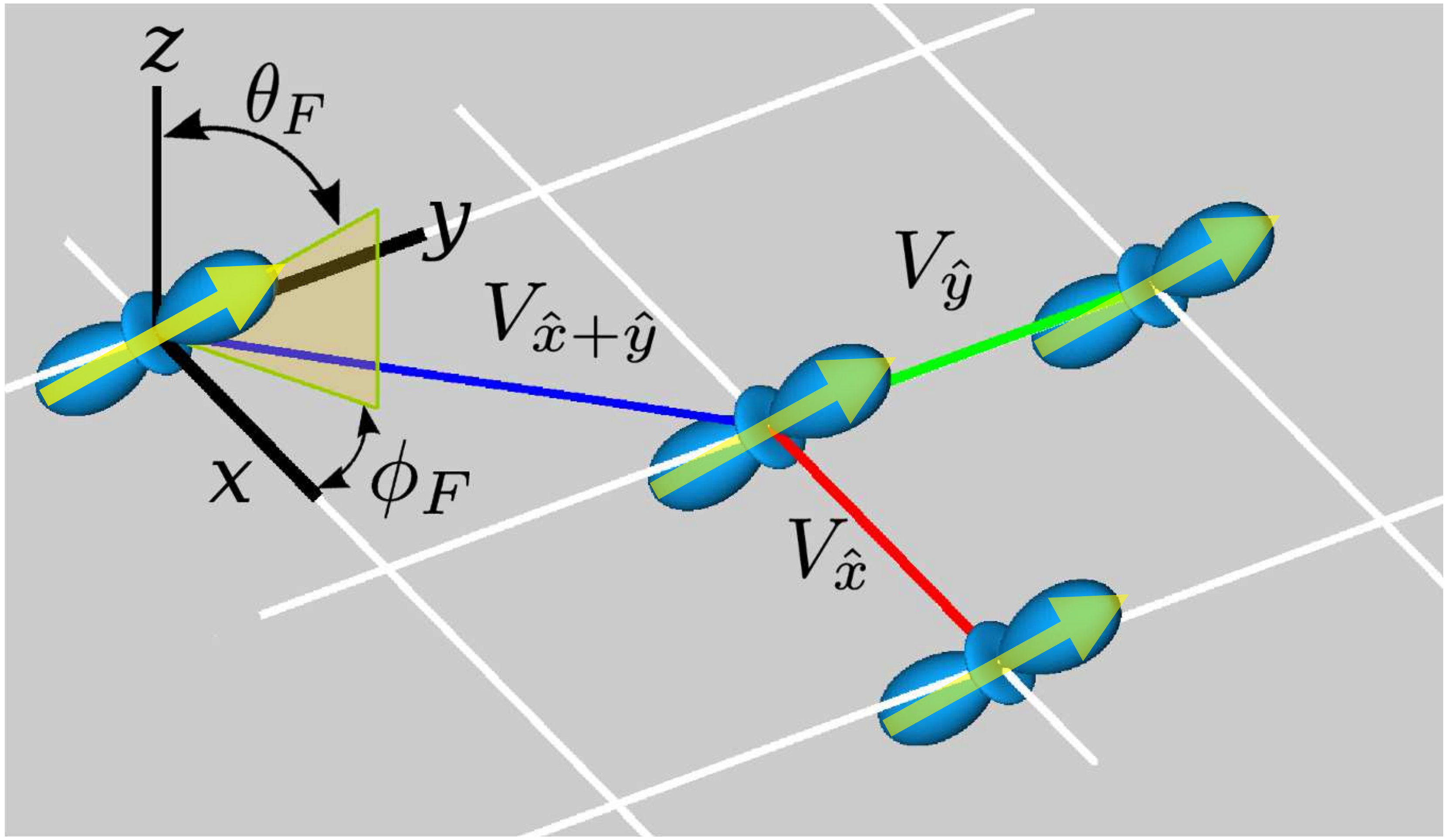
- ★ anisotropic Fermi liquid
- ★ charge density waves (CDW)
- ★ p-wave superfluid
- ★ stripes, quantum liquid crystals?
- ★ supersolid? ...

There has been a large body of work on continuum dipolar Fermi gas.

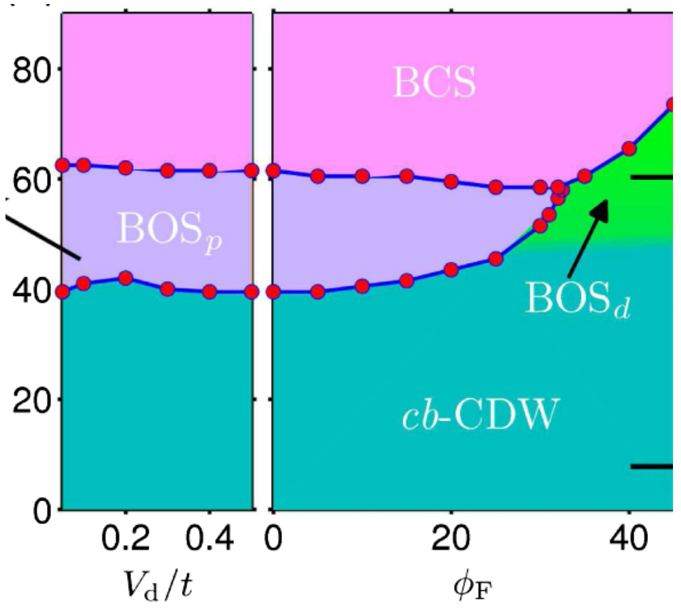
L. You and M. Marinescu. Prospects for p-wave paired Bardeen-Cooper-Schrieffer states of fermionic atoms. *Phys. Rev. A*, 60(3):2324–2329, Sep 1999.

M. A. Baranov, M. S. Mar'enko, V. S. Rychkov, and G. V. Shlyapnikov. Superfluid pairing in a polarized dipolar Fermi gas. *Phys. Rev. A*, 66(1):013606, Jul 2002.

This talk: dipolar fermions on square lattice



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



We will obtain the theoretical phase diagram,
and present evidences for an unusual quantum phase in this system.

Outline

1. Toward degenerate dipolar Fermi gas on optical lattice

   - Ground state polar molecules of KRb in optical lattice (JILA)
   - Degenerate Fermi gas of ^{161}Dy atoms (UIUC-Stanford)

2. Dipolar fermions on 2D square lattice

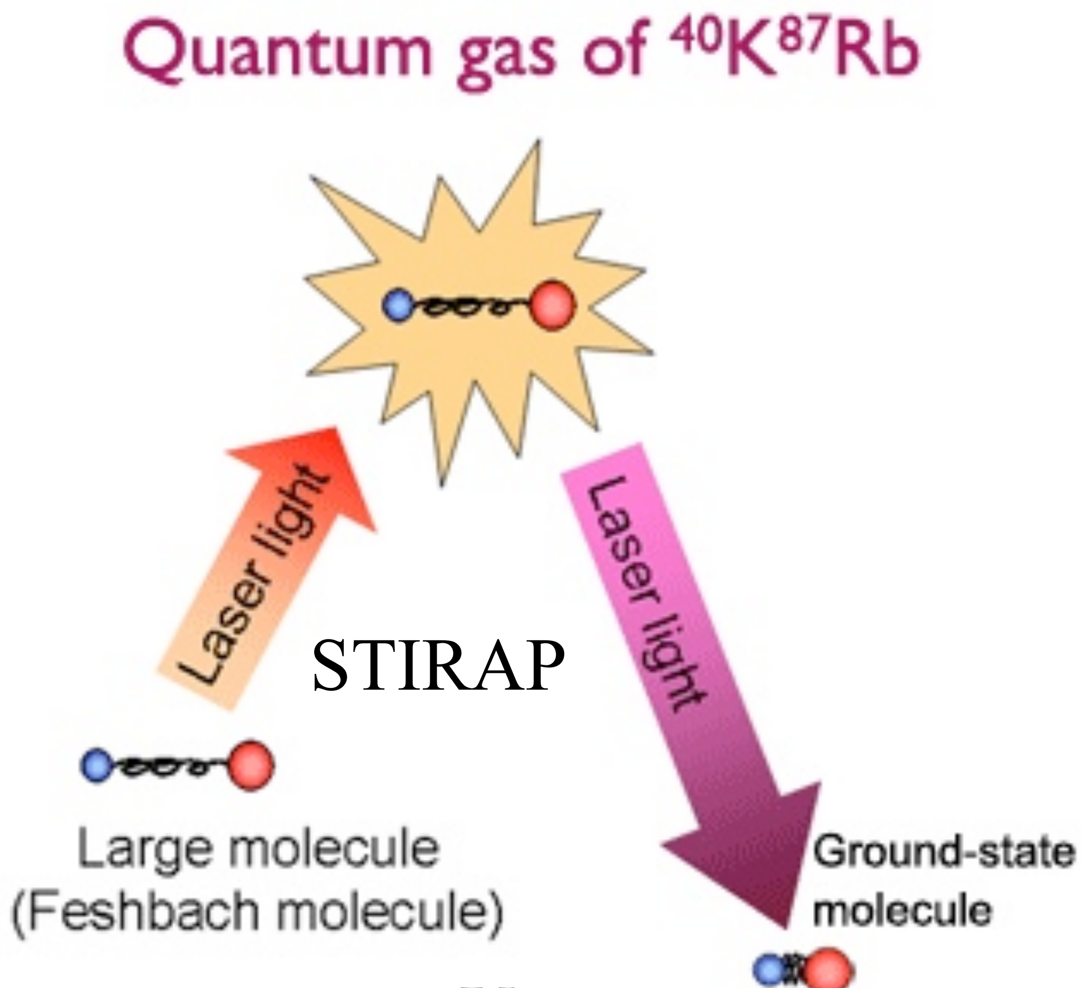
   - Competing orders and how we deal with it
   - What is bond order and when it is favored

3. Generalization: two-component dipolar fermions

   - p-wave spin density waves

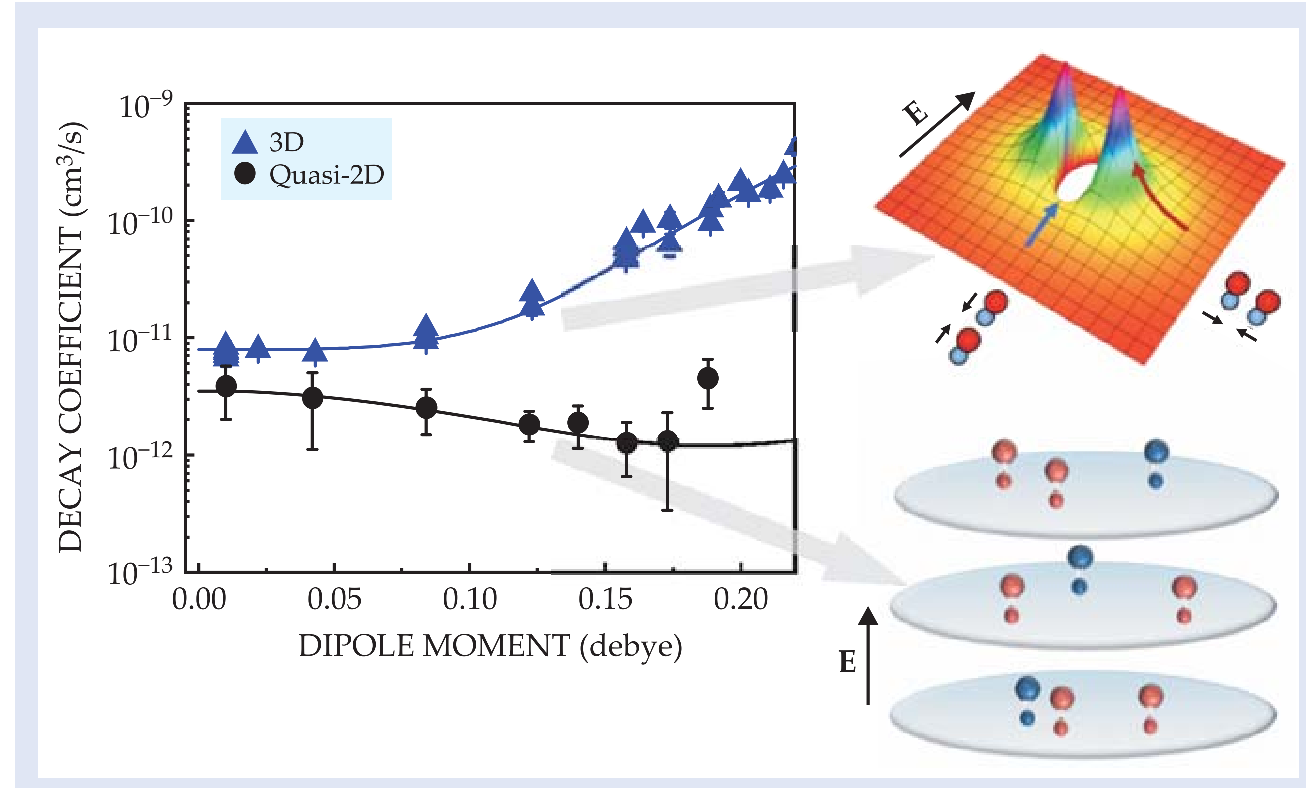
4. Proposal: quadrupolar quantum gases?

Ground state KRb in optical lattice at JILA



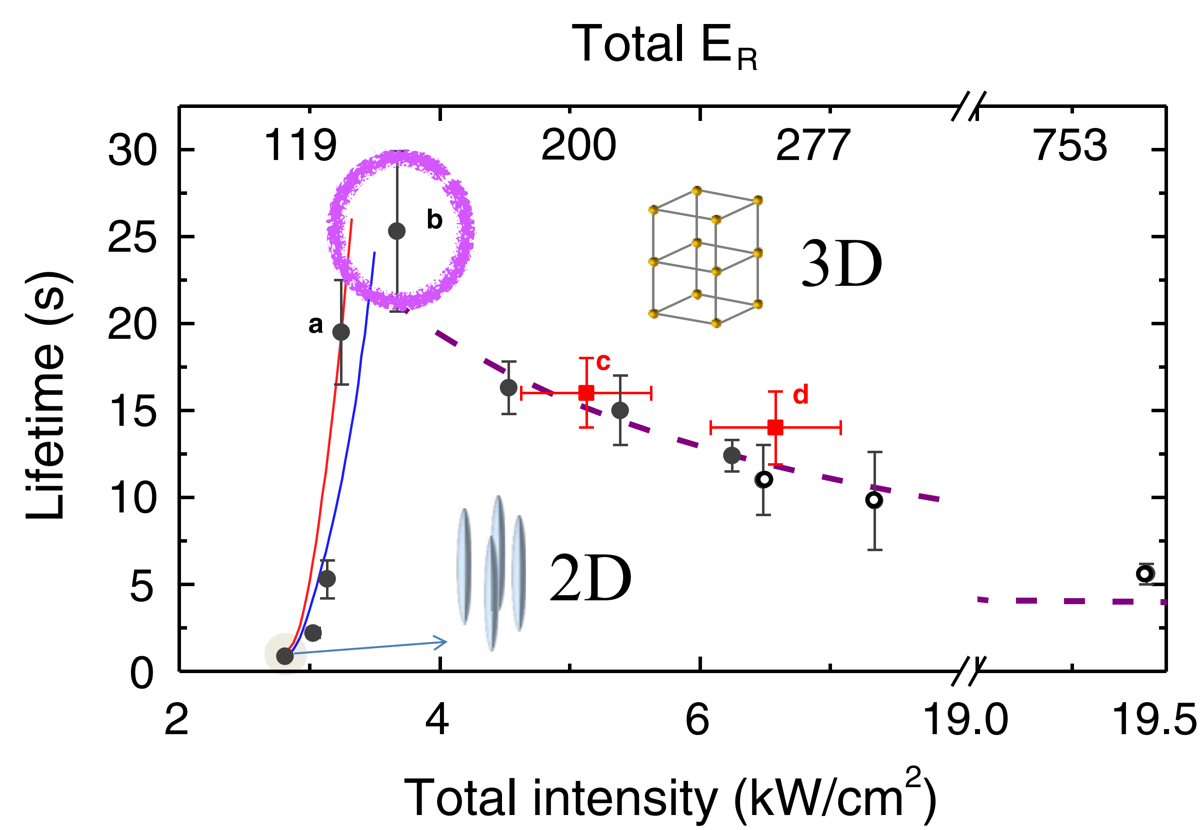
$$T \sim 400nK \sim 3T_F$$
$$d \sim 0.5 \text{ Debye}$$

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



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

Long life time when loaded in 3D and 2D optical lattice:

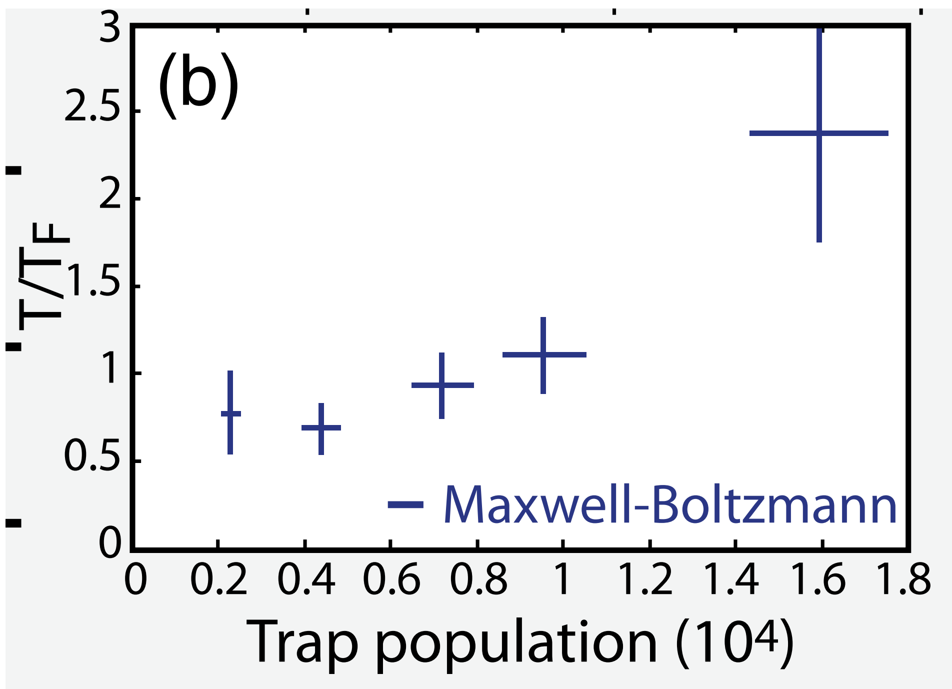


Chotia et al, PRL 108, 080405 (2012)

Quantum degenerate dipolar Fermi gas of ^{161}Dy atoms

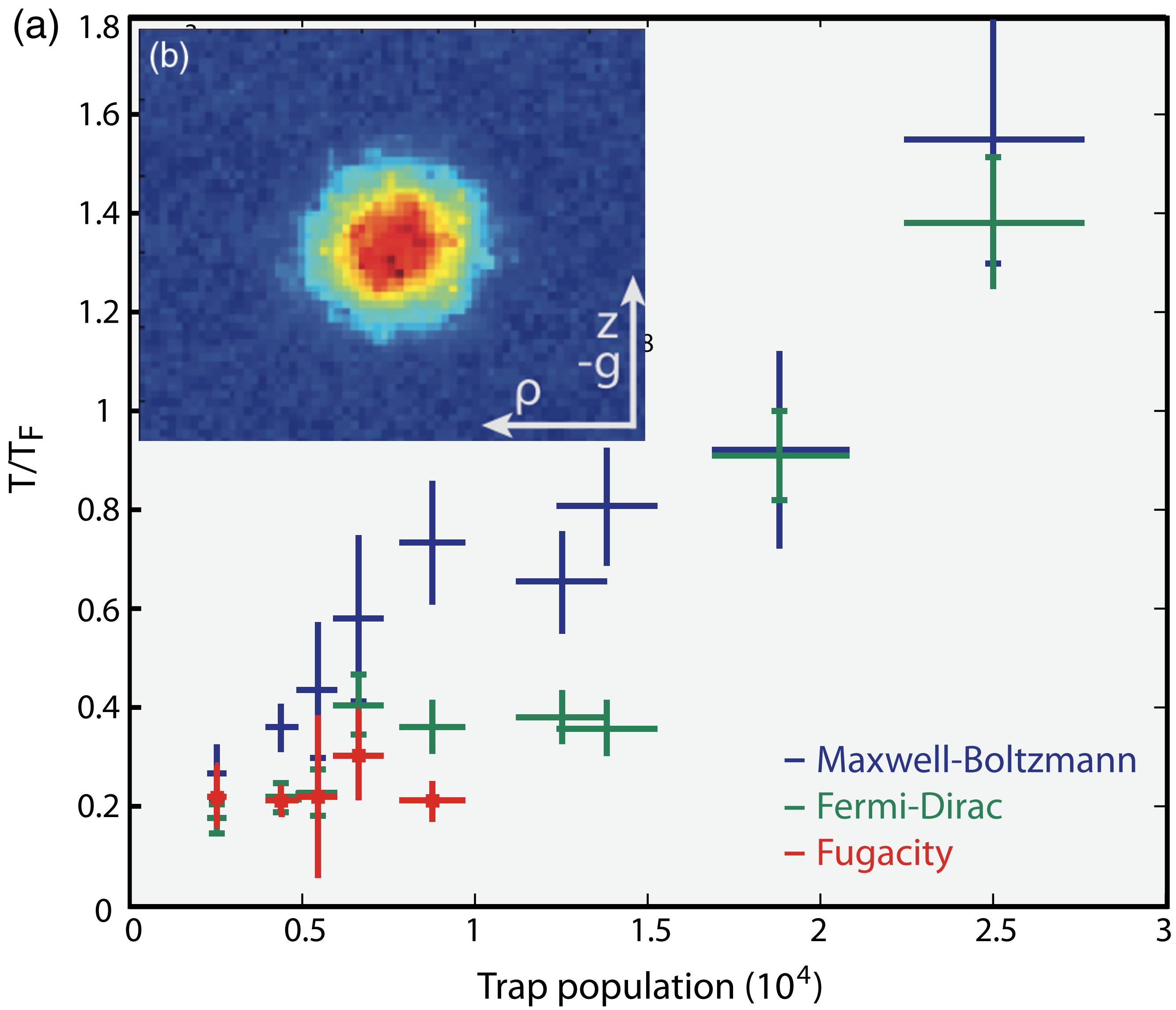
$$\mu = 10\mu_B \qquad |F, m_F\rangle = |21/2, -21/2\rangle.$$

Evaporative cooling of ^{161}Dy below quantum degeneracy:



$$T/T_F = 0.7$$
$$T_F = 500 \text{ nK}$$

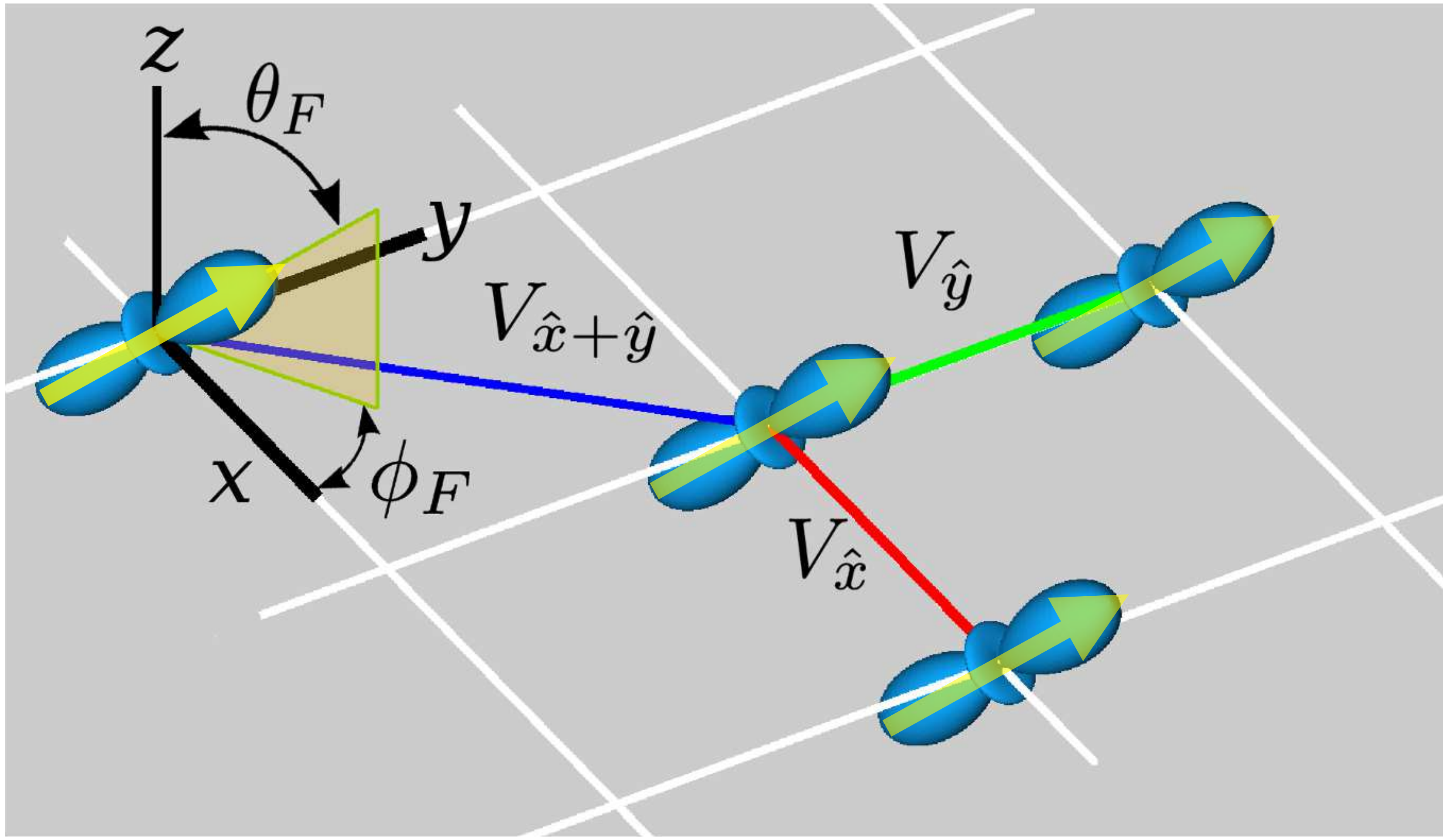
Sympathetic cooling of ^{161}Dy with bosonic ^{162}Dy



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

M. Lu, N. Q. Burdick, B. L. Lev, PRL 108, 215301 (2012)

Dipolar fermions on square lattice: model Hamiltonian



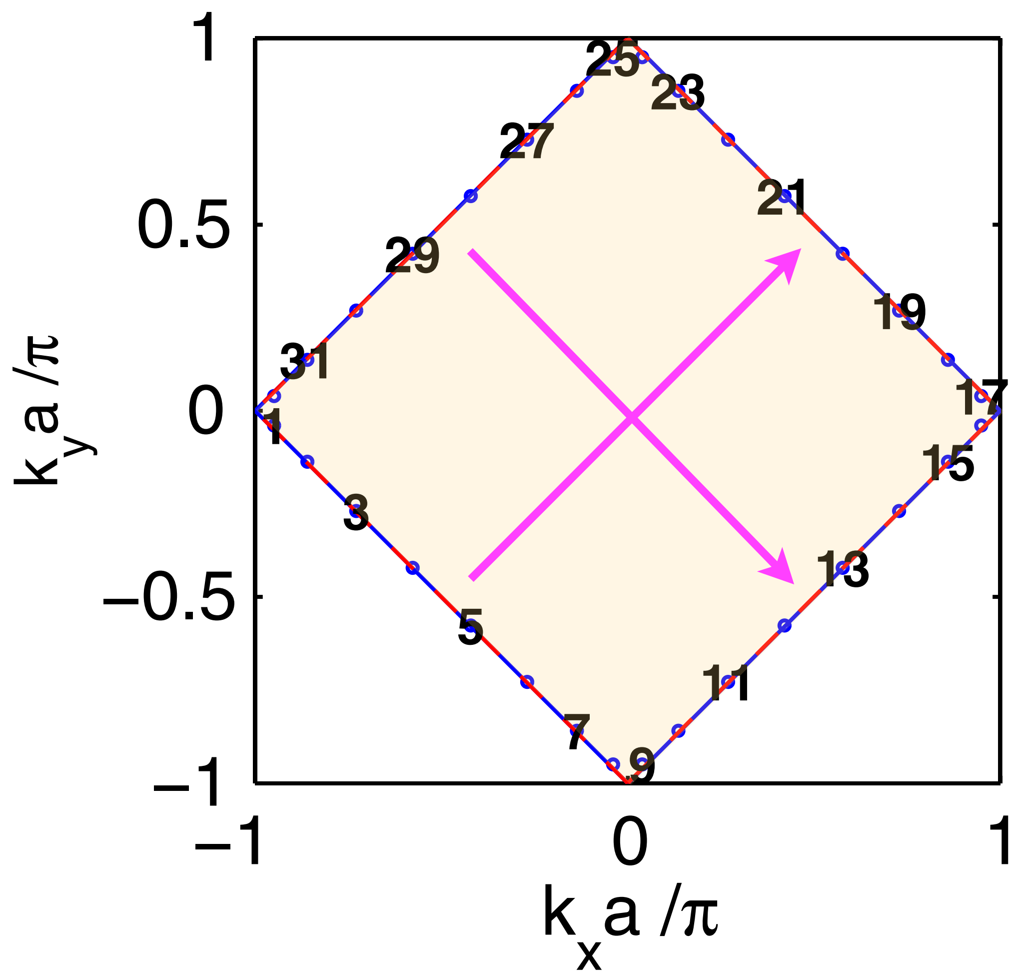
$$H = -t\sum_{\langle ij\rangle} a_i^\dagger a_j + \frac{1}{2}\sum_{i\neq j} V_{dd}(\mathbf{r}_{ij}) n_i n_j,$$

★ 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:



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

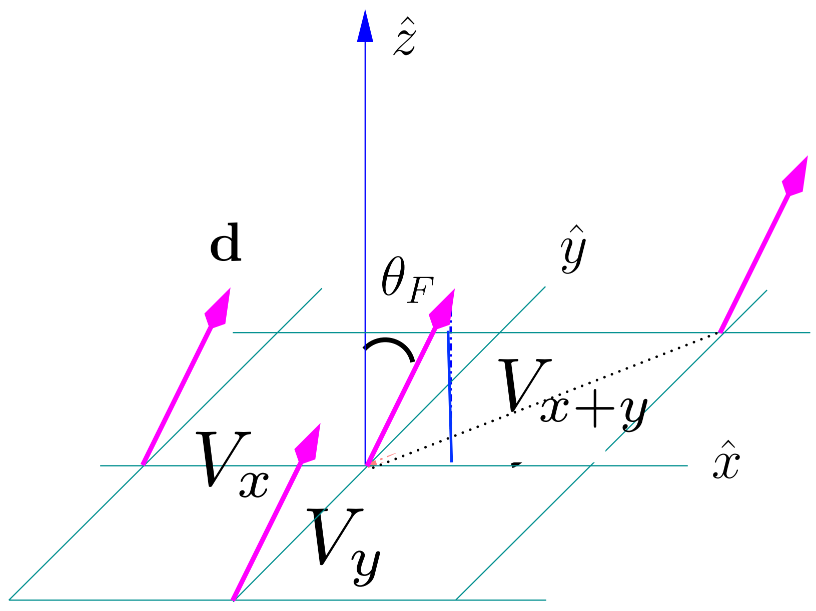
$$(a = 1)$$

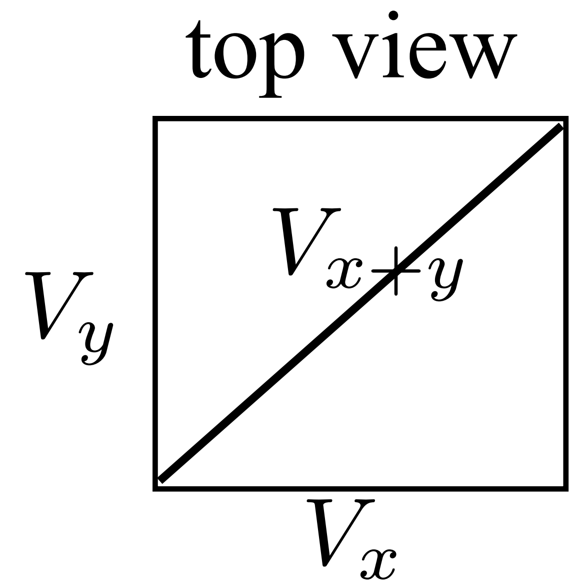
★ Perfect Nesting: **Q** couple **k** points on the opposite sides of the FS.

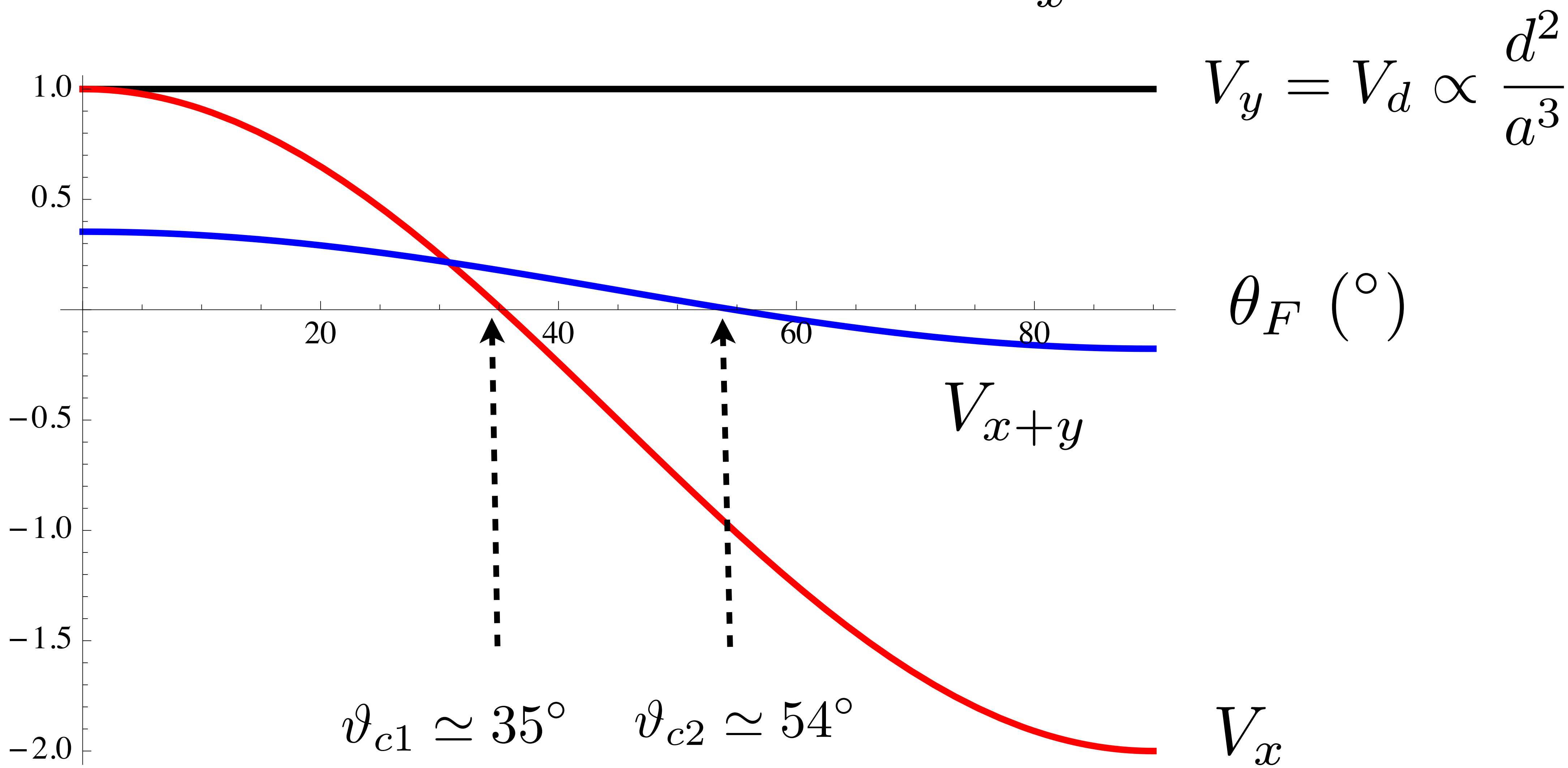
★ Later on, we will discretize the Fermi surface into N patches.

★ The Fermi surface may become unstable when V_{dd} is turned on.

Interactions for dipoles tilting in the x direction







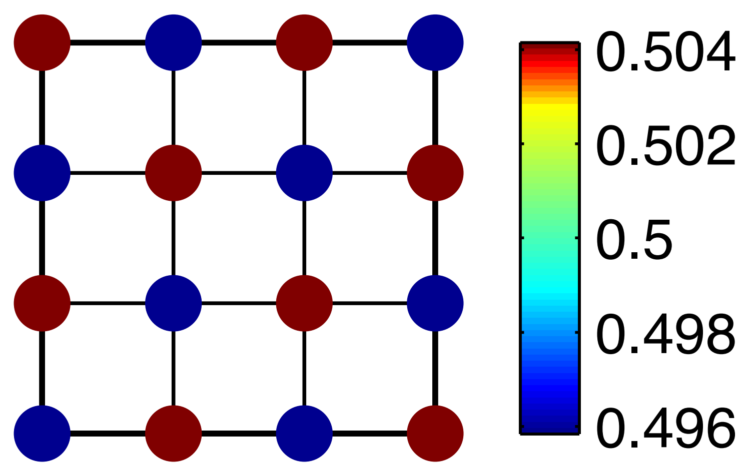
Two limits easy to understand

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 **k** space, this is an instability of FS in the particle-hole channel with **Q**.

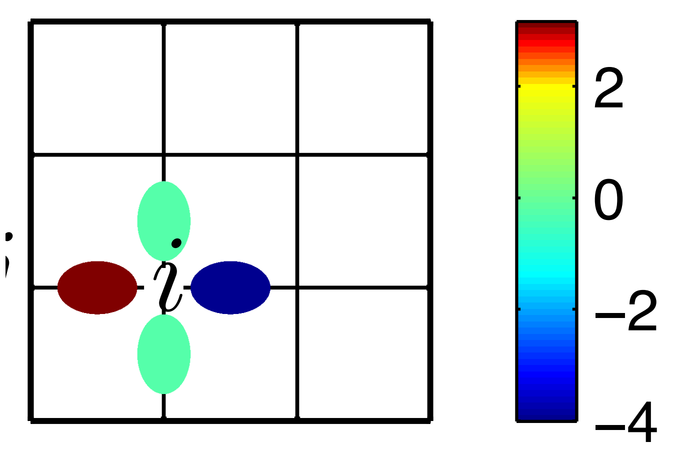


2. Large tilting angle ($\theta_F > \vartheta_{c2}$): V_x and V_{x+y} attractive, but V_y repulsive.

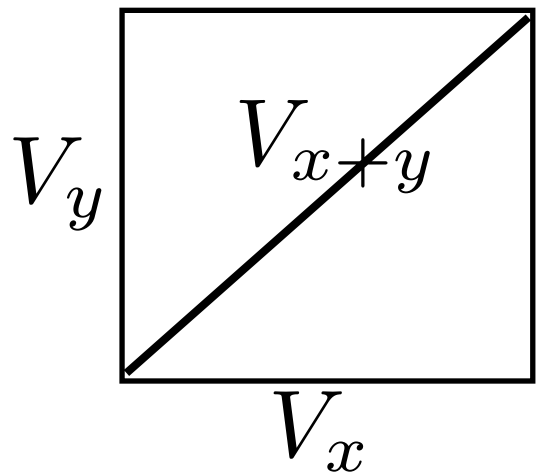
Anisotropic p-wave pairing (BCS):
The pairing order parameter

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

In **k** space, this is an instability of FS in the particle-particle channel.

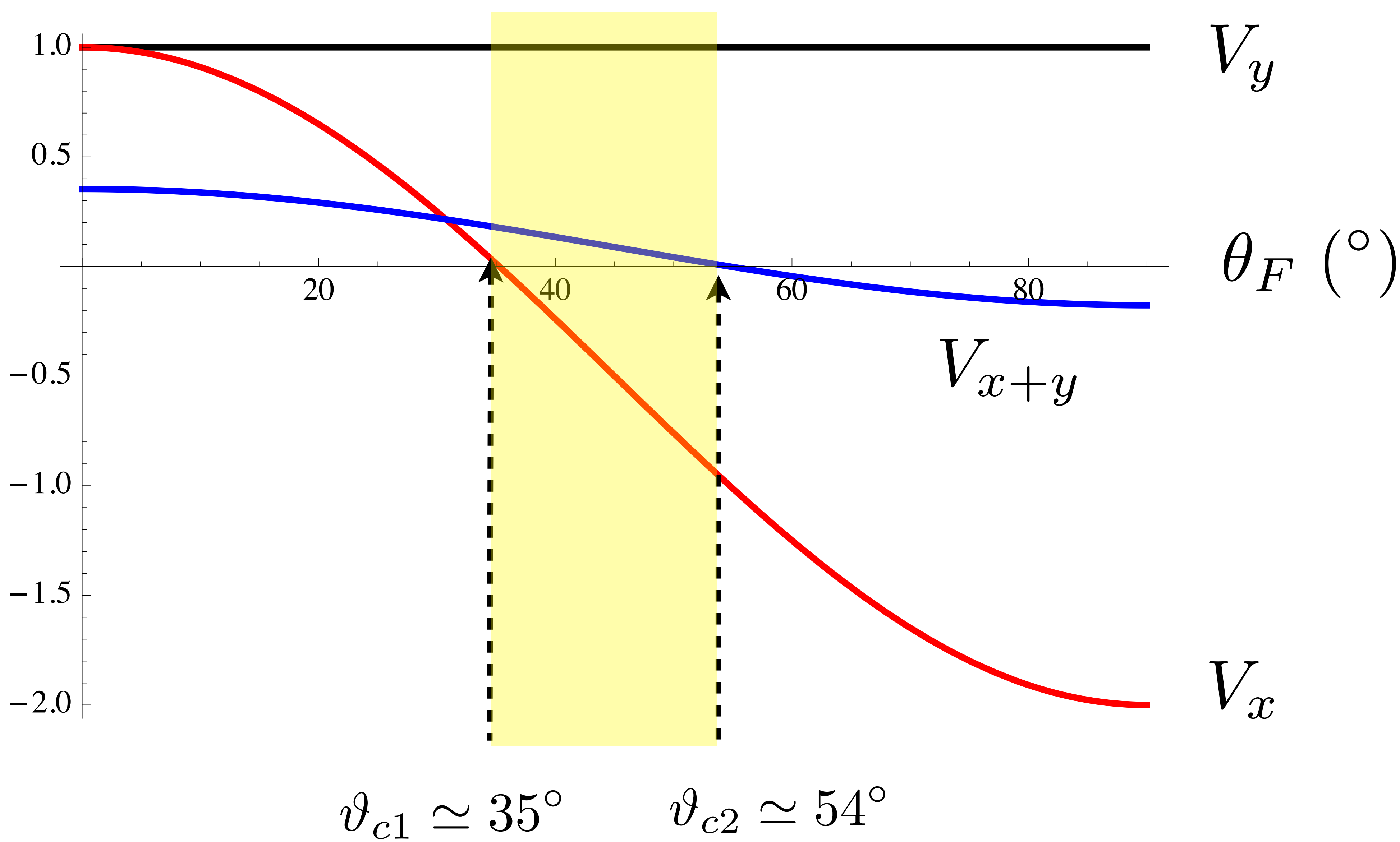


How about the intermediate tilting angle



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.

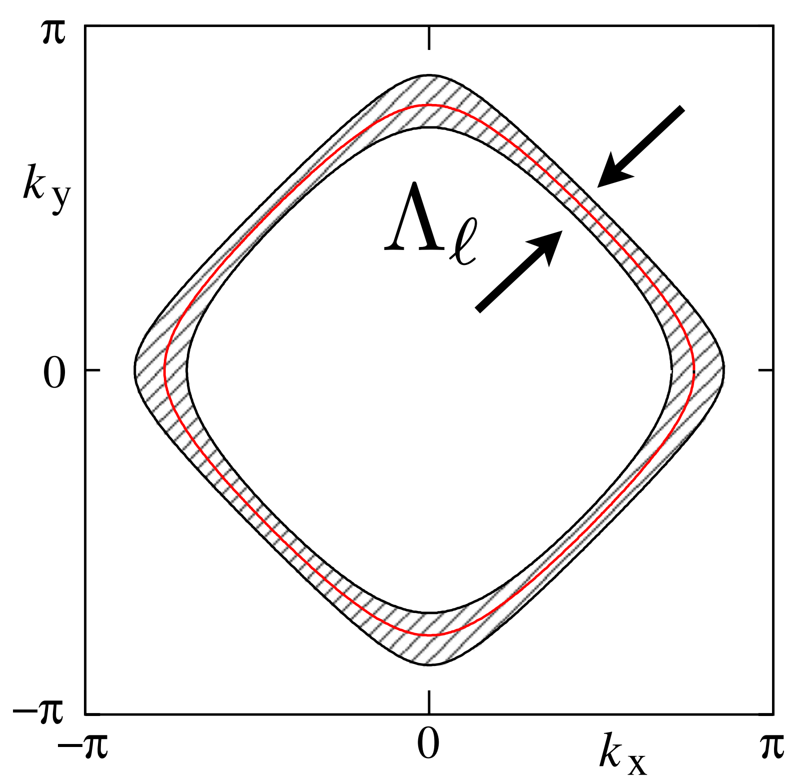
★ Or, some other completely different animal.

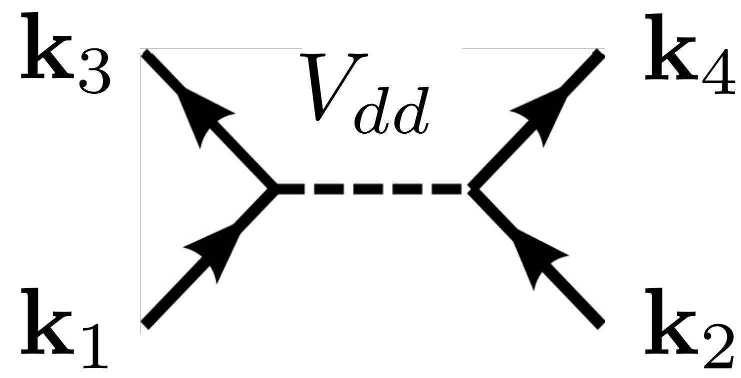
The problem of competing order is at the heart of the many-body physics of dipolar fermions.

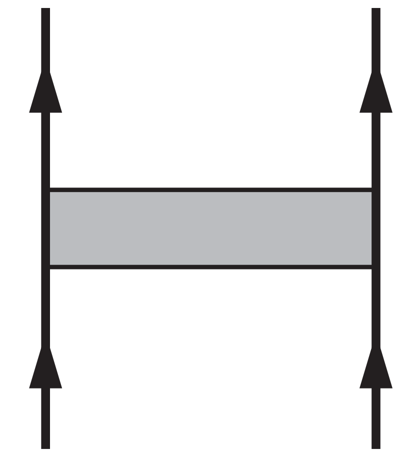
Simple mean field theories or perturbation theories, such as single-channel Renormalization Group or Random Phase Approximation, are insufficient/unreliable to treat competing orders in the regime of intermediate tilting angle.

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

Functional Renormalization Group (FRG)







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

$$\mathbf{k}_4 = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 \qquad \Lambda_\ell = \Lambda_0 e^{-\ell}$$

★ Separate the low-energy modes and high energy modes with scale Λ .

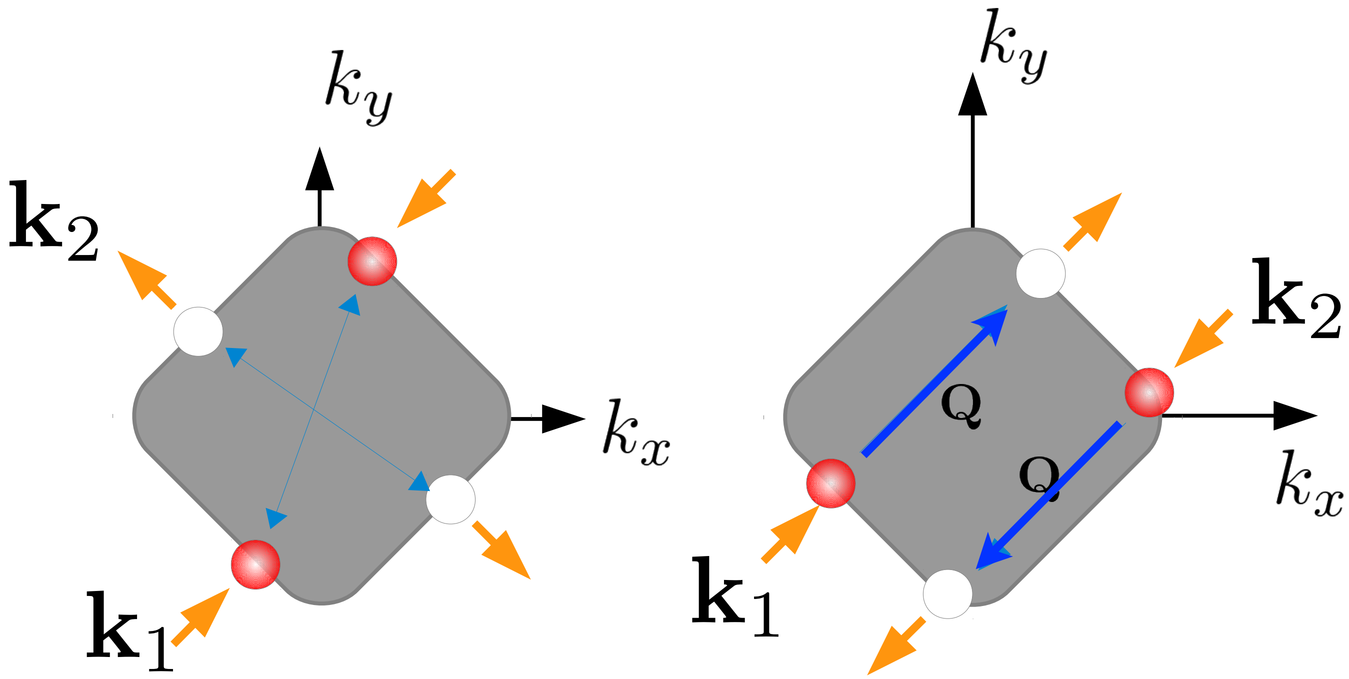
★ At each scale Λ, there is an effective theory description, including the effective interaction (vertex function) *U* between the low energy modes.

★ As Λ 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 **k**.

See e.g. Metzner et al, Rev. Mod. Phys. 84, 299–352 (2012); And reference therein.

FRG applied to interacting dipolar fermions



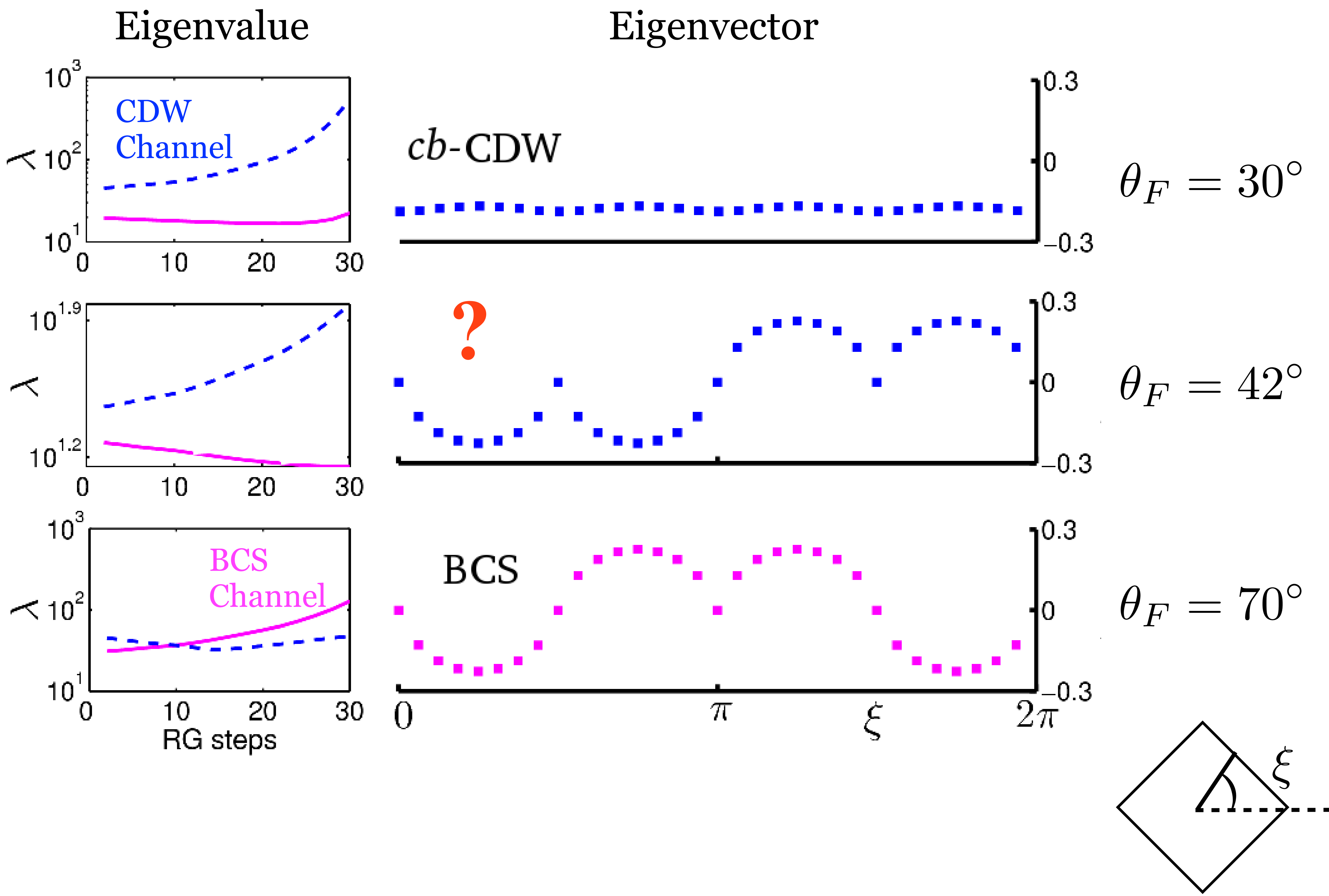
$U_\ell(\mathbf{k}_1, -\mathbf{k}_1, \mathbf{k}_2)$, $\quad$ $U_\ell(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_1 + \mathbf{Q})$,

BCS Channel $\quad$ 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 of the FRG results



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?

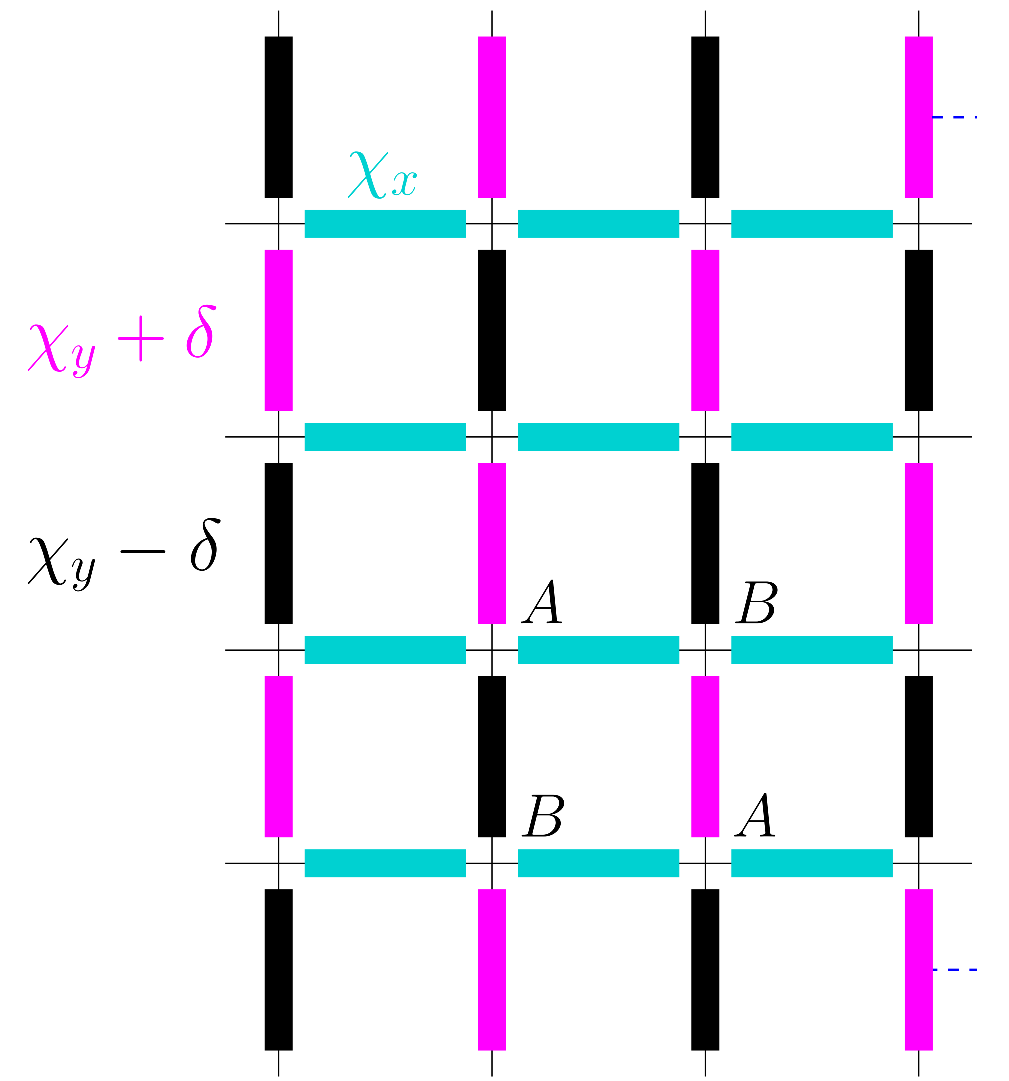
A mean field perspective:

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

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

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

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

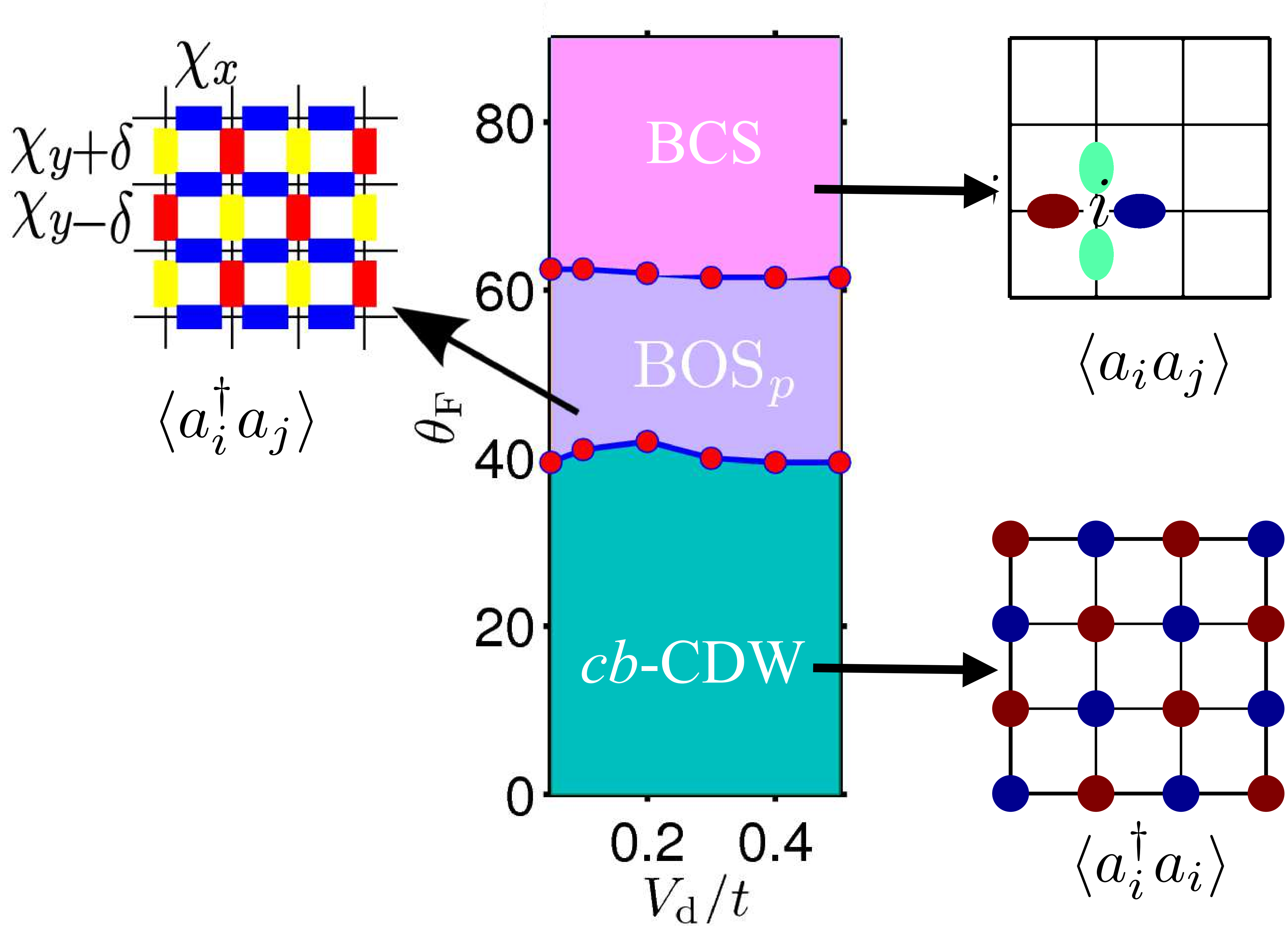


★ Opening up a gap at the Fermi surface.

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

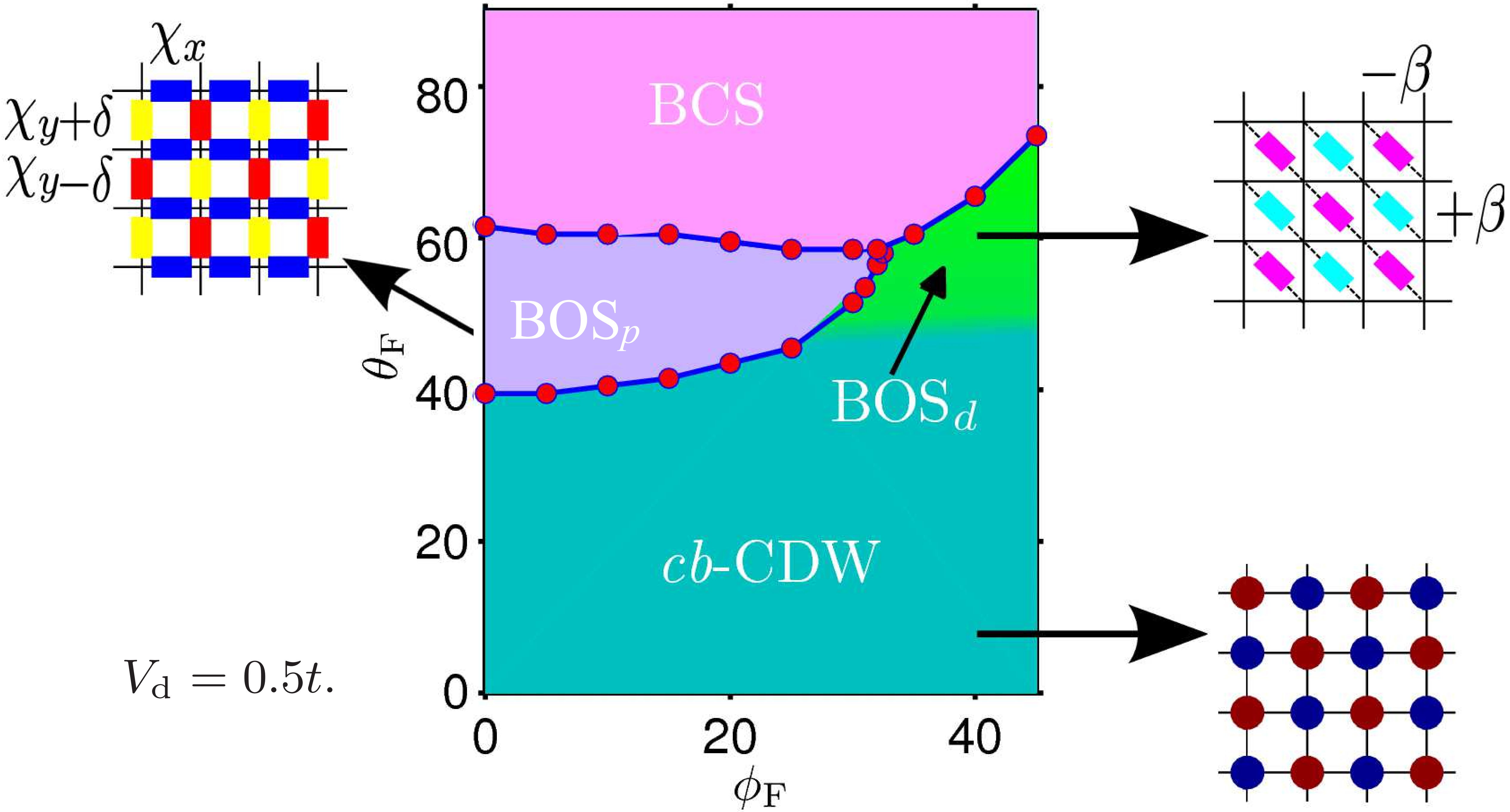
finite bond modulation δ is energetically favored

Phase diagram (T=0, half-filling, ϕ_F=0)



S. G. Bhongale, L. Mathey, S.-W. Tsai, C. W. Clark, EZ, PRL 108, 145301 (2012)

Phase diagram for general dipole tilting

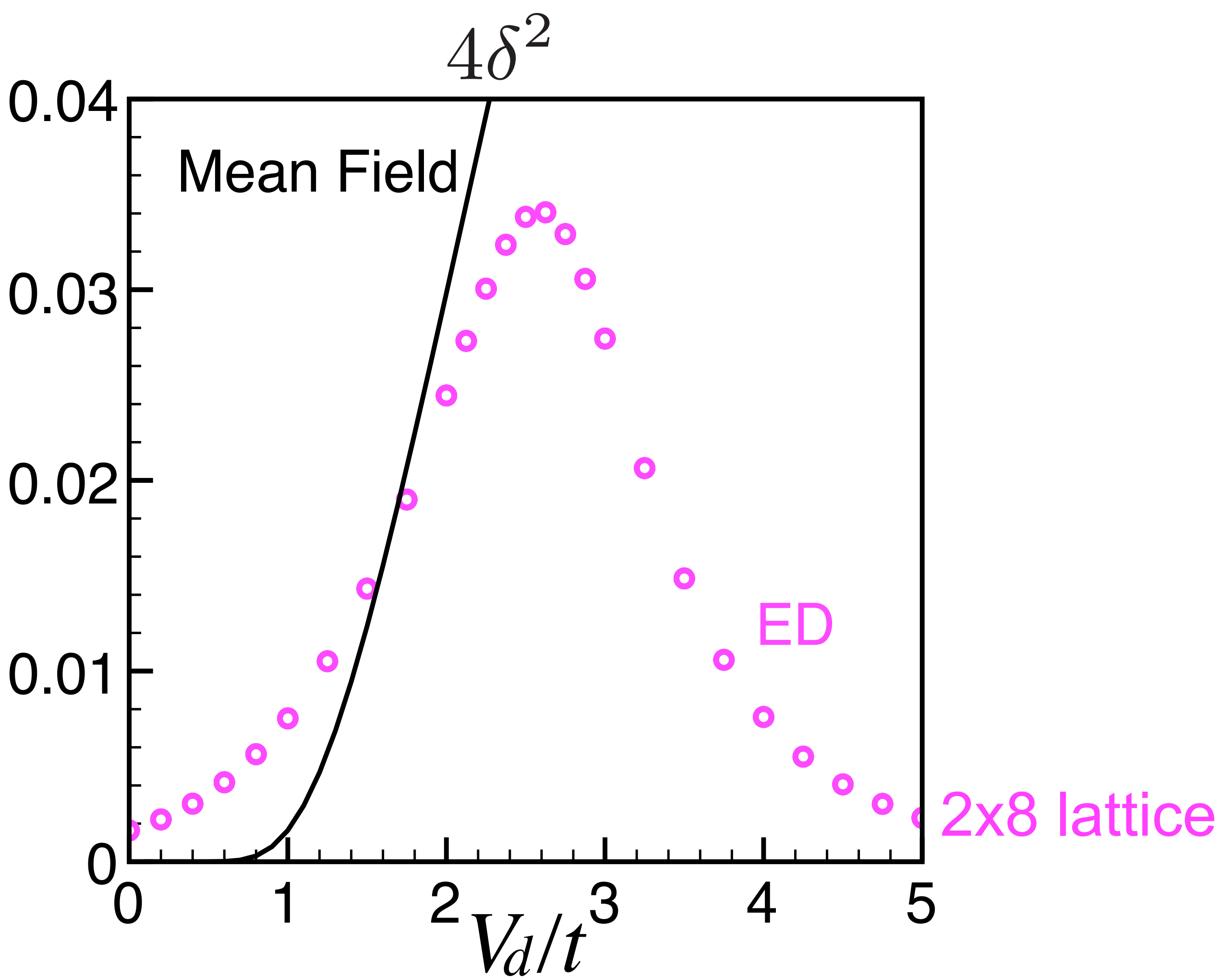


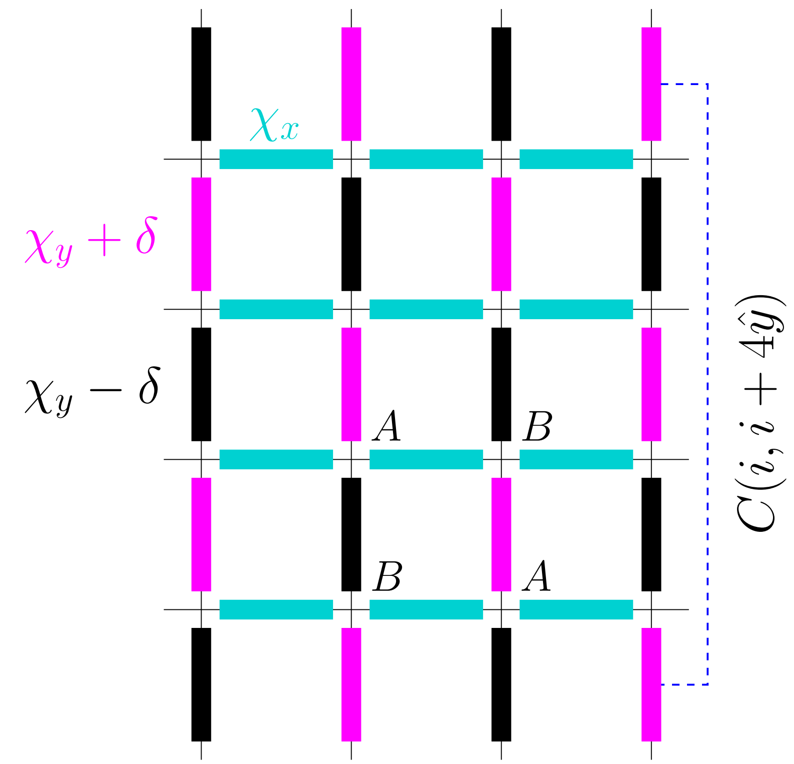
$V_\mathrm{d} = 0.5t.$

S. G. Bhongale, L. Mathey, S.-W. Tsai, C. W. Clark, EZ, PRL 108, 145301 (2012)

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

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

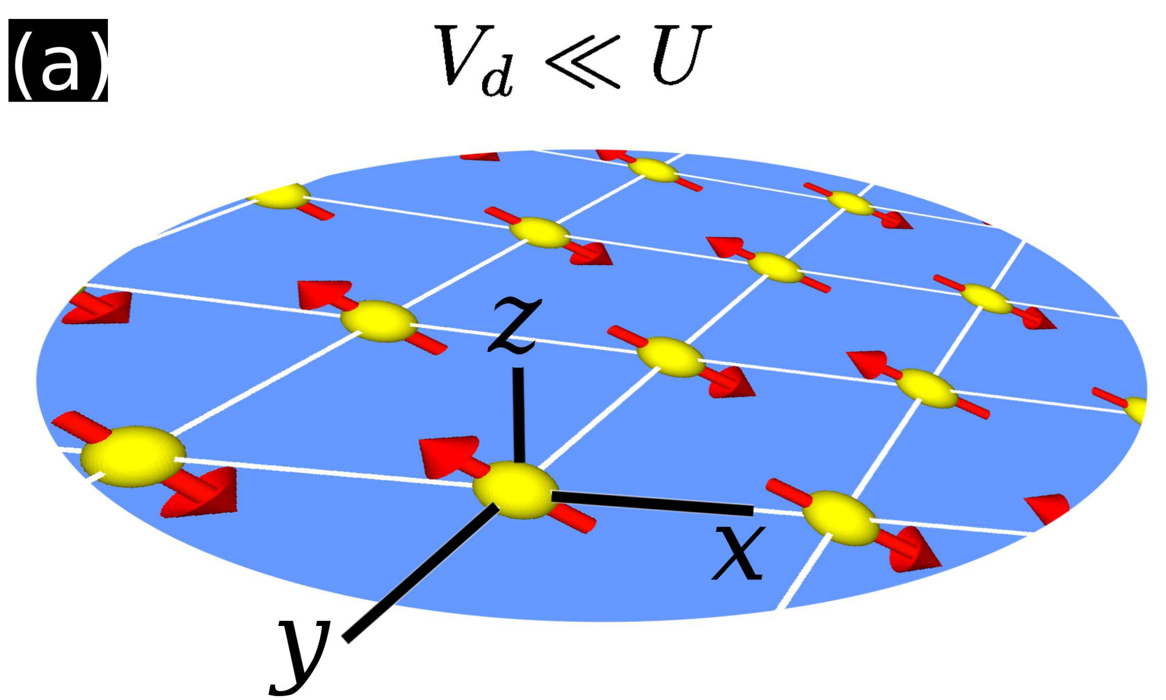
It approaches $4\delta^2$ in the limit of large $|i\text{-}j|$.

Two-component dipolar fermions

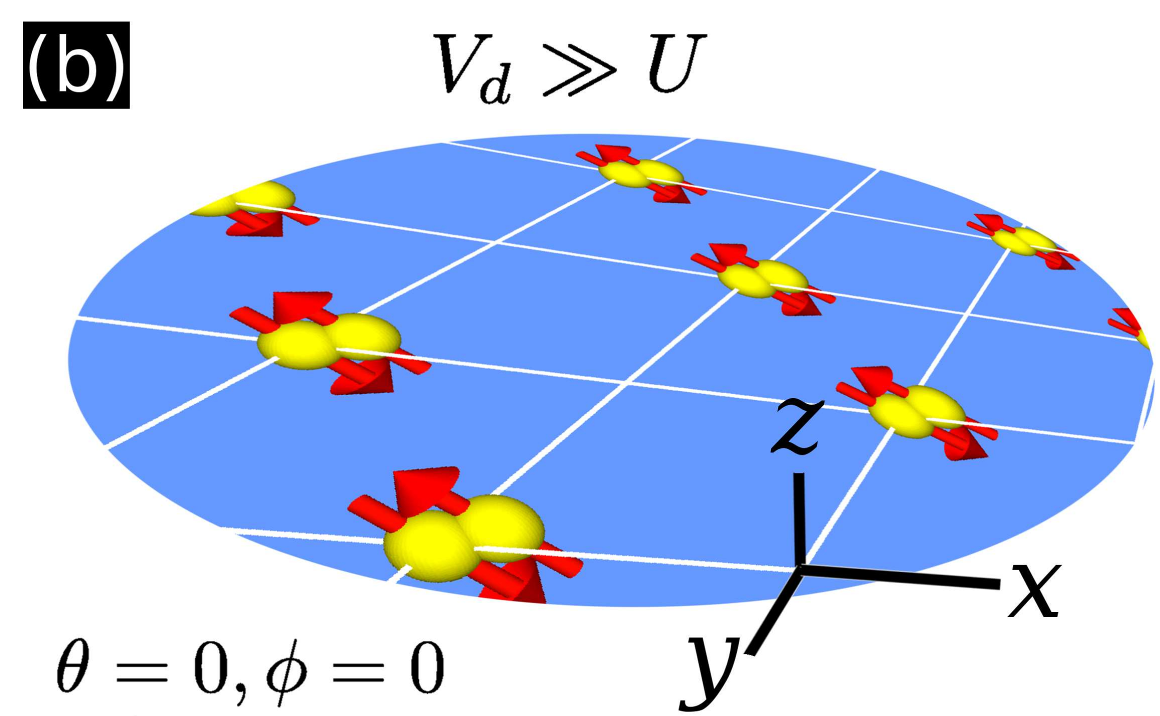
$$\hat{H} = -\sum_{\langle i,j\rangle,\sigma} t\hat{a}^{\dagger}_{j,\sigma}\hat{a}_{i,\sigma} + \frac{U}{2}\sum_{i,\sigma}\hat{n}_{i,\sigma}\hat{n}_{i,-\sigma} + \sum_{i\neq j} V_{ij}\hat{n}_i\hat{n}_j .$$

$$\hat{n}_i = \sum_{\sigma=\uparrow,\downarrow}\hat{n}_{i\sigma} = \sum_{\sigma}\hat{a}^{\dagger}_{i,\sigma}\hat{a}_{i,\sigma} \qquad \hat{\mathbf{S}}_i = \sum_{\alpha\beta}\hat{a}^{\dagger}_{i,\alpha}\boldsymbol{\sigma}_{\alpha\beta}\hat{a}_{i,\beta}$$

Plausible phases at half-filling (one fermion per site on average):



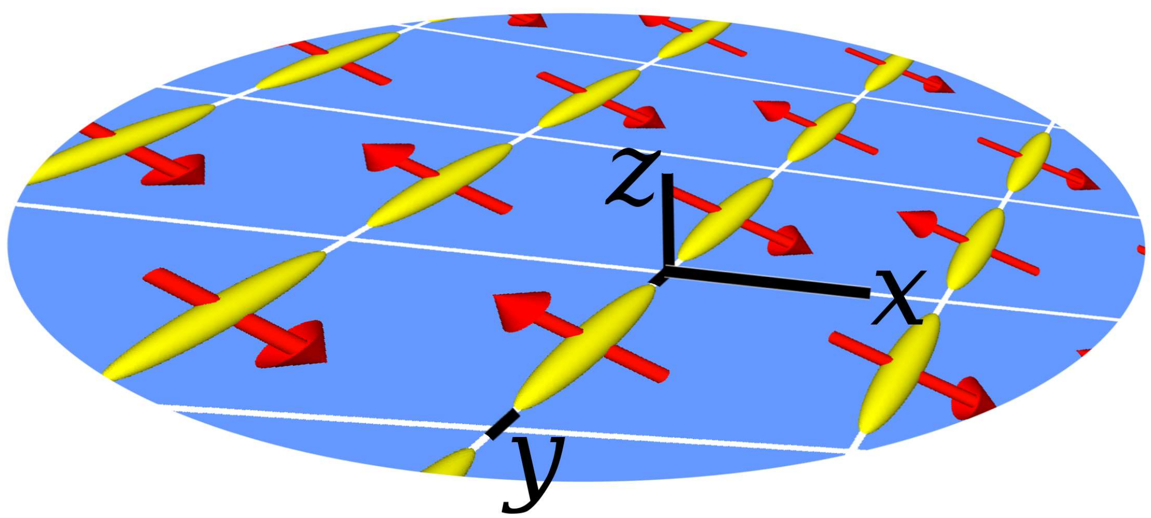
(s-wave) spin density wave $\langle\hat{\mathbf{S}}_i\rangle$



Charge density wave $\langle\hat{n}_i\rangle$

p-wave spin density waves (SDW)

(c) $V_d \gg U$



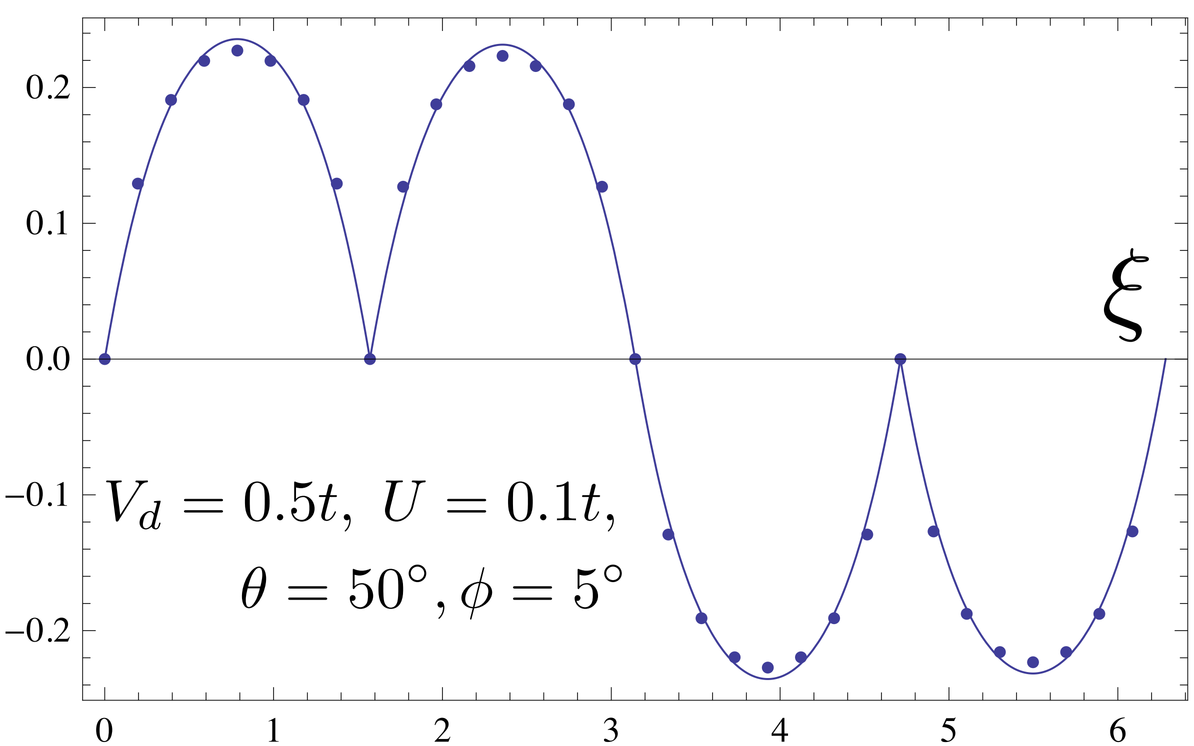
$\vartheta_{c1} < \theta < \vartheta_{c2};\ \phi \sim 0$

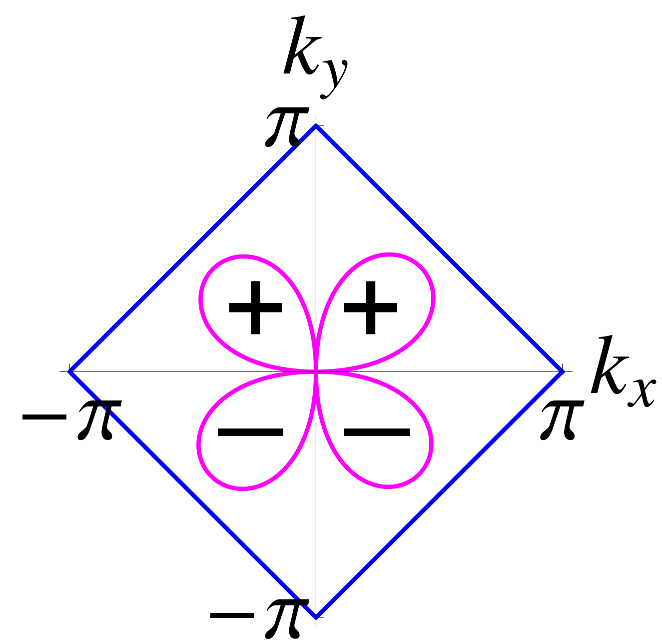
Periodic modulation of bond variable

$$\mathbf{S}_{i,i+y} = \sum_{\alpha\beta} \langle \hat{a}^{\dagger}_{i,\alpha} \boldsymbol{\sigma}_{\alpha\beta} \hat{a}_{i+y,\beta} \rangle$$

The order parameter of this exotic SDW phase is a vector in spin space. It is s defined on lattice bonds rather than on lattice sites.

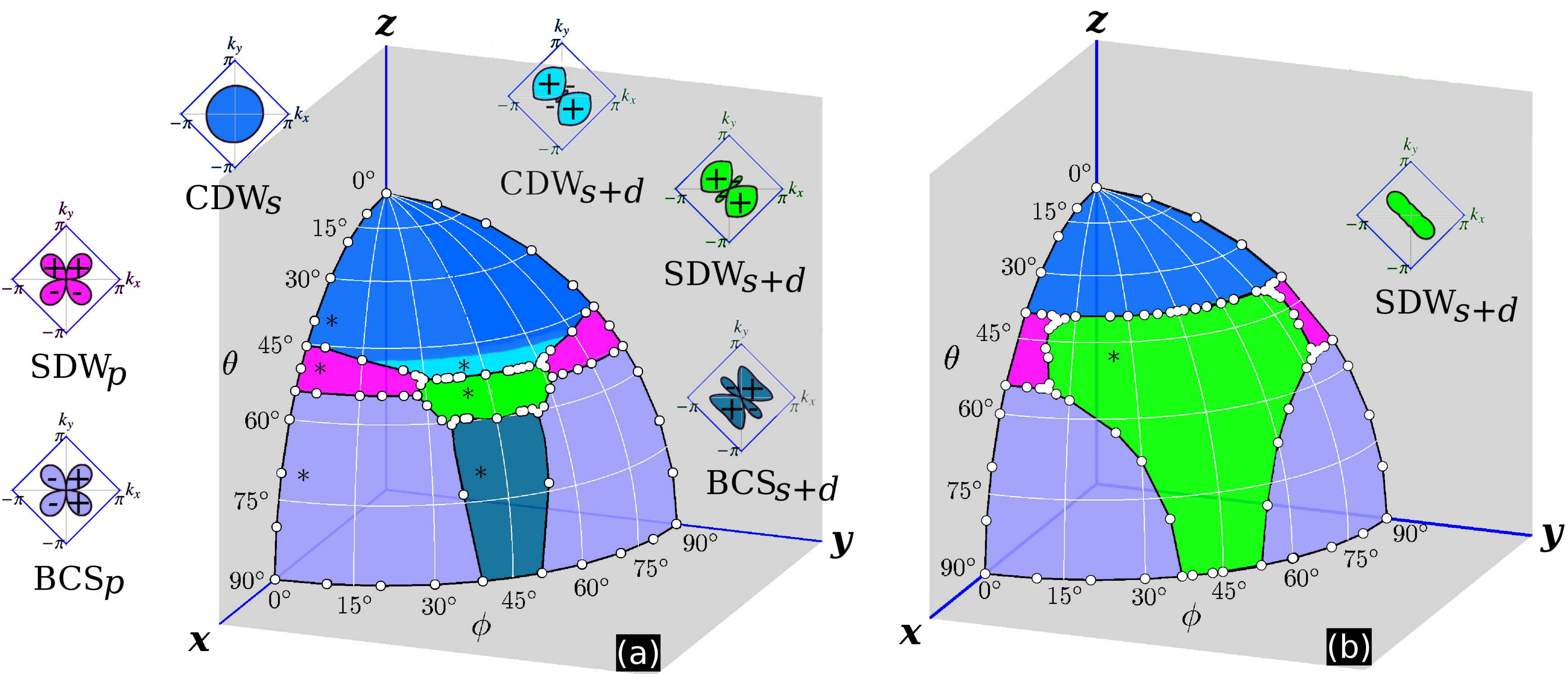
FRG: leading instability is in the SDW channel, and of p-wave symmetry.





$$\mathcal{U}_l^{\mathrm{SDW}}(\mathbf{k}_1, \mathbf{k}_2) = -\hat{X}\mathcal{U}_l^{\perp}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_1 + \mathbf{Q})$$

Phase diagram from FRG



$V_d = 0.5, U = 0.1$

$V_d = 0.5, U = 0.5$

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

S. G. Bhongale, L. Mathey, S.-W. Tsai, C. W. Clark, EZ, arXiv:1209.2671 (2012)

Classification of density waves

Superconductors (condensate of Cooper pairs):

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

s-wave superconductor, l=0
p-wave superconductors, l=1
d-wave superconductors, l=2
......

Density waves (condensate of particle-hole pairs):

$$\langle f_\alpha^\dagger(\mathbf{k}+\mathbf{Q}) f_\beta(+\mathbf{k})\rangle = \Phi(\mathbf{k})\delta_{\alpha\beta}$$

- s-wave CDW (checkerboard)
- p-wave CDW
- d-wave CDW (DDW) ...

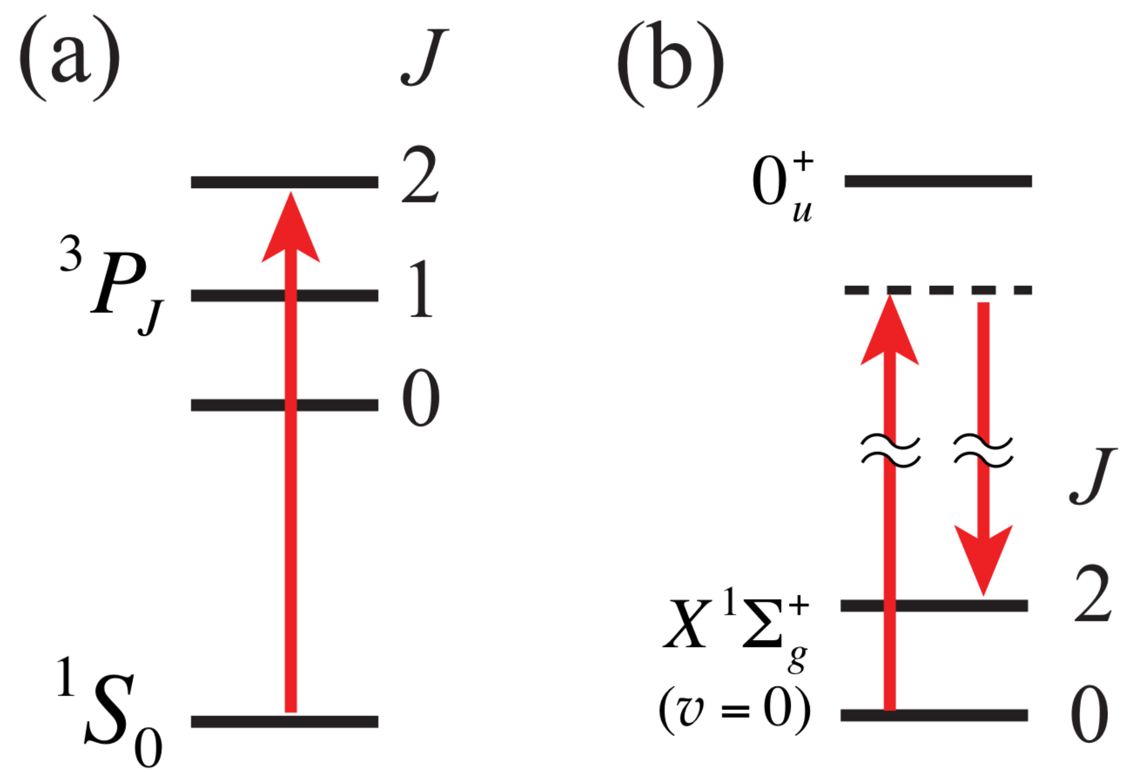
$$\langle f_\alpha^\dagger(\mathbf{k}+\mathbf{Q}) f_\beta(+\mathbf{k})\rangle = \boldsymbol{\Phi}(\mathbf{k}) \cdot \boldsymbol{\sigma}_{\alpha\beta}$$

- s-wave SDW (~Neel order)
- p-wave SDW...

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

They show up in dipolar Fermi gas!

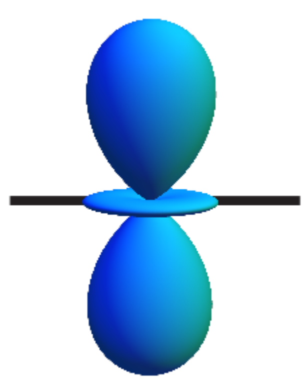
Atoms or molecules with quadrupole moments



Alkaline-earth atoms, such as Sr or Yb, prepared in long-living $^3P_{J=2}$ states.

Homonuclear molecules, such as Cs_2 or Sr_2, prepared in rotational state with J > 0,

External **B** (or **E**) field lifts the *M*-degeneracy, e.g., $|J=2, M=0\rangle$, which has zero dipole moment but a quadrupole moment on the order of 10-40 a.u.



(Proposal by Misha Lemeshko and Susanne Yelin.)

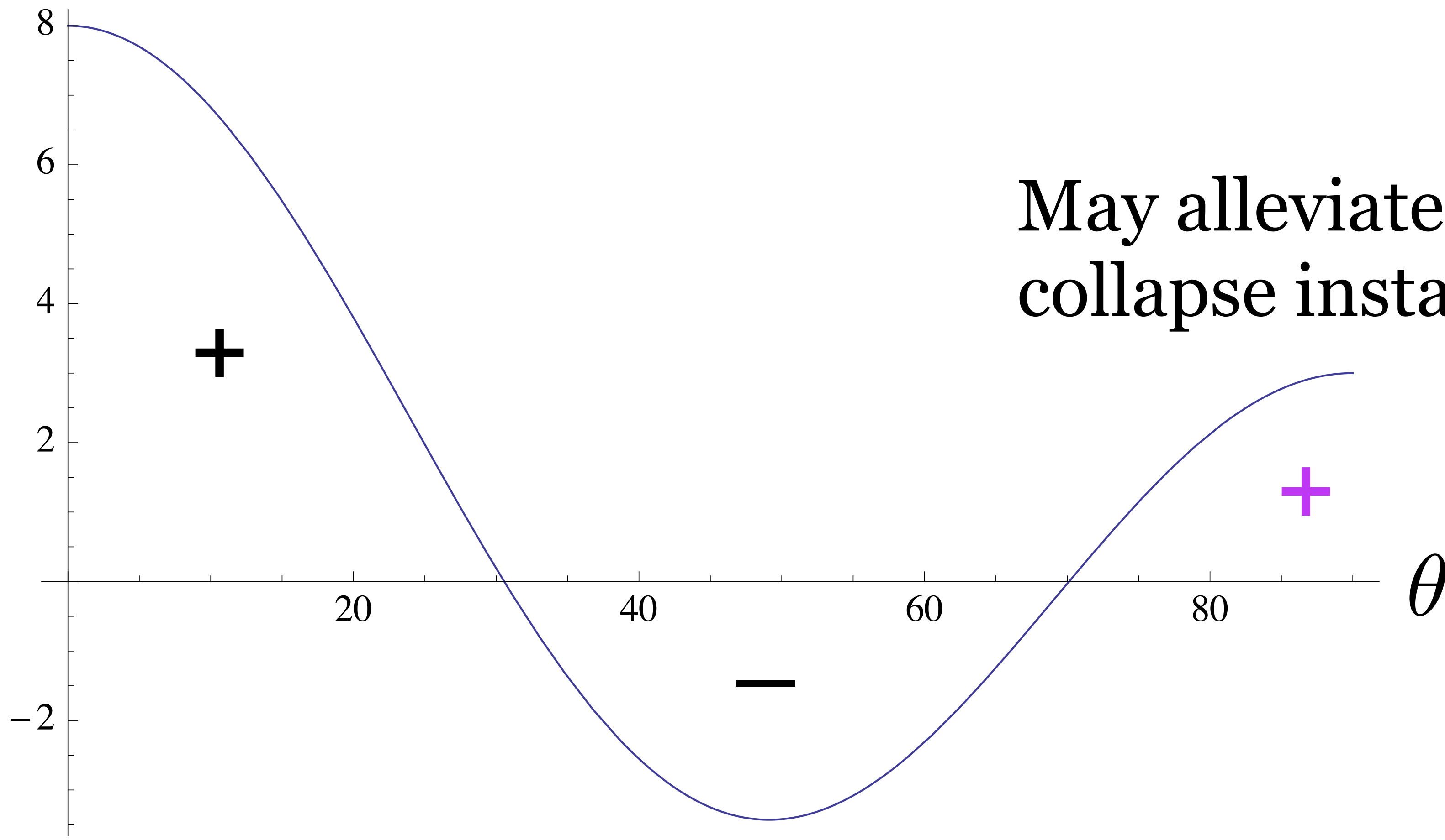
S. G. Bhongale, L. Mathey, EZ, S. F. Yelin, M. Lemeshko, arXiv:1211.3317 (2012)

Interaction between two quadrupoles

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

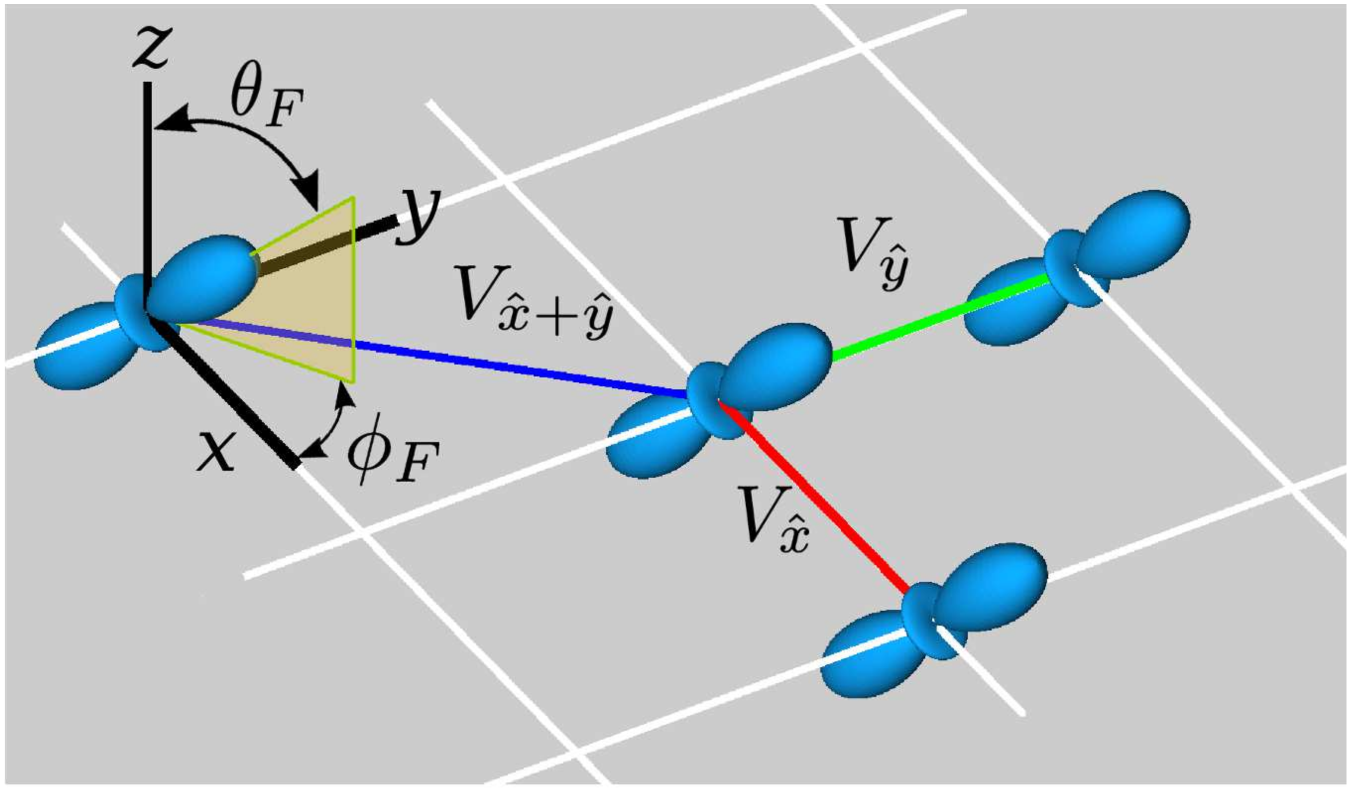
V depends on J,M; in the classical limit, $V = \dfrac{3Q_{zz}^2}{16}$

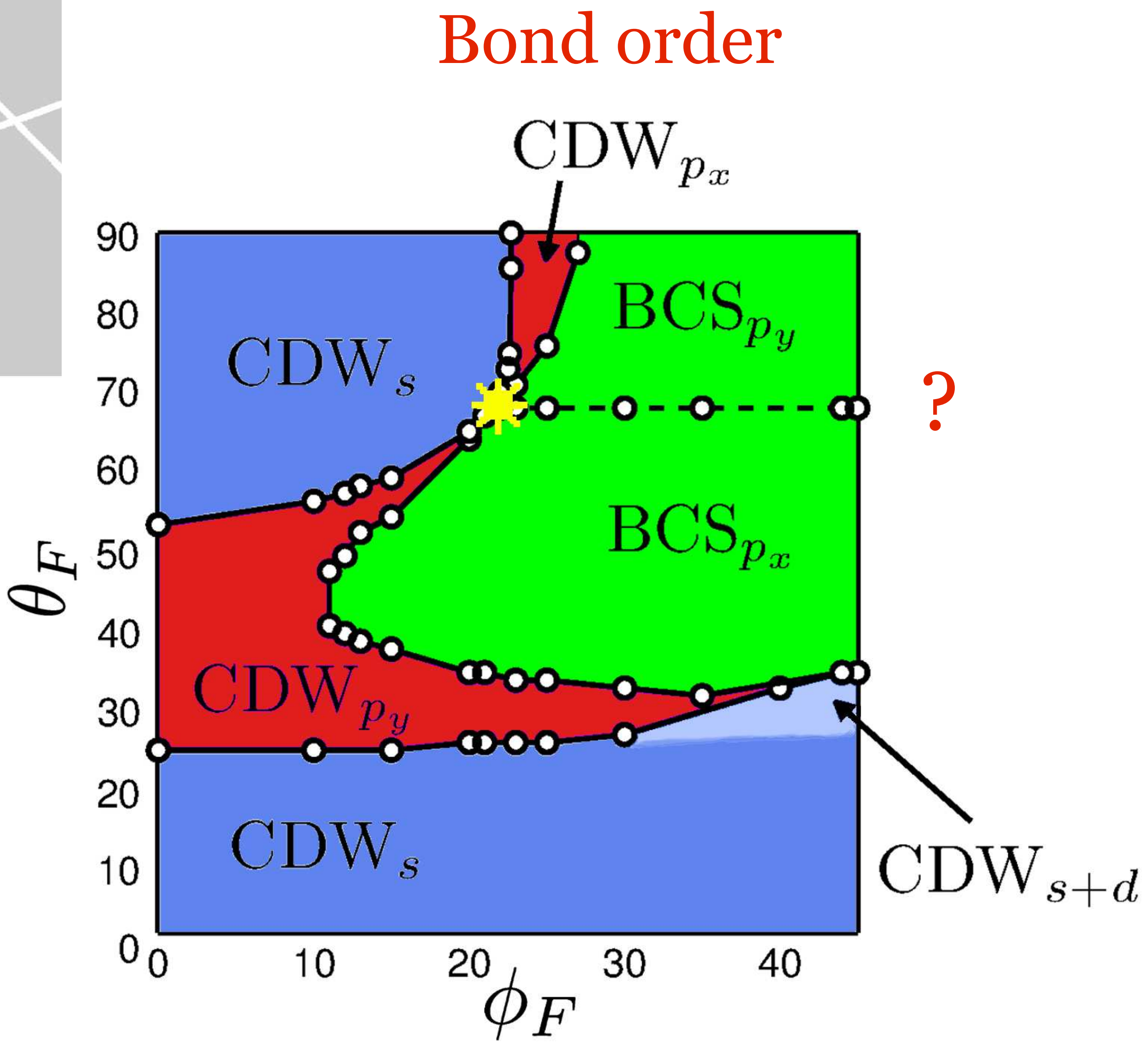
V^{qq} is on the order of Hz for optical lattice spacing of 266 nm (Lemeshko).



May alleviate/avoid collapse instability

Quantum phases of quadrupolar Fermi gas





S. G. Bhongale, L. Mathey, EZ, S. F. Yelin, M. Lemeshko, arXiv:1211.3317 (2012)

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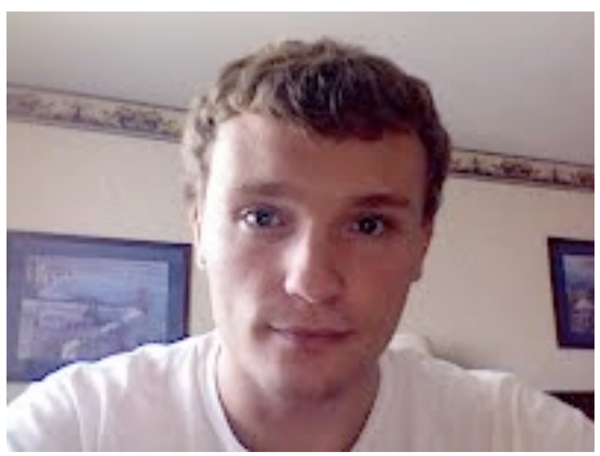

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arXiv:1211.3317 (2012)