

Angle-resolved photoemission spectroscopy (ARPES)

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Momentum conservation

$$\begin{split} H &= \sum_{i} \frac{\mathbf{p}_{i}^{2}}{2m} + \sum_{i} V(\mathbf{r}_{i}) \\ u_{i}e^{-i\mathbf{k}_{i}\mathbf{r}} & u_{f}e^{-i\mathbf{k}_{f}\mathbf{r}} \\ \Delta &= \frac{e}{mc}\mathbf{A}\mathbf{p} \\ w \propto |\langle\psi_{f}|\Delta|\psi_{i}\rangle|^{2}\delta(\varepsilon_{f} - \varepsilon_{i} - h\nu) \propto \left[\int\psi_{f}^{*}\mathbf{A}\cdot\nabla\psi_{i}d^{3}\mathbf{r}\right]^{2}\delta(\varepsilon_{f} - \varepsilon_{i} - h\nu) \\ \int\psi_{f}^{*}\mathbf{A}\cdot\nabla\psi_{i}d^{3}\mathbf{r} \ \delta(\varepsilon_{f} - \varepsilon_{i} - h\nu) = \mathbf{A}\cdot\int u_{f}^{*}e^{-i\mathbf{k}_{f}\mathbf{r}}\nabla(u_{i}e^{i\mathbf{k}_{i}\mathbf{r}})d^{3}\mathbf{r} \ \delta(\varepsilon_{f} - \varepsilon_{i} - h\nu) = \\ &= \mathbf{A}\cdot\int u_{f}^{*}e^{-i\mathbf{k}_{f}\mathbf{r}}(e^{i\mathbf{k}_{i}\mathbf{r}}\nabla u_{i} + u_{i}i\mathbf{k}_{i}e^{i\mathbf{k}_{i}\mathbf{r}})d^{3}\mathbf{r} \ \delta(\varepsilon_{f} - \varepsilon_{i} - h\nu) = \\ &= \mathbf{A}\cdot\int u_{f}^{*}(\nabla u_{i} + u_{i}i\mathbf{k}_{i})e^{i(\mathbf{k}_{i} - \mathbf{k}_{f})\mathbf{r}}d^{3}\mathbf{r} \ \delta(\varepsilon_{f} - \varepsilon_{i} - h\nu) \\ \mathbf{k}_{i} - \mathbf{k}_{f} = \mathbf{G} \end{split}$$

Momentum conservation for semi-infinite case



$$\varepsilon_i = \varepsilon_f - h\nu, \qquad \mathbf{k}_i^{\parallel} = \mathbf{k}_f^{\parallel} + \mathbf{G}$$







Angle-resolved photoemission spectroscopy (ARPES)



BESSY 1³ station



Scienta electron analyzer



Sample preparation



Sample preparation



BESSY 1³ station



Unitary ARPES image

Electronic band dispersion



Unitary ARPES image S 106eV -Kinetic energy (eV) 102 -101 -0.2 0.0 0.2 0.6 -0.8ky, 1/E -0.6 -0.4 0.4 Momentum (1/A) Stöwe et al. В Y D G G

Band dispersion from ARPES



2H-TaSe₂



Another typical experimental data set: 1T-TiSe₂



Another typical experimental data set: 1T-TiSe₂



Beamline



Excitation energy range





hv=200





Fermi surface





Aebi et al. (1996)

Borisenko et al. (1999)





Effects of interaction with bosonic mode







Kondo *et al., Nature* (2009)

ARPES data analysis



Nodal Direction of cuprates



Voigt fit of energy-momentum cut



Evtushinsky et al., PRB (2006)

Spectral Function Extraction from ARPES Data

$l(k, \omega) \propto A(k, \omega) \otimes R(k, \omega)$

We measure $I(k, \omega)$ We are interested in $A(k, \omega)$ We need to remove $R(k, \omega)$



Spectral line shape



Linewidth from Voigt Fit



Evtushinsky et al., PRB (2006)




Comparison to the low-energy highresolution data



Temperature dependence of scattering rate $\Sigma''(\omega=0,T)$



Temperature dependence of scattering rate



ARPES on charge-density-wave compounds

Phase diagram



Morosan et al., Nat. Phys. (2006); PRB (2008)

Electronic structure modification by modulating potential

$$H = \sum_{k} \{\epsilon(k)c_{k}^{+}c_{k} + \sum_{q} [V(q)c_{k+q}^{+}c_{k} + H.c]\} \quad V(\mathbf{x}) \quad V\cos(\frac{\pi}{a}\mathbf{x})$$

$$\hat{H} = \sum_{\mathbf{q} \in \text{RBZ} \atop m,n} (\delta_{m,n}\hat{c}_{\mathbf{q}+\mathbf{g}_{m}} + V_{m,n})\hat{c}_{\mathbf{q}+\mathbf{g}_{m}}^{\dagger}\hat{c}_{\mathbf{q}+\mathbf{g}_{n}}, \quad V_{n,m}(\mathbf{q}) = \begin{pmatrix} 0 & V_{c} \\ V_{c} & 0 \end{pmatrix}$$

$$A_{\mathbf{k}}^{<}(\omega) = \sum_{\mathbf{q} \in \text{RBZ} \atop i,m} \left| D_{m,i}^{*}(\mathbf{k}-\mathbf{g}_{m}) \right|^{2} \delta(E_{i}(\mathbf{k}-\mathbf{g}_{m})-\omega).$$

$$\hat{H} = \sum_{\mathbf{q} \in \text{RBZ} \atop i,m,n} D_{m,i}^{*}(\mathbf{q}) E_{i}(\mathbf{q}) D_{i,n}(\mathbf{q}) \hat{c}_{\mathbf{q}+\mathbf{g}_{n}}^{\dagger} \hat{c}_{\mathbf{q}+\mathbf{g}_{n}} = \sum_{\mathbf{q} \in \text{RBZ} \atop i} E_{i}(\mathbf{q}) \hat{a}_{\mathbf{q},i}^{\dagger} \hat{a}_{\mathbf{q},i}$$
normal state, $V=0$

$$\int_{\mathbf{q} \in \mathbf{q} \in \mathbf{q} \atop i,m,n} \int_{\mathbf{q} \in \mathbf{q} = \mathbf{q} \in \mathbf{q} = \mathbf{q} \in \mathbf{q} = \mathbf{q} \in \mathbf{q} = \mathbf{q} \in \mathbf{q} \in \mathbf{q} = \mathbf{q} = \mathbf{q} \in \mathbf{q} = \mathbf{q} \in \mathbf{q} = \mathbf{q} = \mathbf{q} = \mathbf{q} \in \mathbf{q} = \mathbf{q} \in \mathbf{q} = \mathbf$$

-π/a

0

π/a

Band dispersion of 2H-TMDs



$$2H-TaSe_2$$



CDW-induced Change in Electronic Structure



180K



30K

New Parts of Fermi surface



Fermi surface nesting and superstructure formation

 $\varepsilon(\mathbf{k}) \rightarrow \chi(\mathbf{q})$

nesting vector in the momentum space $\widehat{\mathfrak{V}}$ periodicity of the superstructure in the coordinate space

Charge ordering in 2H-TaSe₂ and NbSe₂

2H-TaSe₂



S. V. Borisenko et al., PRL (2008)

2H-NbSe₂



S. V. Borisenko *et al., PRL* (2009)



D. S. Inosov *et al.*, *NJP* (2008)

2H-NbSe₂



Davis *et al*.

Magnetic ordering in Gd_2PdSi_3 and Tb_2PdSi_3



D. S. Inosov et al., PRL (2009)

Charge-orbital ordering in $La_{0.5}Sr_{1.5}MnO_4$



D. V. Evtushinsky et al., PRL (2010)

Comparison to complementary measurements of electronic structure

ARPES

Electron transport, thermodynamics, etc.

 $\epsilon(\mathbf{k})$

 $\int \Phi[\varepsilon(\mathbf{k})] d\mathbf{k}$

Bloch wave packet <u>Electron</u> dynamics in applied field

$$\begin{aligned} \hbar \frac{d\mathbf{k}}{dt} &= -e\mathbf{E} - e\mathbf{v} \times \mathbf{B} \\ \frac{\partial f(\mathbf{k})}{\partial \mathbf{k}} \cdot \frac{d\mathbf{k}}{dt} &= -\frac{f(\mathbf{k}) - f_0(\mathbf{k})}{\tau(\mathbf{k})} \end{aligned}$$

$$\sigma_{ij} = \frac{e^2}{4\pi^3} \int_{\text{all } \mathbf{k}} \left[-\frac{df_0}{d\varepsilon} \right] \tau(\mathbf{k}) v_i(\mathbf{k}) v_j(\mathbf{k}) d^3 \mathbf{k}$$

$$\sigma_{ij} = \frac{e^2}{4\pi^3} \int_{\{\mathbf{k}| \ \varepsilon(\mathbf{k}) = \varepsilon_{\mathbf{F}}\}} \tau(\mathbf{k}) v_i(\mathbf{k}) v_j(\mathbf{k}) \frac{1}{|\mathbf{v}(\mathbf{k})|} d^2 \mathbf{k}$$

Electronic response to the weak external field

Resistivity ρ , Hall coefficient $R_{\rm H}$, and magnetoresistance $\delta \rho / \rho$

$$\sigma_{xx} = \frac{\tau e^2}{2\pi L_c h} \int v_{\rm F}(\mathbf{k}) dk \qquad \qquad \sigma_{xy} = \frac{\tau^2 B e^3}{L_c h^2} \int \frac{v_{\rm F}^2(\mathbf{k})}{\rho_{\rm F}(\mathbf{k})} dk$$
$$\delta\sigma_{xx} = -\frac{4\pi \tau^3 B^2 e^4}{L_c h^3} \int \left\{ v_{\rm F}(\mathbf{k}) \left[\frac{\mathrm{d}v_{\rm F}(\mathbf{k})}{\mathrm{d}k} \right]^2 + \frac{v_{\rm F}^3(\mathbf{k})}{2\rho^2(\mathbf{k})} \right\} dk$$
$$\rho = \frac{1}{\sigma_{xx}}, \ R_{\rm H} = \frac{\sigma_{xy}}{B \cdot \sigma_{xx}^2}, \ \text{and} \ \frac{\delta\rho}{\rho} = -\frac{\delta\sigma_{xx}}{\sigma_{xx}} - \frac{\sigma_{xy}^2}{\sigma_{xx}^2}$$

where

$$v_{\rm F}(\mathbf{k}) \equiv \frac{1}{\hbar} |\nabla \varepsilon(\mathbf{k})| \qquad \frac{1}{\rho_{\rm F}(\mathbf{k})} \equiv \frac{\nabla \varepsilon(\mathbf{k})}{\hbar v_{\rm F}(\mathbf{k})} - \frac{(\nabla v_{\rm F}(\mathbf{k}), \nabla \varepsilon(\mathbf{k}))}{\hbar v_{\rm F}^2(\mathbf{k})} \qquad \int \equiv \int_{\{\varepsilon(\mathbf{k})=0\}} \frac{\nabla \varepsilon(\mathbf{k})}{\langle \varepsilon(\mathbf{k}) \rangle \langle \varepsilon(\mathbf{k}) \rangle} d\mathbf{k}$$

Seebeck coefficient (thermopower) Nernst effect Electronic specific heat Electronic heat conductivity

Calculated and measured $R_{\rm H}$ for simple metals



	Na	К	Rb	Cu	Nb
Calculation	-2.38	-4.49	-5.4	-0.530	+0.752
Experiment	-2.50	-4.20	-5.0	-0.517	+0.875

 $R_{\rm H} (10^{-10} \, {\rm m}^3/{\rm C})$

T. P. Beaulac, *PRB* (1981) http://www.phys.ufl.edu/fermisurface/

Hall effect in 2H-TaSe₂ and NbS₂



Evtushinsky et al., PRL (2008)

Hall effect in 2H-TaSe₂ and NbS₂



Evtushinsky et al., PRL (2008)

Band dispersion of 2H-TMDs

2H-18552, 2H-NbS2



ARPES on iron-based superconductors

Iron-based superconductors



Fermi surfaces of iron-based superconductors



Fermi surfaces of iron-based superconductors



Electronic bands at Fermi level



Fermi surface of Ba_{1-x}K_xFe₂As₂





Evtushinsky *et al., JPSJ* (2011) Zabolotnyy *et al.,* Nature (2009)



Zabolotnyy *et al., Nature* (2009);*Physica C* (2009) Evtushinsky *et al., NJP* (2009);*JPSJ* (2011)

Propellers again



Hall and FS in parent



LiFeAs: no nesting, no magnetism, superconductivity



Borisenko et al., PRL (2009)

LiFeAs map



Band renormalization in LiFeAs



~3

Superconducting gap extraction from ARPES spectra

Opening of the superconducting gap in electronic dispersion


Superconducting gap in ARPES spectra



Superconducting gap in ARPES spectra



























Gap extraction from ARPES data Fit of IEDC



$$A(k,\omega) = 2\pi [u_{\nu}^{2}\delta(\omega - E_{k}) + v_{\nu}^{2}\delta(\omega + E_{k})],$$

where

$$\begin{split} u_k^2 &= \frac{1}{2} \left(1 + \frac{\xi_k}{E_k} \right), \quad v_k^2 = \frac{1}{2} \left(1 - \frac{\xi_k}{E_k} \right), \\ E_k &= \sqrt{\xi_k^2 + \Delta^2} \end{split}$$







Dynes *et al., PRL* (1978) Evtushinsky *et al., PRB* (2009)

Gap extraction from ARPES data

Fit vs. Symmetrization



Superconducting gap in $Ba_{1-x}K_xFe_2As_2$

Fermi surfaces of iron-based superconductors



Hole-doped BaFe₂As₂



Superconducting gap distribution for $Ba_{1-x}K_xFe_2As_2$ (Γ FS sheets)



Hole-doped BaFe₂As₂



Gap on propeller-like structure



Hole-doped BaFe₂As₂



Gap on propeller-like structure



Gap anisotropy



Anisotropy of gap for Γ -barrels



Momentum dependence of the superconducting gap in $Ba_{1-x}K_xFe_2As_2$



Fermi surface and gap distribution in cuprate superconductors



Superconducting gap in LiFeAs from fit of ARPES spectra



Superconducting gap of 1.7meV in underdoped Ba_{1-x}Na_xFe₂As₂ with T_c =10K





Evtushinsky et al., NJP (2009)

Comparison to complementary measurements of electronic structure in superconducting state

ARPES

μSR, H_{c1}, specific heat, etc.

 $\varepsilon(\mathbf{k}), \Delta(\mathbf{k})$

 $\int \Phi[\varepsilon(\mathbf{k}), \Delta(\mathbf{k})] d\mathbf{k}$

Superfluid density in Ba_{1-x}K_xFe₂As₂ from ARPES



Khasanov *et al., PRL* (2009) Evtushinsky *et al., NJP* (2009)

Inosov et al., PRL (2010)

$$\frac{1}{\lambda^2(T)} = \frac{e^2}{2\pi\varepsilon_0 c^2 h L_c} \cdot \int_{\mathrm{FS}} v_{\mathrm{F}}(\mathbf{k}) \left[1 - \int_{-\infty}^{+\infty} \left(-\frac{\partial f_T(\omega)}{\partial \omega} \right) \left| \operatorname{Re} \frac{\omega}{\sqrt{\omega^2 - \Delta_{\mathbf{k}}^2(T)}} \right| \mathrm{d}\omega \right] \mathrm{d}k$$

Chandrasekhar and Einzel, Ann. Physik (1993)

3D

Sensitivity to 3D electronic structure via scanning hv

$$E_{\rm kin} = (p_{\perp}^2 + p_{\parallel}^2)/2m = hv - E_{\rm bind} - \Phi$$

$$k_{\perp} + n_{\perp}G_{\perp} = \sqrt{\frac{2m}{\hbar^2} (E_{\rm kin} + V_0) - (k_{\parallel} + n_{\parallel}G_{\parallel})^2}$$
$$= \sqrt{0.262 \frac{\text{\AA}^{-2}}{\text{eV}} (hv - E_{\rm bind} + V_0 - \Phi) - (k_{\parallel} + n_{\parallel}G_{\parallel})^2}$$

Inosov et al., PRB (2008)

k_z -dispersion in iron arsenides


k_z -dispersion in iron arsenides



k_z -dependence of the superconducting gap in BKFA



k_z -dependence of the superconducting gap in BKFA



3D band structure



Comparison of calculated and measured band dispersions



Yaresko (2011)

Comparison of calculated and measured band dispersions



Comparison of calculated and measured band dispersions

 $T_{c} = 38 \text{K}$



Hole-doped BaFe₂As₂



Comparison of calculated and measured band dispersions



Zeroing matrix element due to symmetry reasons



Zeroing matrix element due to symmetry reasons



Comparison between of and measured band dispersions



Special role of iron $3d_{xz,yz}$ orbitals in magnetism





Yi et al., PNAS (2011)

Node-like behavior in BFAP







al. et Feng (2011)

$Ba_{1-x}Na_xFe_2As_2$

Fermi surface



 $Ba_{1-x}Na_xFe_2As_2$ *hv*=80eV



Gap on the inner Γ -barrel in Ba_{1-x}Na_xFe₂As₂



Gap on the electron-like pocket in $Ba_{1-x}Na_xFe_2As_2$



Gap on the outer Γ -barrel in Ba_{1-x}Na_xFe₂As₂



Surface sensitivity

Surface component of photoemission signal in YBCO











Absence of surface states in LiFeAs



Absence of surface states in LiFeAs



Lankau et al., PRB (2011)

Surface sensitivity:

•no surface states at the Fermi level observed in 111 and 122 iron arsenides

• surface layer may be non-superconducting, but band dispersion doesn't differ from the bulk

SrPd₂Ge₂



Kim et. al., PRB (2012)







• Likely conventional superconductivity

Kim et. al., PRB (2012)

Mode



DOS of strongly coupled superconductor

FIG. 2. The effective tunneling density of states $N_T(\omega)/N(0)$ vs $(\omega - \Delta_0)/\omega_1^t$ (solid) and the density of states of the simplified BCS model $\omega/(\omega^2 - \Delta_0^2)^{1/2}$ (short dash). The ratio of the differential conductance of Pb in the superconducting to that in the normal state,

$$\frac{\frac{dI_s(\omega)}{d\omega}}{\frac{dI_n(\omega)}{d\omega}},$$

is plotted (long dash) as a function of $(\omega - \Delta_0)/\omega_1^t$ for $T = 1.3^{\circ}$ K. These data were obtained from the tunneling experiments reported by Rowell, Anderson, and Thomas.



kink_energy = 23 meV $\Delta = 10$ meV





Christianson et al., Nature (2008)

Kink in $Ba_{1-x}Na_xFe_2As_2$



Mode effect at X-pocket in $Ba_{1-x}K_xFe_2As_2$




Fusion of bogoliubons



Fusion of bogoliubons



Fusion of bogoliubons





Fine structure of electronic spectrum below $T_{\rm c}$



Temperature dependence: faster saturation for the larger gap



Relation between energy scales of band structure and superconductivity



Conclusions for iron-based

- Various Fermi surface shape for different iron-based superconductors
- Large and small superconducting gaps in $Ba_{1-x}K_xFe_2As_2$ and other materials, large $2\Delta/kT_c$
- Correlation of superconducting gap magnitude with orbital composition: importance of iron $3d_{xz,yz}$

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