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Effect of electron-phonon interactions on orbital fluctuations in iron-based superconductors

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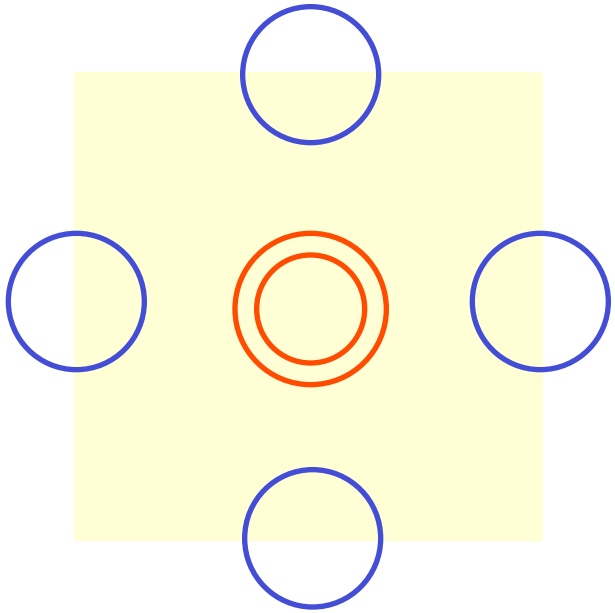
Motivation

$S_{\pm}$ vs S_{++} pairing in iron-based superconductor

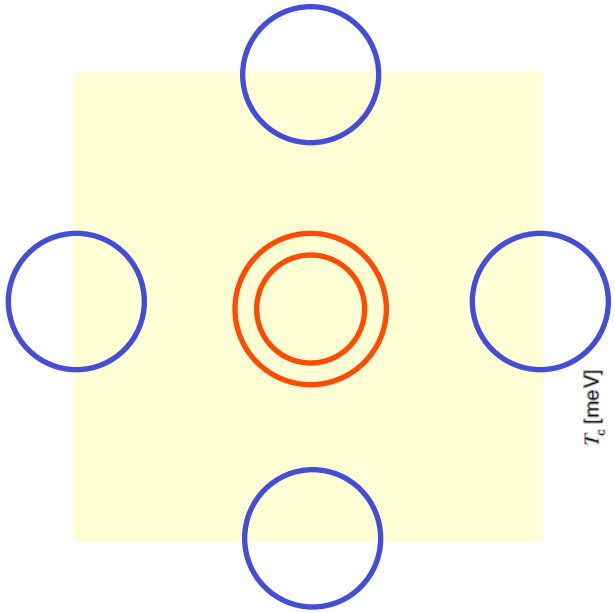


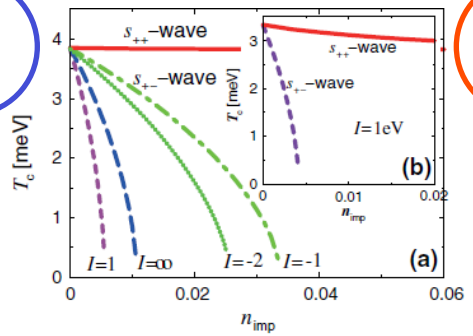
Spin fluctuation mediated SC

Mazin et al., Kuroki et al., …

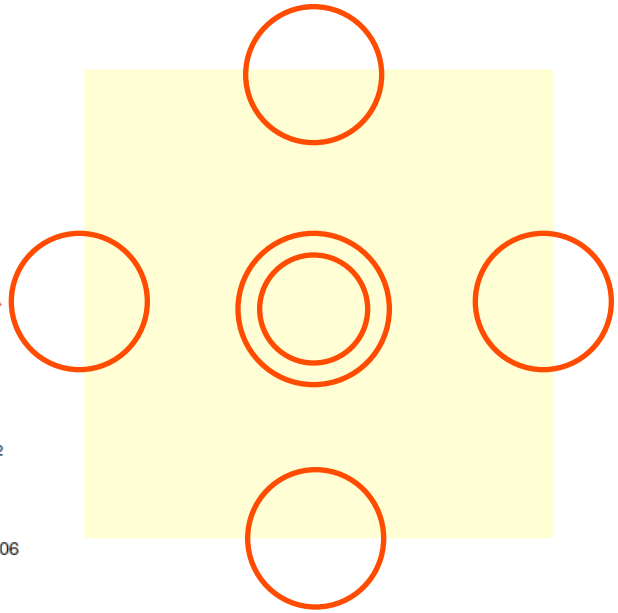
Motivation

$S_{\pm}$ vs S_{++} pairing in iron-based superconductor





Onari-Kontani PRL10



Spin fluctuation mediated SC

Mazin et al., Kuroki et al., …

Orbital fluctuation mediated SC

Onari-Kontani, …

Motivation

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Linearized Eliashberg equation:

$$\lambda_E \Delta_{ll'}(k) = \frac{T}{N} \sum_{k' m_i} W_{l m_1 m_4 l'}(k-k') G^0_{m_1 m_2}(k') \Delta_{m_2 m_3}(k') G^0_{m_4 m_3}(-k')$$

Pairing interaction

$$\hat{W}(q) = -\frac{3}{2}\hat{\Gamma}^s \hat{\chi}^s \hat{\Gamma}^s + \frac{1}{2}\hat{\Gamma}^c \hat{\chi}^c \hat{\Gamma}^c - \frac{1}{2}(\hat{\Gamma}^s - \hat{\Gamma}^c)$$

$$\hat{\chi}^s(q) = \frac{\hat{\chi}^0(q)}{1 - \hat{\Gamma}^s \hat{\chi}^0(q)}$$

$$\hat{\chi}^c(q) = \frac{\hat{\chi}^0(q)}{1 - \hat{\Gamma}^c(\omega_l) \hat{\chi}^0(q)}$$

Usually, $\chi^c < \chi^s$, but the situation can be different if

$$\hat{\Gamma}^c(\omega_l) = -\hat{C} - 2\hat{V}(\omega_l)$$

Phonon mediated attraction

H. Kontani and S. Onari, PRL 104, 157001 (2010).
T. Saito *et al.*, PRB 82, 144510 (2010).

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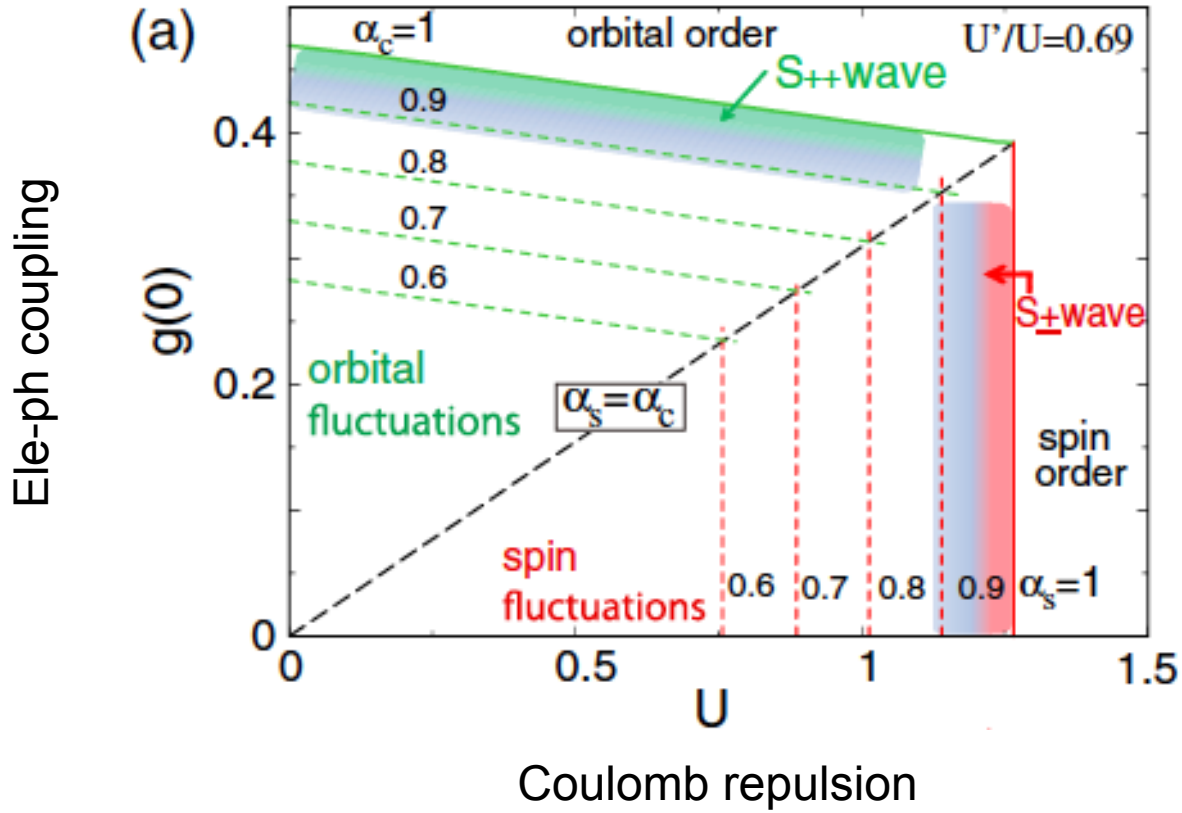
Motivation

H. Kontani and S. Onari, PRL 104, 157001 (2010).
T. Saito *et al.*, PRB 82, 144510 (2010).



Where does iron-based superconductors locate in the phase diagram ?

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Outline

Y. Nomura, K. Nakamura and RA, arXiv:1305.2995

- *Ab initio* derivation of low-energy Hamiltonians for iron-based superconductors

$$\mathcal{H} = \sum_{\mathbf{k}} \sum_{ij} \left[\mathcal{H}_0^{(\mathrm{w})}(\mathbf{k})\right]_{ij} c_{i\mathbf{k}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} + \sum_{\mathbf{q}} \sum_{\mathbf{k}\mathbf{k}'} \sum_{ij,i'j'} \sum_{\sigma\sigma'} U_{ij,i'j'}^{(p)}(\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{i'\mathbf{k}'}^{\sigma'\dagger} c_{j'\mathbf{k}'+\mathbf{q}}^{\sigma'} c_{j\mathbf{k}}^{\sigma}$$
$$+ \sum_{\mathbf{q}\nu} \sum_{\mathbf{k}} \sum_{ij} \sum_{\sigma} g_{ij}^{(p)\nu}(\mathbf{k},\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} \left(b_{\mathbf{q}\nu} + b_{-\mathbf{q}\nu}^{\dagger}\right) + \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu}^{(p)} b_{\mathbf{q}\nu}^{\dagger} b_{\mathbf{q}\nu}$$

  - Electronic one-body part — Kuroki et al., PRL 101 087004 (08)
  - Electron correlation part: cRPA method — Miyake et al., JPSJ 79 045705(10)
  - Phonon part: cDFPT method

- Effect of electron-phonon coupling on orbital fluctuations
  - Ele-ph coupling does not induce orbital-fluctuation-mediated SC

Ab initio downfolding

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Low-energy models for electron-phonon coupled systems

$$\mathcal{H} = \sum_{\mathbf{k}} \sum_{ij} \left[\mathcal{H}_0^{(\mathrm{w})}(\mathbf{k})\right]_{ij} c_{i\mathbf{k}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} + \sum_{\mathbf{q}} \sum_{\mathbf{k}\mathbf{k}'} \sum_{ij,i'j'} \sum_{\sigma\sigma'} U_{ij,i'j'}^{(p)}(\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{i'\mathbf{k}'}^{\sigma'\dagger} c_{j'\mathbf{k}'+\mathbf{q}}^{\sigma'} c_{j\mathbf{k}}^{\sigma}$$
$$+ \sum_{\mathbf{q}\nu} \sum_{\mathbf{k}} \sum_{ij} \sum_{\sigma} g_{ij}^{(p)\nu}(\mathbf{k},\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} \left(b_{\mathbf{q}\nu} + b_{-\mathbf{q}\nu}^{\dagger}\right) + \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu}^{(p)} b_{\mathbf{q}\nu}^{\dagger} b_{\mathbf{q}\nu}$$

Ab initio downfolding

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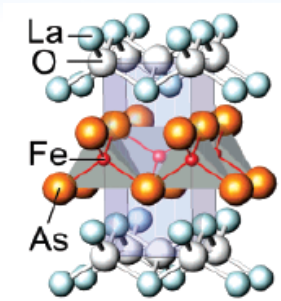
Low-energy models for electron-phonon coupled systems

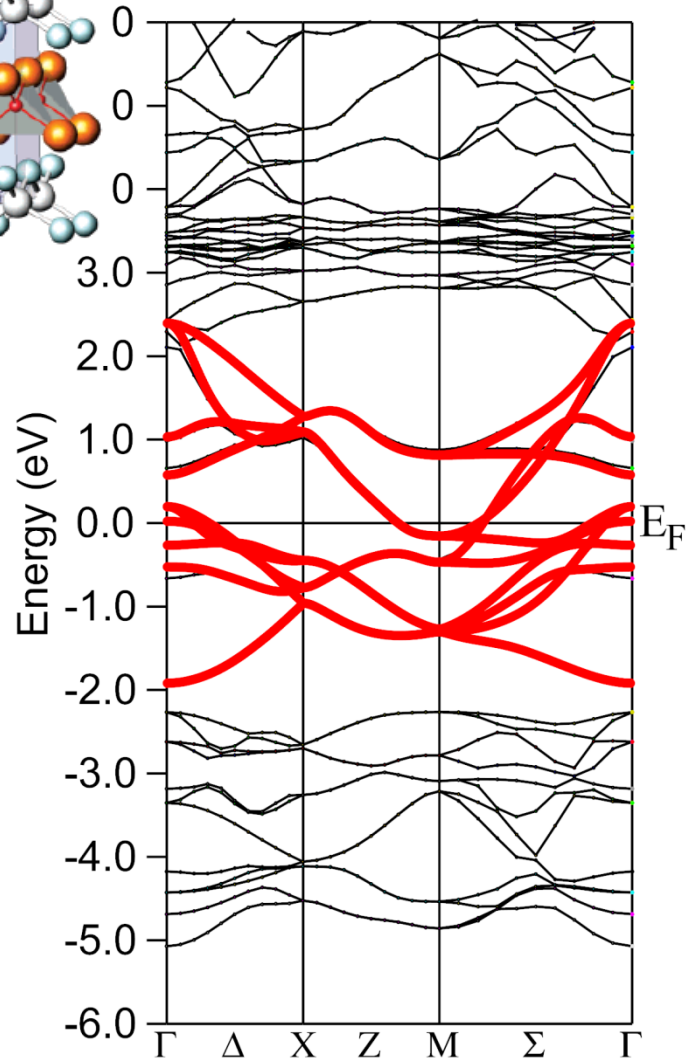
Electronic one body part

$$\mathcal{H} = \boxed{\sum_{\mathbf{k}} \sum_{ij} \left[\mathcal{H}_0^{(\mathrm{w})}(\mathbf{k})\right]_{ij} c_{i\mathbf{k}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma}} + \sum_{\mathbf{q}} \sum_{\mathbf{k}\mathbf{k}'} \sum_{ij,i'j'} \sum_{\sigma\sigma'} U_{ij,i'j'}^{(p)}(\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{i'\mathbf{k}'}^{\sigma'\dagger} c_{j'\mathbf{k}'+\mathbf{q}}^{\sigma'} c_{j\mathbf{k}}^{\sigma}$$
$$+ \sum_{\mathbf{q}\nu} \sum_{\mathbf{k}} \sum_{ij} \sum_{\sigma} g_{ij}^{(p)\nu}(\mathbf{k},\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} \left(b_{\mathbf{q}\nu} + b_{-\mathbf{q}\nu}^{\dagger}\right) + \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu}^{(p)} b_{\mathbf{q}\nu}^{\dagger} b_{\mathbf{q}\nu}$$

Kuroki, Onari, RA et al.
Phys. Rev. Lett. 101 087004 (08)

One-body part of the Hamiltonian



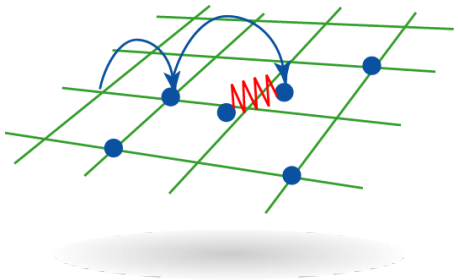


La 4f

Fe 3d

O 2p
As 4p

$$H_0 = \sum_{\sigma} \sum_{RR'} \sum_{nm} t_{mRnR'} c^{\dagger}_{\sigma nR} c_{\sigma mR'}$$



$$\left| w_{\sigma nR} \right\rangle = c^{\dagger}_{\sigma nR} \left| 0 \right\rangle$$

MaxLoc Wannier

Ab initio downfolding

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Low-energy models for electron-phonon coupled systems

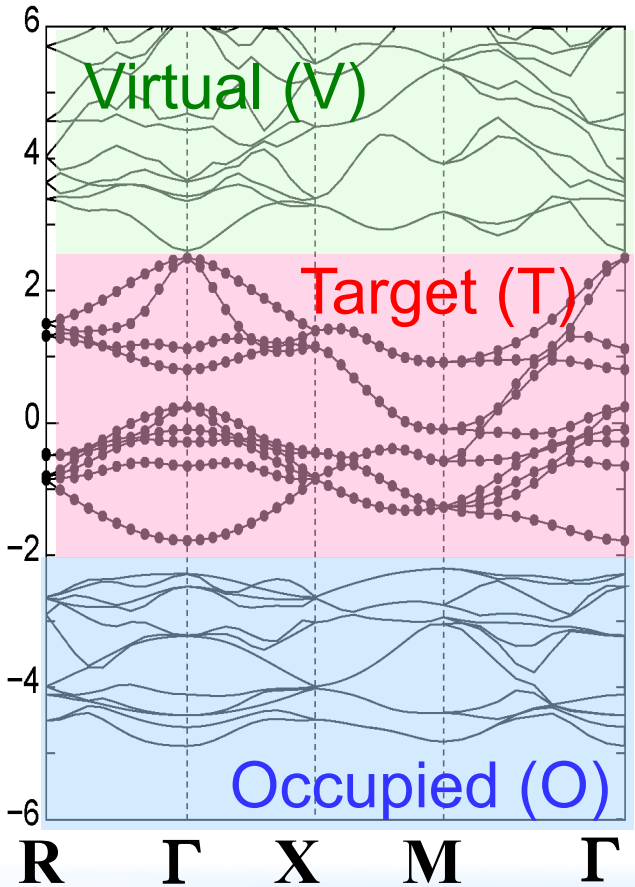
Correlation part

$$\mathcal{H} = \sum_{\mathbf{k}} \sum_{ij} \left[\mathcal{H}_0^{(\mathrm{w})}(\mathbf{k})\right]_{ij} c_{i\mathbf{k}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} + \boxed{\sum_{\mathbf{q}} \sum_{\mathbf{k}\mathbf{k}'} \sum_{ij,i'j'} \sum_{\sigma\sigma'} U_{ij,i'j'}^{(p)}(\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{i'\mathbf{k}'}^{\sigma'\dagger} c_{j'\mathbf{k}'+\mathbf{q}}^{\sigma'} c_{j\mathbf{k}}^{\sigma}}$$
$$+ \sum_{\mathbf{q}\nu} \sum_{\mathbf{k}} \sum_{ij} \sum_{\sigma} g_{ij}^{(p)\nu}(\mathbf{k},\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} \left(b_{\mathbf{q}\nu} + b_{-\mathbf{q}\nu}^{\dagger}\right) + \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu}^{(p)} b_{\mathbf{q}\nu}^{\dagger} b_{\mathbf{q}\nu}$$

Miyake-Nakamura-RA-Imada, JPSJ10
Nakamura-RA-Imada, JPSJ09

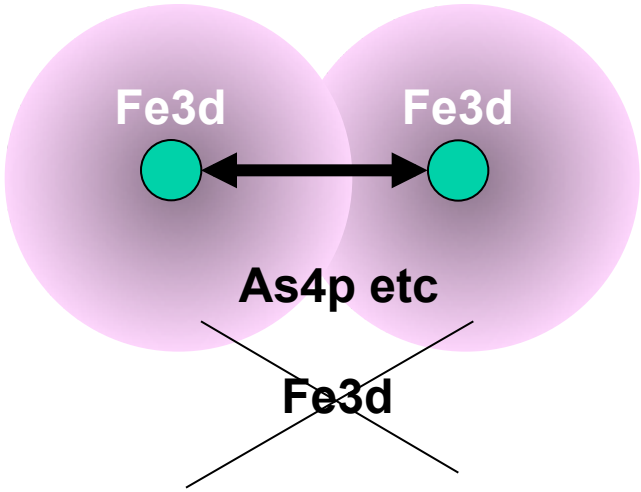
Constrained RPA

$$W = \left(1 - v\chi\right)^{-1} v$$



Full RPA polarizability:

$$\chi = \sum_{i}^{occ} \sum_{j}^{unocc} \frac{\psi_i(r)\psi_j^*(r)\psi_i^*(r')\psi_j(r')}{\omega - \varepsilon_j + \varepsilon_i \pm i\delta}$$



Constrained RPA method

Aryasetiawan et al, PRB 70, 195104 (2004)
Solovyev-Imada, PRB 71, 045103 (2005)

Constrained RPA

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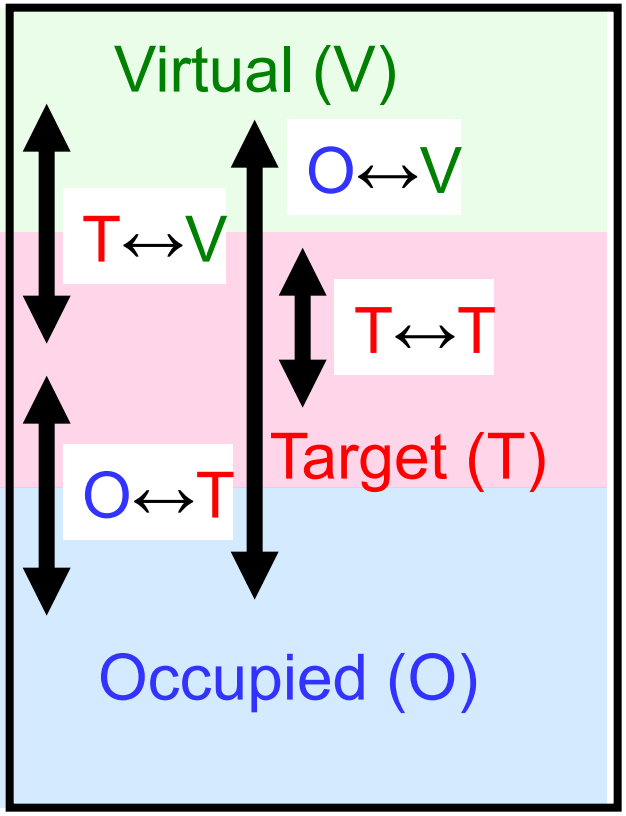
$$W = \left(1 - v\chi\right)^{-1} v$$



Full RPA polarizability:

$$\chi = \sum_{i}^{occ} \sum_{j}^{unocc} \frac{\psi_i(r)\psi_j^*(r)\psi_i^*(r')\psi_j(r')}{\omega - \varepsilon_j + \varepsilon_i \pm i\delta}$$

$$\chi = \sum_{O\leftrightarrow T} + \sum_{T\leftrightarrow V} + \sum_{O\leftrightarrow V} + \sum_{T\leftrightarrow T}$$

$$\chi_{\mathrm{r}} = \sum_{O\leftrightarrow T} + \sum_{T\leftrightarrow V} + \sum_{O\leftrightarrow V} \qquad \chi_{\mathrm{d}} = \sum_{T\leftrightarrow T}$$

$$W_{eff} = \left(1 - v\chi_{\mathrm{r}}\right)^{-1} v$$

$$U_{\mathbf{R}} = \left\langle w_{\mu\mathbf{0}} w_{\mu\mathbf{0}} \middle| W_{eff} \middle| w_{\nu\mathbf{R}} w_{\nu\mathbf{R}} \right\rangle$$

Interaction Parameters

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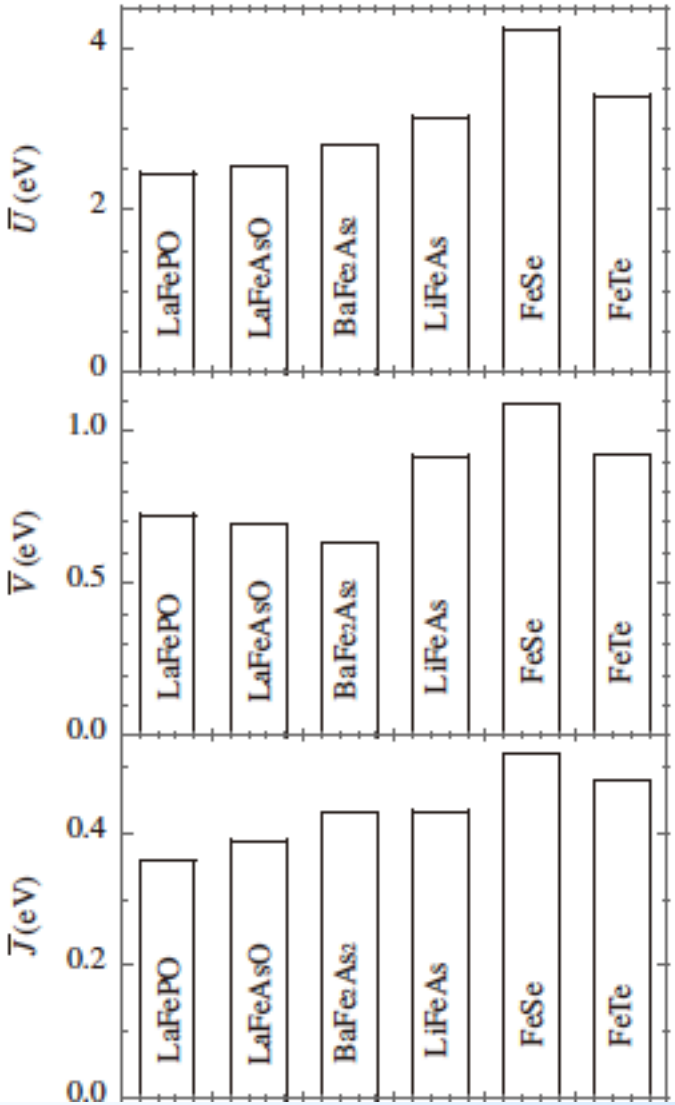
Miyake-Nakamura-RA-Imada, JPSJ10
Nakamura-RA-Imada, JPSJ09



- 1111, 122, 111 are moderately correlated (U~W)
- Correlation in 11 system is stronger

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Ab initio downfolding

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Low-energy models for electron-phonon coupled systems

$$\mathcal{H} = \sum_{\mathbf{k}} \sum_{ij} \left[\mathcal{H}_0^{(\mathrm{w})}(\mathbf{k})\right]_{ij} c_{i\mathbf{k}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} + \sum_{\mathbf{q}} \sum_{\mathbf{k}\mathbf{k}'} \sum_{ij,i'j'} \sum_{\sigma\sigma'} U_{ij,i'j'}^{(p)}(\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{i'\mathbf{k}'}^{\sigma'\dagger} c_{j'\mathbf{k}'+\mathbf{q}}^{\sigma'} c_{j\mathbf{k}}^{\sigma}$$

$$+ \sum_{\mathbf{q}\nu} \sum_{\mathbf{k}} \sum_{ij} \sum_{\sigma} g_{ij}^{(p)\nu}(\mathbf{k},\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} \left(b_{\mathbf{q}\nu} + b_{-\mathbf{q}\nu}^{\dagger}\right) + \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu}^{(p)} b_{\mathbf{q}\nu}^{\dagger} b_{\mathbf{q}\nu}$$

How to evaluate $g_{ij}^{(p)\nu}(\mathbf{k},\mathbf{q})$ and $\omega_{\mathbf{q}\nu}^{(p)}$?

We have to exclude the effect of low-energy screening
(we need to estimate partially screened values)

Y. Nomura, K. Nakamura and RA, arXiv:1305.2995

Ab initio downfolding

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Low-energy models for electron-phonon coupled systems

$$\mathcal{H} = \sum_{\mathbf{k}} \sum_{ij} \left[\mathcal{H}_0^{(\mathrm{w})}(\mathbf{k})\right]_{ij} c_{i\mathbf{k}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} + \sum_{\mathbf{q}} \sum_{\mathbf{k}\mathbf{k}'} \sum_{ii'jj'} \sum_{\sigma\sigma'} U_{ij,i'j'}^{(p)}(\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{i'\mathbf{k}'}^{\sigma'\dagger} c_{j'\mathbf{k}'+\mathbf{q}}^{\sigma'} c_{j\mathbf{k}}^{\sigma}$$

$$+ \sum_{\mathbf{q}\nu} \sum_{\mathbf{k}} \sum_{ij} \sum_{\sigma} g_{ij}^{(p)\nu}(\mathbf{k},\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} \left(b_{\mathbf{q}\nu} + b_{-\mathbf{q}\nu}^{\dagger}\right) + \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu}^{(p)} b_{\mathbf{q}\nu}^{\dagger} b_{\mathbf{q}\nu}$$

How to evaluate $g_{ij}^{(p)\nu}(\mathbf{k},\mathbf{q})$ and $\omega_{\mathbf{q}\nu}^{(p)}$?

We have to exclude the effect of low-energy screening
(we need to estimate partially screened values)

Let us first consider to evaluate fully screened $g_{ij}^{(f)\nu}(\mathbf{k},\mathbf{q})$ and $\omega_{\mathbf{q}\nu}^{(f)}$

➡ Density functional perturbation theory, Baroni RMP 2001

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Phonon spectrum

Matrix of Interatomic force constants

$$C^{\alpha\alpha'}_{p\kappa,p'\kappa'} = C^{\alpha'\alpha}_{p'\kappa',p\kappa} = \left.\frac{\partial^2 E}{\partial u^{\alpha}_{p\kappa}\partial u^{\alpha'}_{p'\kappa'}}\right|_{u=0}$$

Displacements of the atoms

$$\sum_{\kappa'\alpha'} C^{\alpha\alpha'}_{\kappa\kappa'}(\mathbf{q})u^{\alpha'}_{\kappa'}(\mathbf{q}) = M_{\kappa}\underline{\omega^2}(\mathbf{q})u^{\alpha}_{\kappa}(\mathbf{q})$$

Phonon frequency

Mass

Electron-phonon coupling

Displacements of the atoms → ΔV → electron scattering

$$\sum \underline{\Delta V} c^\dagger_{k+q} c_k$$

$$\boxed{\langle \psi_{k+q} | \frac{\partial V}{\partial u} | \psi_k \rangle \underline{\Delta u}}$$

$$\boxed{(b_q + b^\dagger_{-q})}$$

$$\mathcal{H}_{el-ph} = \sum \underline{g(k,q)} c^\dagger_{k+q} c_k (b_q + b^\dagger_{-q})$$

$$\boxed{\langle \psi_{k+q} | \frac{\partial V}{\partial u} | \psi_k \rangle}$$

Density functional perturbation theory

Electron-phonon coupling g $\quad \langle \psi_{k+q} | \frac{\partial V}{\partial u} | \psi_k \rangle$

Phonon frequency ω $\quad \frac{\partial^2 E}{\partial u \partial u}$

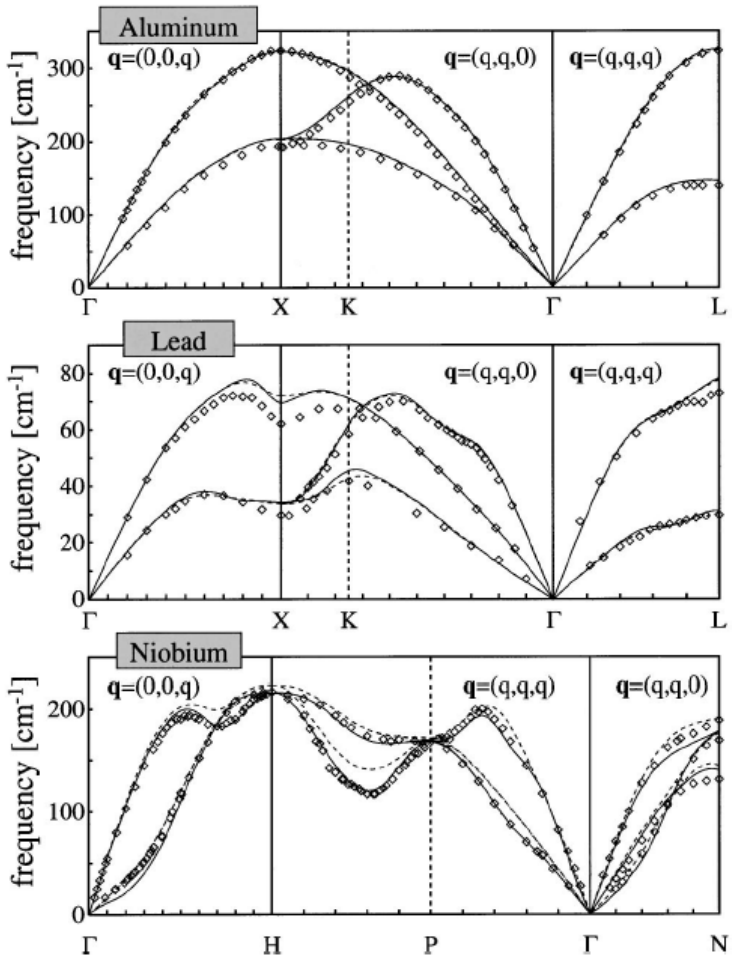
In DFT, physical quantities are represented in terms of ρ

$$E[\rho] \qquad V[\rho]$$

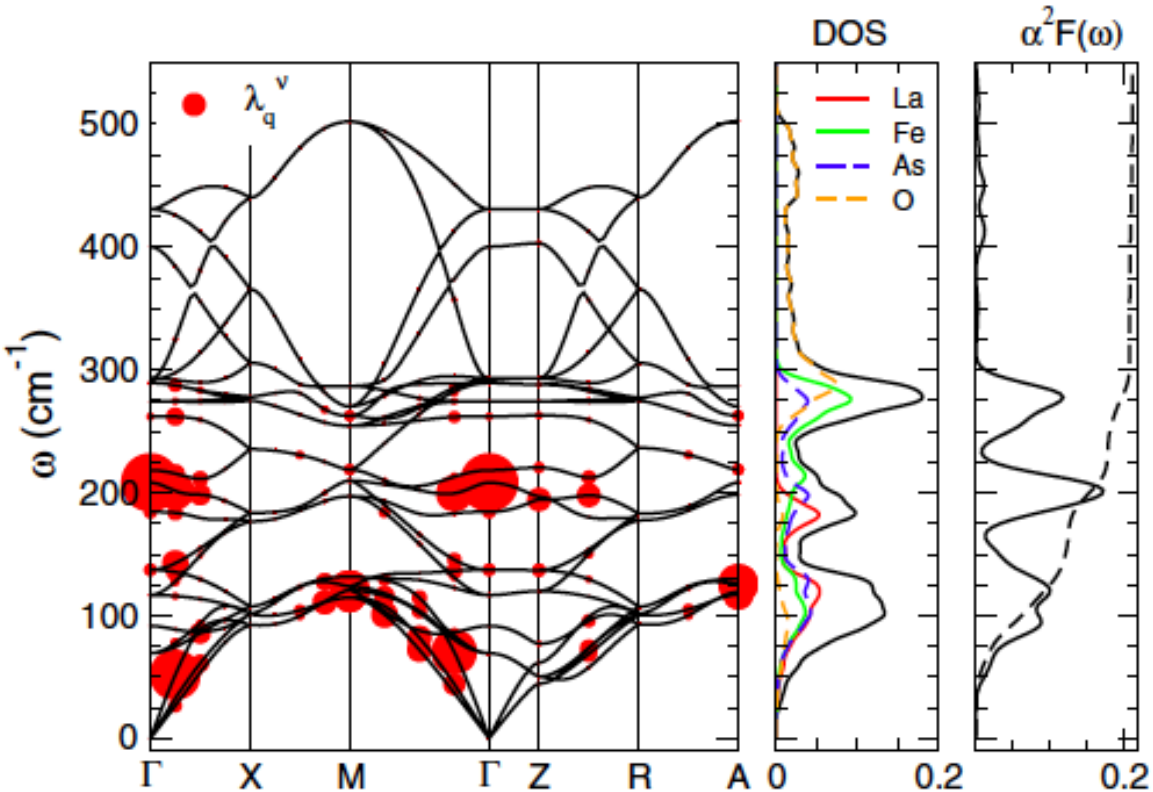
$$\frac{\partial}{\partial u} = \boxed{\frac{\partial \rho}{\partial u}} \frac{\partial}{\partial \rho} \Rightarrow$$

from $\frac{\partial \rho}{\partial u}$, we can estimate g and ω

Density functional perturbation theory



Density functional perturbation theory



Fully screened ele-ph coupling λ=0.2
Energy scale of fully screened phonon frequency ~205K
→ McMillan's formula gives T_c=0.5K

Boeri *et al.*, Phys. Rev. Lett. 101, 026403 (2008)

Ab initio downfolding

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$$+ \sum_{\mathbf{q}\nu} \sum_{\mathbf{k}} \sum_{ij} \sum_{\sigma} g_{ij}^{(p)\nu}(\mathbf{k},\mathbf{q}) c_{i\mathbf{k}+\mathbf{q}}^{\sigma\dagger} c_{j\mathbf{k}}^{\sigma} \left(b_{\mathbf{q}\nu} + b_{-\mathbf{q}\nu}^{\dagger}\right) + \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu}^{(p)} b_{\mathbf{q}\nu}^{\dagger} b_{\mathbf{q}\nu}$$

How to evaluate $g_{ij}^{(p)\nu}(\mathbf{k},\mathbf{q})$ and $\omega_{\mathbf{q}\nu}^{(p)}$?

We have to exclude the effect of low-energy screening in

$g_{ij}^{(f)\nu}(\mathbf{k},\mathbf{q})$ and $\omega_{\mathbf{q}\nu}^{(f)}$

➡ Constrained DFPT

Y. Nomura, K. Nakamura and RA, arXiv:1305.2995

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Density functional perturbation theory

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Electron-phonon coupling g $\langle \psi_{k+q} | \frac{\partial V}{\partial u} | \psi_k \rangle$

Phonon frequency ω $\frac{\partial^2 E}{\partial u \partial u}$

$$\frac{\partial}{\partial u} = \boxed{\frac{\partial \rho}{\partial u}} \frac{\partial}{\partial \rho}$$

we can easily exclude the effect of low-energy screening

Constrained DFPT

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$$\Delta\rho = 2\sum_n \psi_n^* \Delta\psi_n$$

$$\Delta\psi_n(\mathbf{r}) = \sum_{m\neq n} \psi_m(\mathbf{r}) \frac{\langle\psi_m|\Delta V_{SCF}|\psi_n\rangle}{\epsilon_n - \epsilon_m}$$

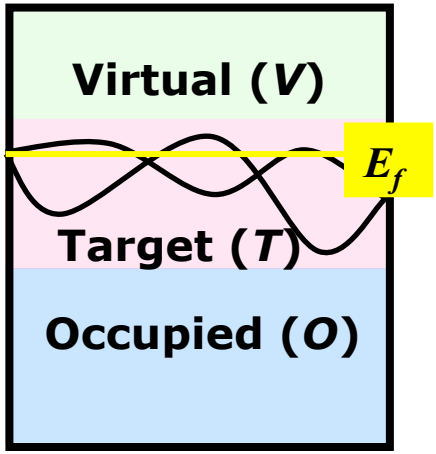
If ψ_n belongs to the target subspace, we modify the sum over *m* as

$$\sum_m \longrightarrow \sum_{m\in occ.,vir.}$$

exclude the target-target processes

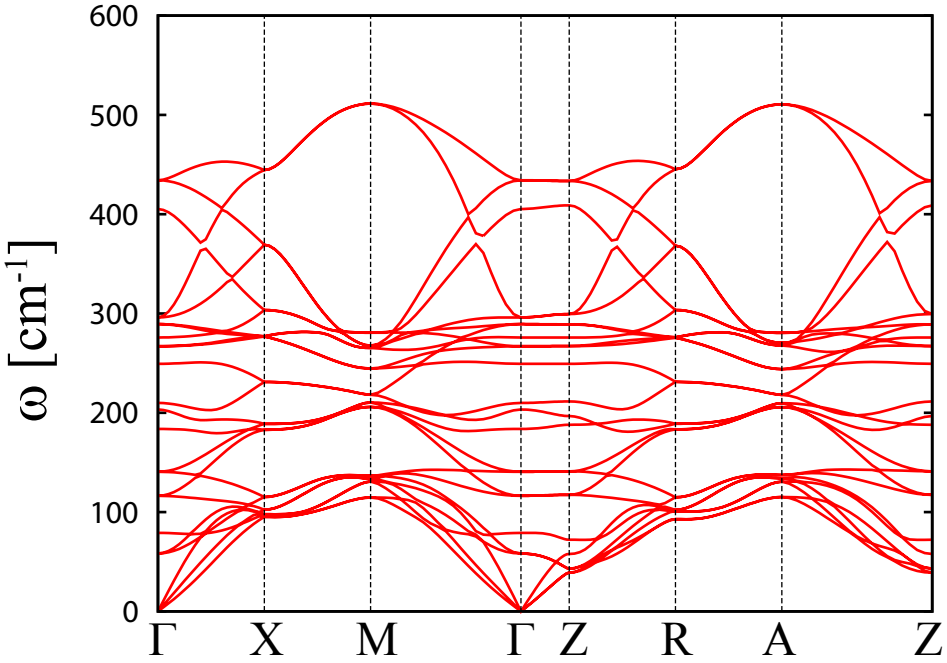
We can obtain $\Delta\rho^{(p)}$ and then

$\omega^{(p)}$ and $g^{(p)}$

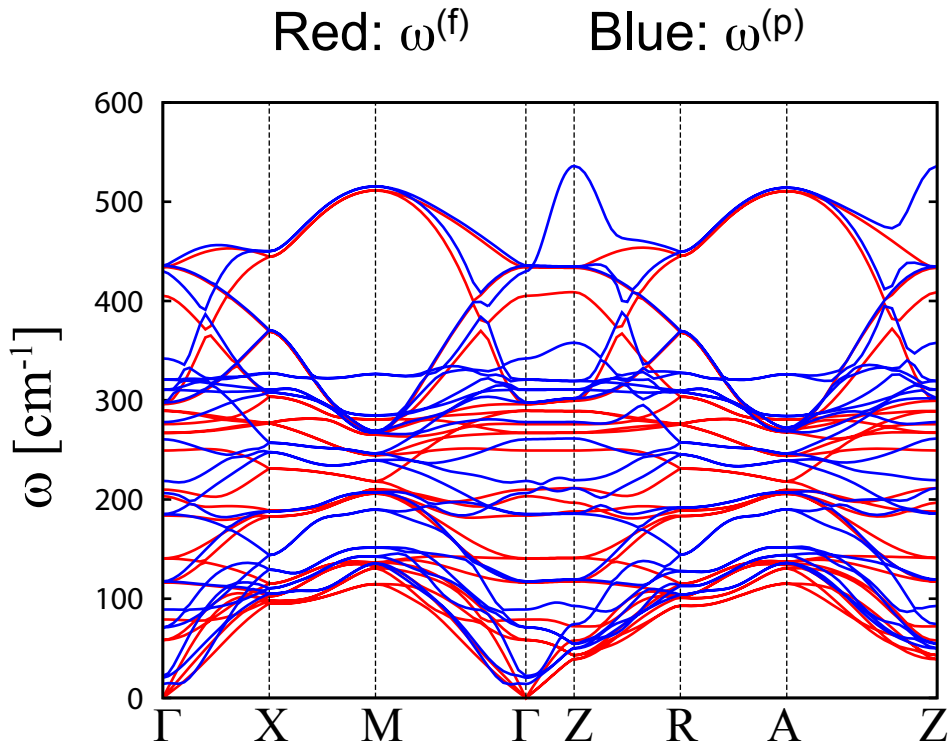


Phonon dispersion: LaFeAsO

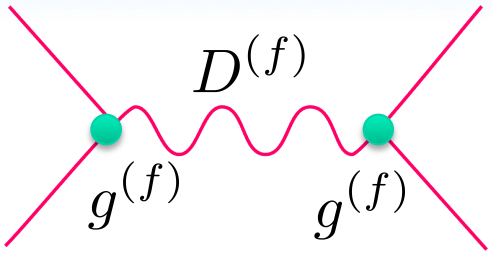
Fully screened $\omega^{(f)}$



Comparison between $\omega^{(f)}$ and $\omega^{(p)}$



Phonon-mediated interactions



Fully screened

$-V_{ii,ii}(0)$ and $-V_{ii,jj}(0)$

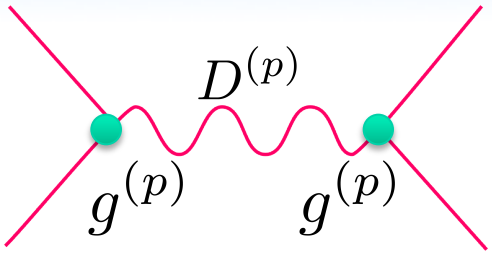
	$3z^2$-r^2	xz	yz	x^2-y^2	xy
$3z^2$-r^2	0.027	0.028	0.028	0.024	0.021
xz		0.037	0.024	0.027	0.021
yz			0.037	0.027	0.021
x^2-y^2				0.039	0.011
xy					0.028

$-V_{ij,ij}(0)$ and $-V_{ij,ji}(0)$

	$3z^2$-r^2	xz	yz	x^2-y^2	xy
$3z^2$-r^2	-	0.025	0.025	0.024	0.001
xz		-	0.003	0.014	0.018
yz			-	0.014	0.018
x^2-y^2				-	0.004
xy					-

U_{ph}, J_{ph}~ -0.03eV

Phonon-mediated interactions



Partially screened

$-V_{ii,ii}(0)$ and $-V_{ii,jj}(0)$

	$3z^2$-r^2	xz	yz	x^2-y^2	xy
$3z^2$-r^2	0.47	0.44	0.44	0.38	0.44
xz		0.43	0.41	0.36	0.42
yz			0.43	0.36	0.42
x^2-y^2				0.32	0.35
xy					0.43

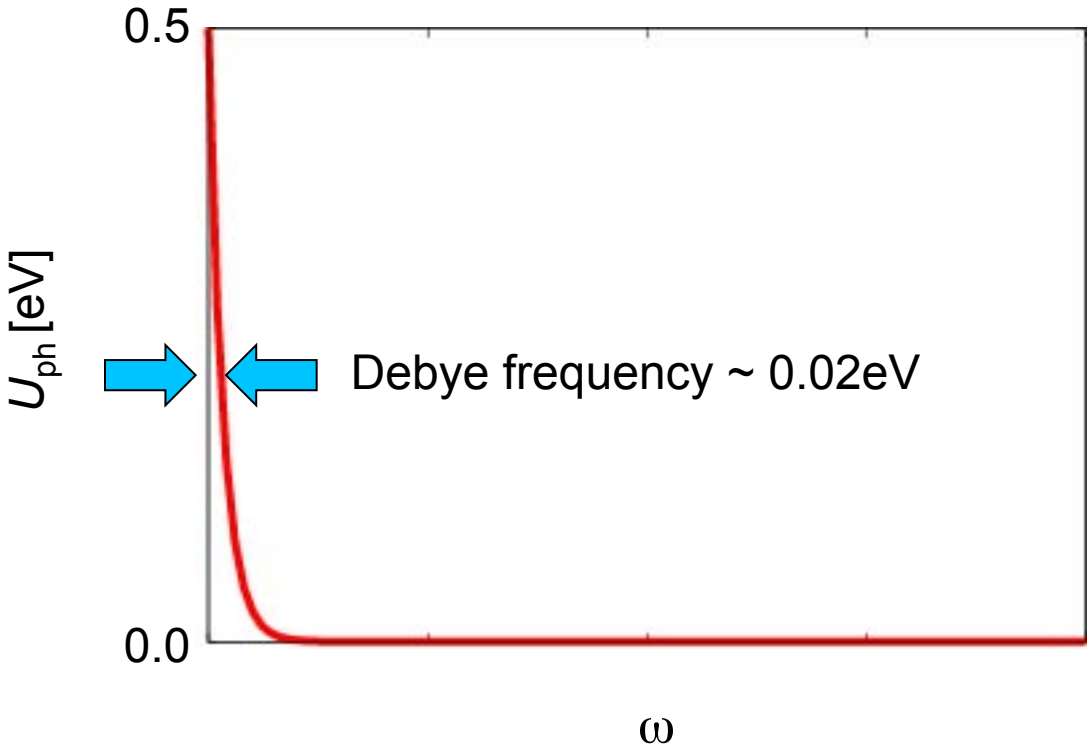
$-V_{ij,ij}(0)$ and $-V_{ij,ji}(0)$

	$3z^2$-r^2	xz	yz	x^2-y^2	xy
$3z^2$-r^2	-	0.023	0.023	0.021	0.003
xz		-	0.006	0.020	0.023
yz			-	0.023	0.023
x^2-y^2				-	0.003
xy					-

U_{ph} ~ -0.4eV J_{ph}~ -0.01eV

cf) U_{ph} = J_{ph}~ -0.4eV (Onari-Kontani PRL10, point charge model)

Phonon-mediated interactions



RPA analysis

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Linearized Eliashberg equation:

$$\lambda_E \Delta_{ll'}(k) = \frac{T}{N} \sum_{k' m_i} W_{l m_1 m_4 l'}(k-k') G^0_{m_1 m_2}(k') \Delta_{m_2 m_3}(k') G^0_{m_4 m_3}(-k')$$

Pairing interaction

$$\hat{W}(q) = -\frac{3}{2}\hat{\Gamma}^s \hat{\chi}^s \hat{\Gamma}^s + \frac{1}{2}\hat{\Gamma}^c \hat{\chi}^c \hat{\Gamma}^c - \frac{1}{2}(\hat{\Gamma}^s - \hat{\Gamma}^c)$$

$$\hat{\chi}^s(q) = \frac{\hat{\chi}^0(q)}{1 - \hat{\Gamma}^s \hat{\chi}^0(q)}$$

$$\hat{\chi}^c(q) = \frac{\hat{\chi}^0(q)}{1 - \hat{\Gamma}^c(\omega_l) \hat{\chi}^0(q)}$$

$$\hat{\Gamma}^c(\omega_l) = -\hat{C} - 2\hat{V}(\omega_l)$$

Phonon mediated attraction

Onari-Kontani PRL10

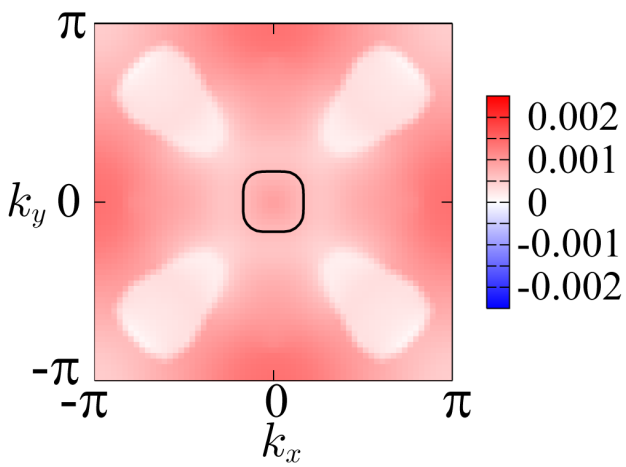
R.Arita

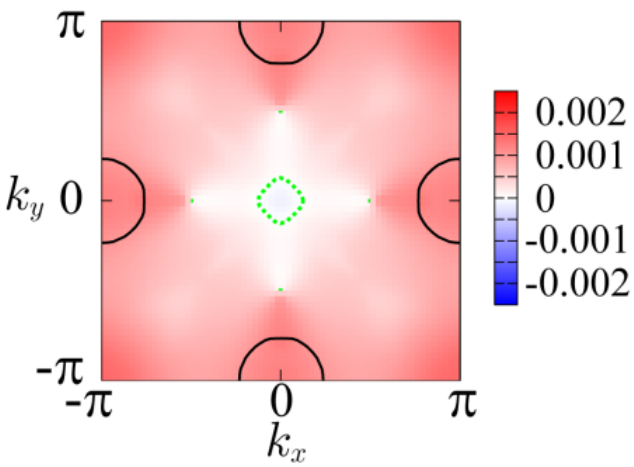
RPA analysis

U = 0.8 eV, U'/U = 0.69, J/U = J'/U = 0.16, T = 0.02 eV, n = 6.1

$V(\omega_l) = V(0)\ \omega_D^2 / (\ \omega_D^2 + \omega_l^2\ )$, $V(0)$ = -0.385 eV, ω_D = 0.02 eV

$U_{ph} = -U'_{ph} = J_{ph} = V(\omega_l)$ → S++ Onari-Kontani





RPA analysis

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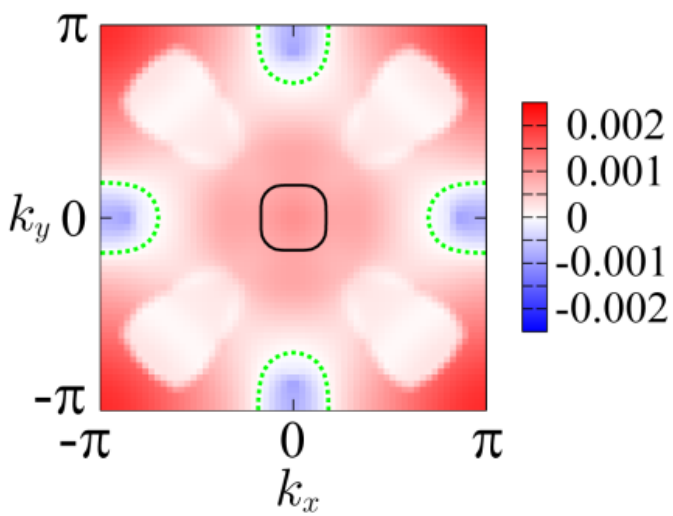
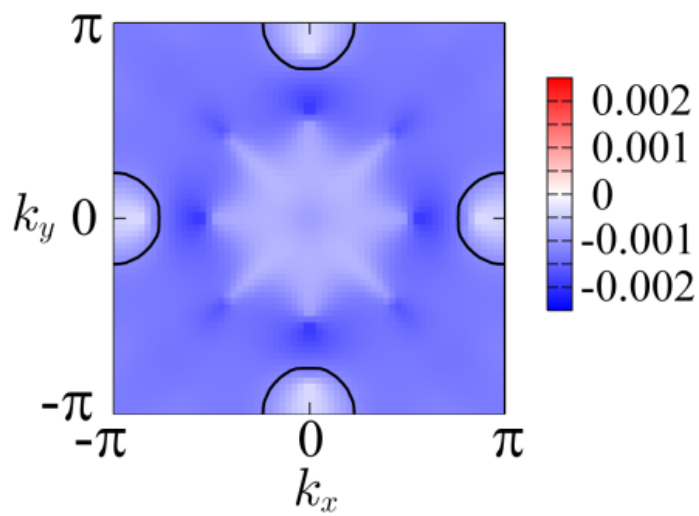
$U_{ph} = U'_{ph} = 20\text{x}\ J_{ph} = V(\omega_l)$ → S±





RPA analysis

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U = 0.8 eV, U'/U = 0.69, J/U = J'/U = 0.16, T = 0.02 eV, n = 6.1

$V(\omega_l) = V(0)\ \omega_D^2 / (\ \omega_D^2 + \omega_l^2\ )$, $V(0)$ = -0.385 eV, ω_D = 0.02 eV

1. $U_{ph} = -U'_{ph} = J_{ph} = V(\omega_l)$ → S++ Onari-Kontani

2. $U_{ph} = -U'_{ph} = 20\text{x}\ J_{ph} = V(\omega_l)$ → $S\pm$

3. $U_{ph} = U'_{ph} = J_{ph} = V(\omega_l)$ → S++

4. $U_{ph} = U'_{ph} = 20\text{x}\ J_{ph} = V(\omega_l)$ → $S\pm$

U'_{ph} is not important. Size of J_{ph} is important.

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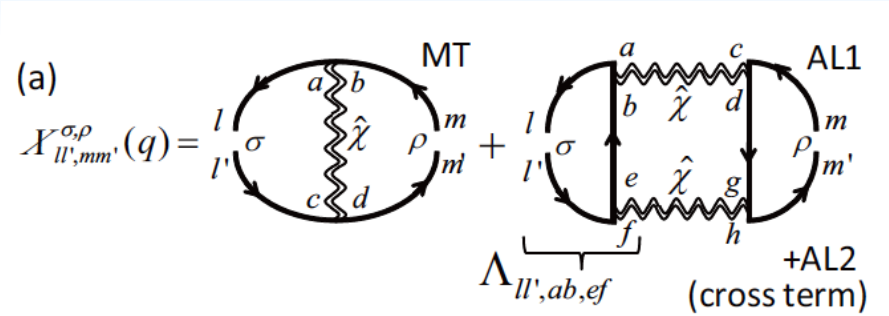
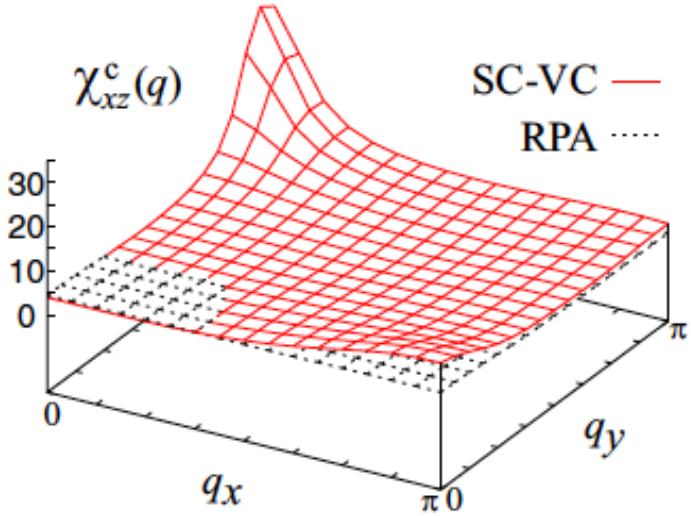
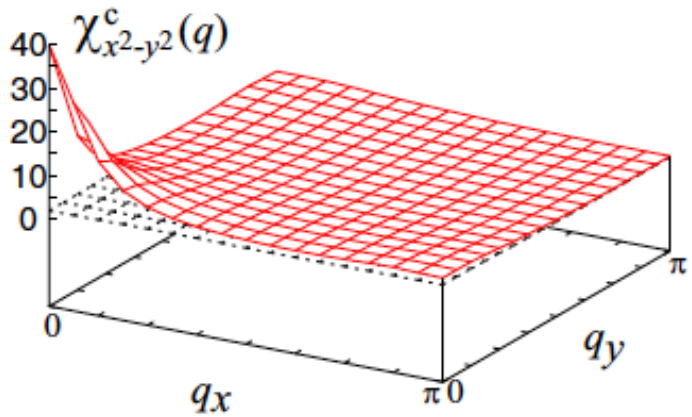
Beyond RPA analysis: role of vertex corr.







Orbital fluctuation mediated s_{++} pairing

Orthorhombic structure transition C_{66} elastic constant softening

Onari-Kontani, PRL 109, 137001 (2012)

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Beyond RPA analysis: role of vertex corr.

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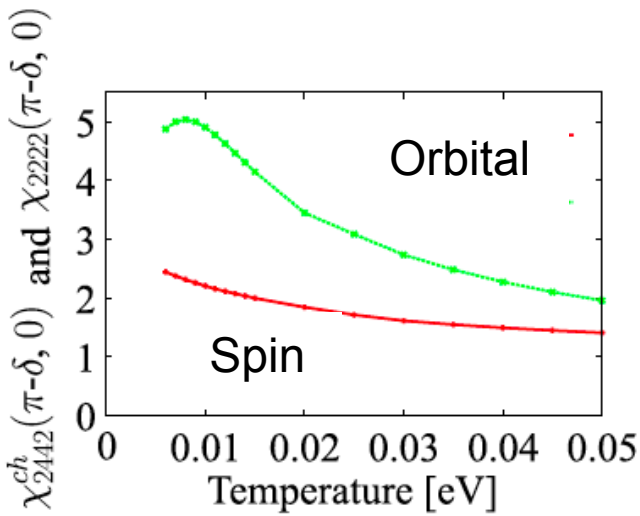
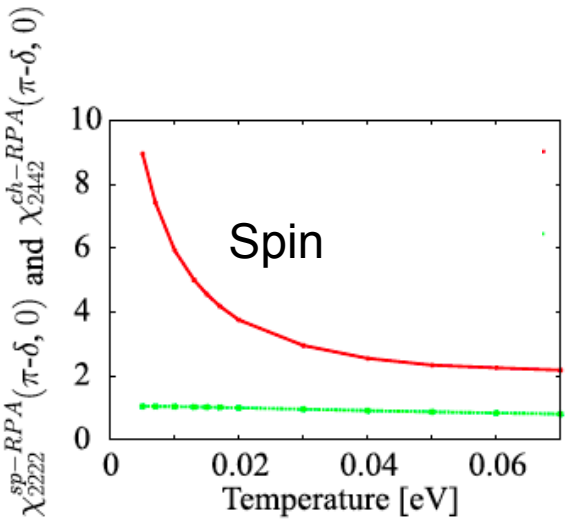
Vilk and Tremblay, J. Phys. I. France 7, 1309-1368 (1997)

Determine the local vertex correction so that the susceptibility satisfies its sum rule

$$\chi_{\rm sp} = \frac{\chi^0(q)}{1 - U_{\rm sp}\chi^0(q)} \qquad \chi_{\rm sp}(1,1^+) = \frac{T}{N}\sum_{\mathbf{q},\mathrm{i}q_n} \chi_{\rm sp}(\mathbf{q},\mathrm{i}q_n) = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle - 2\langle n_\uparrow n_\downarrow\rangle$$





Orbital

Miyahara, RA, Ikeda, PRB13

R.Arita

Beyond RPA analysis: role of vertex corr.

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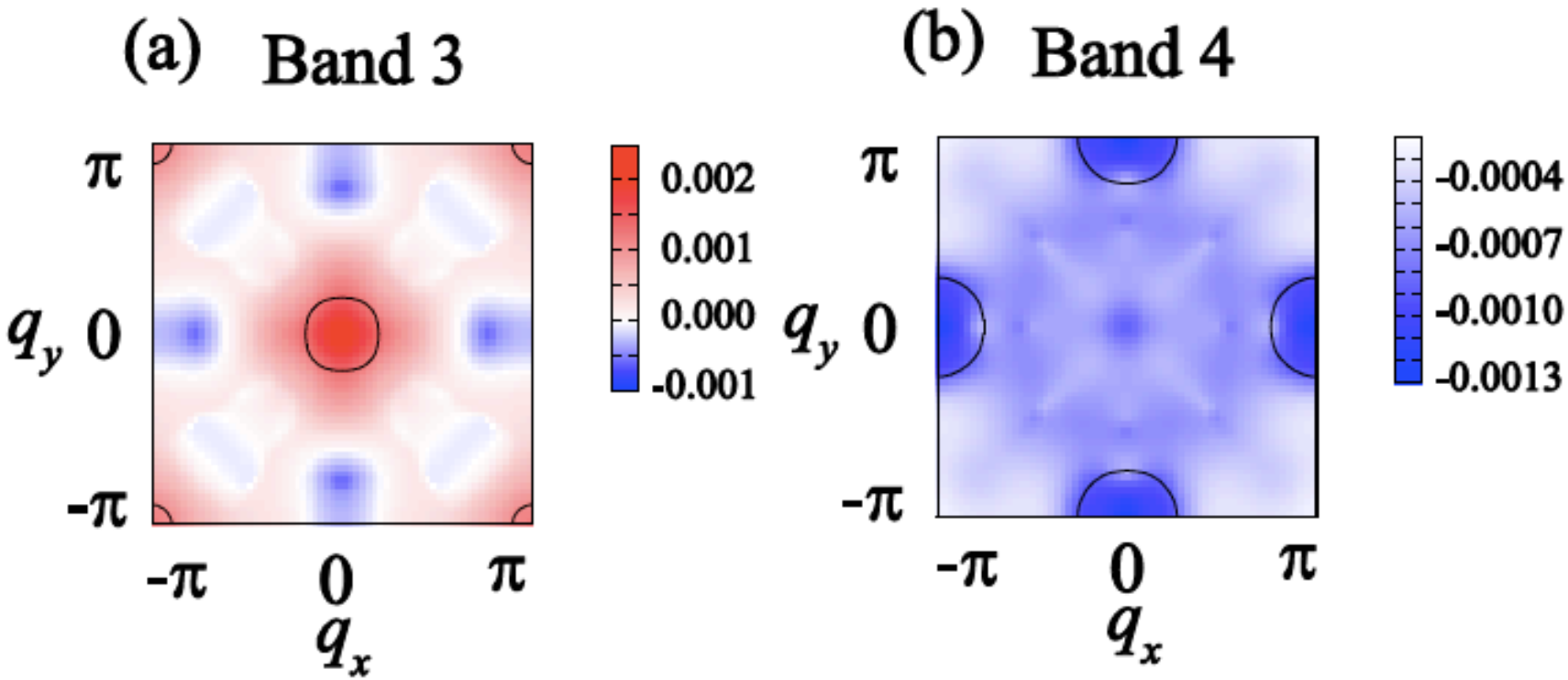
$s_{\pm}$



Oribtal fluctuation is not strong enough
local vertex correction does not favor s++
Miyahara, RA, Ikeda, PRB13

R.Arita

Conclusion

- *Ab initio* derivation of low-energy Hamiltonians for iron-based superconductors
  - New method to derive the phonon terms: cDFPT method

- Effect of electron-phonon coupling on orbital fluctuations
  - Ele-ph coupling does not induce orbital-fluctuation-mediated SC
  - If orbital-fluctuation-mediated s_{++}-wave is realized, the driving force is electronic, not electron-phonon coupling

Y. Nomura, K. Nakamura and RA, arXiv:1305.2995