

Correlated superconductivity comes in (at least) two varieties:

- Strongly correlated normal state exhibiting a "BCS-ish" pairing instability (?pnictides, ³He, heavy fermions, organics, e-doped cuprates, ...)
- Intrinsic strongly correlated SC, exerting major influence on surrounding "normal" state(s) (?pnictides, h-doped cuprates, ...)





Correlated Superconductors: Cu-oxides vs Fe-pnictides



Both have d-electrons in key role (Cu vs Fe) Both are layered (CuO₂ vs FeAs) Both have AF and SC in close proximity

However, there are also many differences! This may add up to new and interesting physics

Key Difference: 9 versus 6 d-electrons

ZT, Physics 2, 60 (2009)



In CuO_2 a single hole in a filled 3d orbital shell

 \rightarrow A suitable single band model might work

In FeAs large and even number of d-holes

 \rightarrow A multiband model is likely necessary

Cu-oxides: Mott Insulators \rightarrow Superconductors



In a half-filled band Coulomb repulsion $Un_{i\uparrow}n_{i\downarrow}$ $(U \gg t)$ keeps holes in place \Rightarrow Mott insulator + Neel antiferomagnet !!

> Only when doped with holes (or electrons) do cuprates turn into superconductors





How Mott insulators turn into superconductors, particularly in the pseudogap region, remains one of great intellectual challenges of condensed matter physics

Fe-pnictides: Semimetals \rightarrow Superconductors



semiconductor \rightarrow semimetal

 $\rightarrow \qquad FeAs are less$ correlated than CuO₂(correlations are stillimportant !!)

Phase diagram of Fe-pnictides

C. de la Cruz, et al., Nature 453, 899 (2008)



SC coexists with SDW (AF) in 122 compounds \rightarrow



Like CuO₂, phase diagram of FeAs has SDW (AF) in proximity to the SC state.

H. Chen, et al., arXiv/0807.3950



However, unlike CuO₂, all regions of FeAs phase diagram are (bad) metals !!



Minimal Model of FeAs Layers

V. Cvetkovic and ZT, EPL 85, 37002 (2009) C. Cao, P. J. Hirschfeld, and H.-P. Cheng, PRB 77, 220506 (2008) K. Kuroki et al, PRL 101, 087004 (2008)

Tight-binding model optimized Only nearest neighbor Fe-As, Fe-Fe,

for band structure + exps. and As-As hoppings are used. -1eV d_{xx-yy} d_{2zz-xx-yy} hole FS electron FS 2 pockets (valleys) 2 pockets (valleys)

Important: Near E_{F} e and h bands contain significant admixture of all five Wannier dorbitals, d_{xz} and d_{yz} of odd parity (in FeAs plane) and the remaining three d-orbitals of even parity in FeAs plane

Р,

a)

As one goes around the FS there is strong mixing of odd and even d-orbitals no simple orbital "topology" \Rightarrow

even parity







 d_{xz}

odd parity

d_{yz}

Nesting in Fe-pnictides

Cvetkovic & ZT, Korshunov & Eremin



If hole (Γ) and electron bands (M) are identical \Rightarrow perfect nesting at $\mathbf{q} = \mathbf{M} = (\pi, \pi) \Rightarrow$ strongly enhanced electron-hole excitations

$$\chi_0'(\mathbf{q}, \omega = 0) = 2\frac{m_e}{2\pi} \log \frac{\Lambda}{|\mathbf{q} - \mathbf{M}|},$$



Turning on moderate interactions \rightarrow VDW = itinerant multiband CDW (structural), SDW (AF) and orbital orders at **q** = **M** = (π , π)



Interactions in FeAs I

V. Cvetkovic and ZT, PRB **80**, 024512 (2009); J. Kang and ZT, arXiv:1011.2499

High multiband itinerancy implies significant metallic screening

Yang *et al*, PRB **80**, 014508 (2009): U_d not larger than ~ 2 eV, $J_{Hund} \sim 0.8$ eV from X-ray absorption \Rightarrow moderate correlations $U_d \sim t$, $J_{Hund} < U_d$

Consider $\frac{1}{2} \int d^2r d^2r' V(\mathbf{r}, \mathbf{r}') n(\mathbf{r}) n(\mathbf{r}')$, where $V(\mathbf{r}, \mathbf{r}')$ is the screened Coulomb repulsion \Leftrightarrow Hubbard-like Hamiltonian with U_d and J_{Hund} reflecting atomic limit Coulomb correlations

$$H_{\text{FeAs}} = -\sum_{ij,\alpha\beta} t_{ij}^{\alpha\beta} c_{i\alpha}^{\dagger} c_{j\beta} + \sum_{i,\alpha} \epsilon_{i}^{\alpha} c_{i\alpha}^{\dagger} + \frac{1}{2} U_d \sum_{i} n_{di}^2 - J_{\text{Hund}} \sum_{i} \mathbf{S}_{di}^2 + (\cdots)$$

Sawatzky et al discuss various interorbital interactions (\cdots)

Effective interaction at the Fermi surface:

$$\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \mathsf{\Gamma}_{lpha,eta,\gamma,\delta}(\mathbf{k},\mathbf{k}';\mathbf{q}) f^{\dagger}_{\mathbf{k}+\mathbf{q},lpha} f^{\dagger}_{\mathbf{k}'-\mathbf{q},eta} f_{\mathbf{k}',\delta} f_{\mathbf{k},\gamma}$$

 $\Gamma_{\alpha,\beta,\gamma,\delta}(\mathbf{k},\mathbf{k}';\mathbf{q}) \rightarrow U,W,G_1,G_2$

All flavor conserving (U, W) and flavor mixing (G_1, G_2) vertices

Interactions in FeAs II



Two Kinds of Interband Superconductivity



Interactions in FeAs III

V. Cvetkovic & ZT (RG) ; A. V. Chubukov, I. Eremin *et al* (parquet); F. Wang, H. Zhai, Y. Ran, A. Vishwanath & DH Lee (fRG) R. Thomale, C. Platt, J. Hu, C. Honerkamp & A. Bernevig (fRG)



The condition for interband SC is actually milder: suffices to have G₂* > U* even if G₂ << U

RG Theory of Interband Mechanism of SC in FeAs



In Fe-pnictides interband superconductivity (s' or s+- state) is a strong possibility but there is some fine tuning with SDW/CDW/ODW

What is a (THE) Model for Iron-Pnictides ? \rightarrow U(4)×U(4) Theory of Valley-Density Wave (VDW)



The first question: Itinerant or Localized? \Rightarrow Itinerant starting point for high T_c Fe-pnictides

> All e and h bands are identical \Rightarrow H_0 has SU(8) internal symmetry

$$H_0 = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}^{(0)} \left[\sum_{\alpha} h_{\mathbf{k}}^{(\alpha)\dagger} h_{\mathbf{k}}^{(\alpha)} + \sum_{\beta} e_{\mathbf{k}}^{(\beta)\dagger} e_{\mathbf{k}}^{(\beta)} \right]$$

This is highly idealized. In the real world:

- Pockets are not of same size (particularly h_2)
- Their shape differs ("elliptical" e versus "circular" h) Eremi

Eremin, Knolle

Key assumption I:

Differences among (e, h) pockets \ll effective bandwidth $D \sim E_F$

Furthermore, in real world, Γ s have strong orbital content:

- Vertices U, W, G_1 , and G_2 differ for e(h) pockets
- They have significant angular variation $\delta\Gamma$ around FS

Key assumption II:



Hirschfeld, Kuroki, Bernevig, Thomale, Chubukov, Eremin,

for moderate correlations $U_d \sim t, ~J_{\rm Hund} \ll U_d$

U(4)×U(4) Theory of Valley-Density Wave (VDW)

All e and h bands are identical \Rightarrow H_0 has SU(8) internal symmetry

 $H_0 = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}^{(0)} \left[\sum_{\alpha} h_{\mathbf{k}}^{(\alpha)\dagger} h_{\mathbf{k}}^{(\alpha)} + \sum_{\beta} e_{\mathbf{k}}^{(\beta)\dagger} e_{\mathbf{k}}^{(\beta)} \right]$

Effective interaction at the Fermi surface: $\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \Gamma_{\alpha,\beta,\gamma,\delta}(\mathbf{k},\mathbf{k}';\mathbf{q}) f^{\dagger}_{\mathbf{k}+\mathbf{q},\alpha} f^{\dagger}_{\mathbf{k}'-\mathbf{q},\beta} f_{\mathbf{k}',\delta} f_{\mathbf{k},\gamma} \rightarrow U, W, G_1, G_2$

Flavor-conserving vertices U and W

$$U, W \sim D$$

erving

$$U^{h} = J^{h} J^{h}$$

 $U^{h} = J^{h} J^{h}$
 $W = J^{h} J^{h} = G_{h} = M_{h} J^{h}$
 $W = J^{h} J^{h} = G_{h} = M_{h} J^{h}$

Flavor-changing vertices G_2 and G_1

V. Cvetkovic and ZT, PRB 80, 024512 (2009);

J. Kang and ZT, arXiv:1011.2499



 $H_{\text{int}} \to U^{(h)} \sum_{\alpha \alpha' \sigma \sigma'} h_{\sigma}^{(\alpha)\dagger} h_{\sigma'}^{(\alpha')\dagger} h_{\sigma'}^{(\alpha')} h_{\sigma}^{(\alpha)} + U^{(e)} \sum_{\beta \beta' \sigma \sigma'} e_{\sigma}^{(\beta)\dagger} e_{\sigma'}^{(\beta')\dagger} e_{\sigma'}^{(\beta')} e_{\sigma'}^{(\beta)} + 2W \sum_{\alpha \beta \sigma \sigma'} e_{\sigma'}^{(\beta)\dagger} h_{\sigma}^{(\alpha)\dagger} h_{\sigma}^{(\alpha)} e_{\sigma'}^{(\beta)} + (\cdots)$

 \rightarrow U(4)×U(4) symmetry \rightarrow unified spin and pocket/orbital flavors

Hierarchy of RG Energy Scales U, W >> $G_1, G_2 \rightarrow U(4) \times U(4)$ Theory of Valley-Density Wave (VDW) ^{V. Cvetkovic and ZT, PRB 80, 024512 (2009);} J. Kang and ZT, arXiv:1011.2499



$$H_{0} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}^{(0)} \left[\sum_{\alpha} h_{\mathbf{k}}^{(\alpha)\dagger} h_{\mathbf{k}}^{(\alpha)} + \sum_{\beta} e_{\mathbf{k}}^{(\beta)\dagger} e_{\mathbf{k}}^{(\beta)} \right]$$

All e and h bands are identical \Rightarrow H_0 has SU(8) internal symmetry

Orbital flavor-conserving vertices (U, W)reduce this to U(4)×U(4):

	<i>T</i> _s (K)	<i>T</i> _N (K)	$m_{ m ord}(\mu_{ m B})$
LaFeAsO	155	137	0.36
CeFeAsO	155	140	0.83
PrFeAsO	153	127	0.48
NdFeAsO	150	141	0.9
CaFeAsF	134	114	0.49
SrFeAsF	175	120	
CaFe ₂ As ₂	173	173	0.8
SrFe ₂ As ₂	220	220	0.94-1.0
BaFe ₂ As ₂	140	140	0.9

W do not vary much in different (e, h) channels

Finally, flavor-mixing vertices $G_{1,2}(\ll U, W)$ have the highest symmetry that physics will allow:

$$(\dots) \rightarrow 2G_1 \sum_{\substack{\alpha\beta\sigma\sigma'\\\alpha\beta'\sigma\sigma'}} (\sigma\sigma') e_{\sigma}^{(\beta)\dagger} h_{-\sigma}^{(\alpha)\dagger} h_{-\sigma'}^{(\alpha)} e_{\sigma'}^{(\beta)} + G_2 \sum_{\substack{\alpha\alpha'\beta\beta'\sigma\sigma'\\\alpha\sigma'}} (\sigma\sigma') h_{-\sigma}^{(\alpha)} e_{\sigma}^{(\beta)} h_{-\sigma'}^{(\alpha')} e_{\sigma'}^{(\beta')} \epsilon^{\alpha\alpha'} \epsilon^{\beta\beta'} + h.c.$$

	(h1)	(h2)	(e1)	(e2)	(h1,e1)	(h1,e2)	(h2,e1)	(h2,e2)	(h1,e1)	(h1,e1)
s	0.44	0.31	0.35	0.3 <mark>5</mark>	0.21	0.25	0.27	0.29	0.14	0.14
p	0.04	0.21	0.17	0.20	0.22	0.21	0.22	0.22	0.01	0.01
d	0.22	0.12	0.09	0.10	0.11	0.13	0.09	0.11	0.03	0.02

VDW in Fe-pnictides is a (nearly) U(4)×U(4) symmetric combination: SDW/CDW/ODW

Hierarchy of RG Energy Scales U, W \gg G₁, G₂ \rightarrow U(4) \times U(4) Theory of Valley-Density Wave (VDW)

Key assumptions:

V. Cvetkovic and ZT, PRB **80**, 024512 (2009); J. Kang and ZT, arXiv:1011.2499



Flavor-conserving vertices $(U, W) \sim D$; $\delta U, \delta W \ll D$; Flavor-changing vertices $G_1, G_2 \ll D$; Similarly, differences among (e, h) pockets $\ll D \rightarrow U(4) \times U(4)$ symmetric theory at high energies:

$$\exp\left(-W\sum c^{\dagger}_{\mu}c_{\mu}d^{\dagger}_{\nu}d_{\nu}
ight) \rightarrow \Delta_{\mu
u}\leftrightarrow\langle c^{\dagger}_{\mu}d_{\nu}
angle$$



$$\int \mathcal{D}\Delta \exp\left\{-\sum_{\mu\nu} \left[\frac{1}{W}|\Delta_{\mu\nu}|^2 - \Delta^*_{\mu\nu}c^{\dagger}_{\mu}d_{\nu} + h.c.\right]\right\}$$

U(4)×U(4) symmetric free energy: $F = \alpha \mathcal{T}r(\Delta^{\dagger}\Delta) + \frac{1}{2}\beta \mathcal{T}r(\Delta^{\dagger}\Delta\Delta^{\dagger}\Delta) \rightarrow \Delta = \Delta_{0}\mathcal{U}$

 $\mathcal U$ is a 4 \times 4 unitary matrix \rightarrow all combinations SDW/CDW/PDW

U(4)×U(4) symmetry at high energies \rightarrow Spin and pocket/orbital flavors all mixed \rightarrow VDW ground state (any combination of SDW/CDW/ODW)

At low energies, numerous terms break this $U(4) \times U(4)$ symmetry

$U(4) \times U(4)$ Symmetry vs Reality

J. Kang and ZT, arXiv:1011.2499

At low energy, numerous terms break $U(4) \times U(4)$ symmetry. We consider their influence at the leading order

Most important symmetry breaking terms are $G_{1,2} \ (\ll U, W)$. $G_1 < G_2$ for $J_{\text{Hund}} \ll U_d$.

 $\sim \Pi(0)^{2} \left\{ G_{2}^{eh_{1}} \left(\Delta_{11} \Delta_{22} + \Delta_{13} \Delta_{24} - \Delta_{12} \Delta_{21} - \Delta_{14} \Delta_{23} \right) \\ + G_{2}^{eh_{2}} \left(\Delta_{31} \Delta_{42} + \Delta_{33} \Delta_{44} - \Delta_{32} \Delta_{41} - \Delta_{34} \Delta_{43} \right) + h.c \right\},$ i) G_{2} fixes phases of different DWs. One expects $G_{2}^{eh_{1}}, G_{2}^{eh_{2}} > 0$, as prerequisite for high $T_{c} s^{+-}$ SC. Hence, the ground state is either real SDW or imaginary spin-singlet DW(s)

$$\begin{array}{c} \Gamma = (0,0) \\ \hline h_{1} \\ h_{2} \\ \hline h_{2} \\ \hline e_{y} \end{array} \begin{array}{c} M_{1} = (\pi,0) \\ R_{2} \\ \hline e_{y} \end{array} \begin{array}{c} M_{1} = (\pi,0) \\ R_{1} = \begin{pmatrix} G_{1}^{11} & \mathcal{R}eG_{1}^{12} \\ \mathcal{R}eG_{1}^{21} & G_{1}^{22} \end{pmatrix} \\ \hline For \ J_{\text{Hund}} \ll U_{d} \\ \text{typically} \ \lambda_{1} \sim 0 \end{array} \begin{array}{c} \Pi(0)^{2} \left\{ G_{1}^{11} \left(|\Delta_{11} + \Delta_{22}|^{2} + |\Delta_{13} + \Delta_{24}|^{2} \right) + \\ G_{1}^{22} \left(|\Delta_{31} + \Delta_{42}|^{2} + |\Delta_{33} + \Delta_{44}|^{2} \right) + \\ \left[G_{1}^{12} (\Delta_{11}^{*} + \Delta_{22}^{*}) (\Delta_{31} + \Delta_{42}) + h.c. \right] + \\ \left[G_{1}^{12} (\Delta_{13}^{*} + \Delta_{24}^{*}) (\Delta_{33} + \Delta_{44}) + h.c. \right] \right\} .$$

ii) Two real eigenvalues of $G_1 \rightarrow \lambda_1$, λ_2 if $\lambda_1, \lambda_2 > 0 \rightarrow two$ real SDWs. if $\lambda_1, \lambda_2 < 0 \rightarrow two$ imaginary SSDWs. if $\lambda_1 < 0$ and $\lambda_2 > 0 \rightarrow$ one real SDW and one imaginary SSDW.

Correction to free energy $\delta F[G_2]$:

Since $\lambda_1 \sim 0$ el-ph interaction or dynamical polarization from Pn bands could easily lead to $\lambda_1 < 0$ \rightarrow Pnictides are near $\lambda_1 = 0$ QCP !!

"Near" U(4)×U(4) Symmetry and Experiments

J. Kang and ZT, arXiv:1011.2499

"Direction" of U(4)×U(4) symmetry breaking fixed by flavor-mixing vertices $G_{1,2} (\ll U, W)$:



 $2G_1 \sum (\sigma\sigma') e_{\sigma}^{(\beta)\dagger} h_{-\sigma}^{(\alpha)\dagger} h_{-\sigma'}^{(\alpha)} e_{\sigma'}^{(\beta)} +$ $G_2 \sum (\sigma\sigma') h^{(\alpha)}_{-\sigma} e^{(\beta)}_{\sigma} h^{(\alpha')}_{-\sigma'} e^{(\beta')}_{\sigma'} \epsilon^{\alpha\alpha'} \epsilon^{\beta\beta'} + h.c.$ $\alpha \alpha' \beta \beta' \sigma \sigma'$ Two main predictions: i) SDW along x accompanied by imaginary PWD along y \rightarrow orbital/charge currents ii) Structural transition driven by PDW $\rightarrow T_s > T_N$. Fe As PHYSICAL REVIEW B 81, 014501 (2010)

Universal magnetic and structural behaviors in the iron arsenides

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Orbital "AF" \rightarrow Can this modulated current pattern be observed by neutrons? μ SR?



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A New Century of Superconductivity: Iron Pnictides and Beyond

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With the first century of superconductivity drawing to a close, a new frontier arose – the iron-based high-temperature superconductors. These materials have deep implications for fundamental physics. Their discovery opens a new path to explore the still-elusive phenomenon of high-Tc superconductivity and to address many fundamental questions related to the origin of the electron pairing in other unconventional superconductors, such as the cuprates, the heavy-fermions and the organics: What is the origin of the pairing and does it lead to the same or different pairing gap symmetries and why? What are the possible competing orders, like magnetism, and their origins? What are the limits on superconducting transition temperatures? The Workshop will focus on an in-depth theoretical exploration of these and related issues, assisted by guidance from several leading experimentalists, and in high celebratory spirit as we enter the new century of superconductivity.