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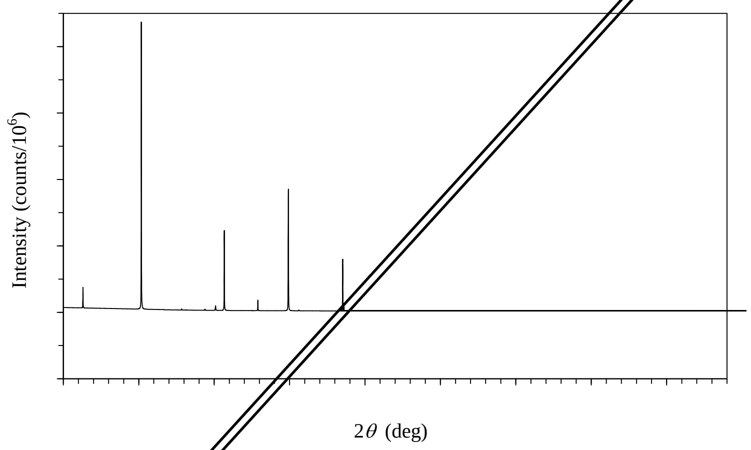

Observed (crosses), calculated (solid line), and difference synchrotron X-ray powder diffraction patterns of $BaOsO_3$ at 300 K. Bragg reflections are indicated by tick marks. The lower tick marks are given for reflections from the Os impurity (2.9 weight %).

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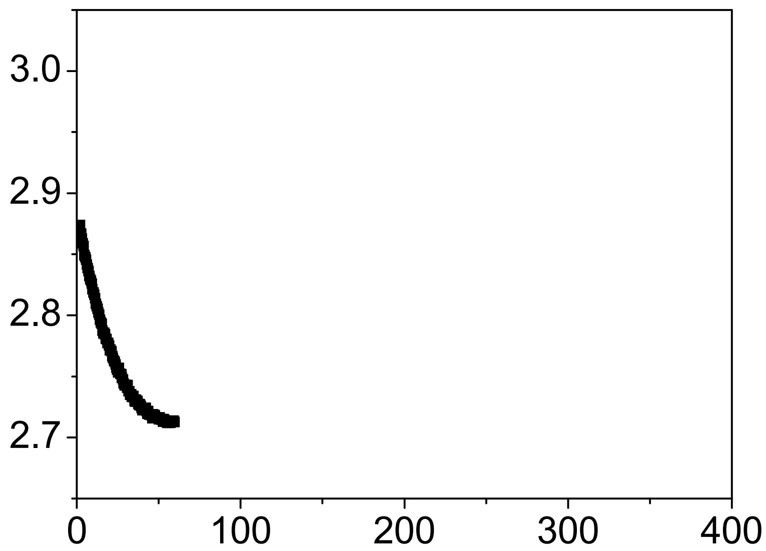
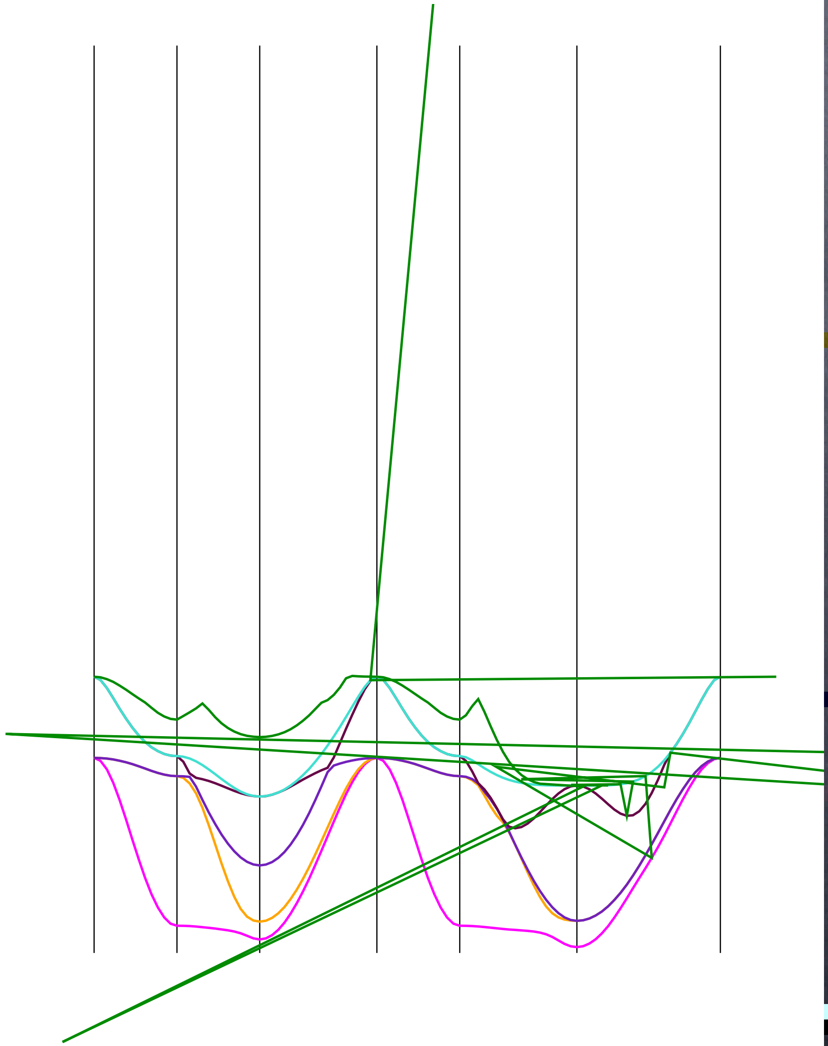
2 - '$3+- 2 -45$)





First-prin iples al ulations: within GGA SOC U (U . eV)

Ferromagneti ase

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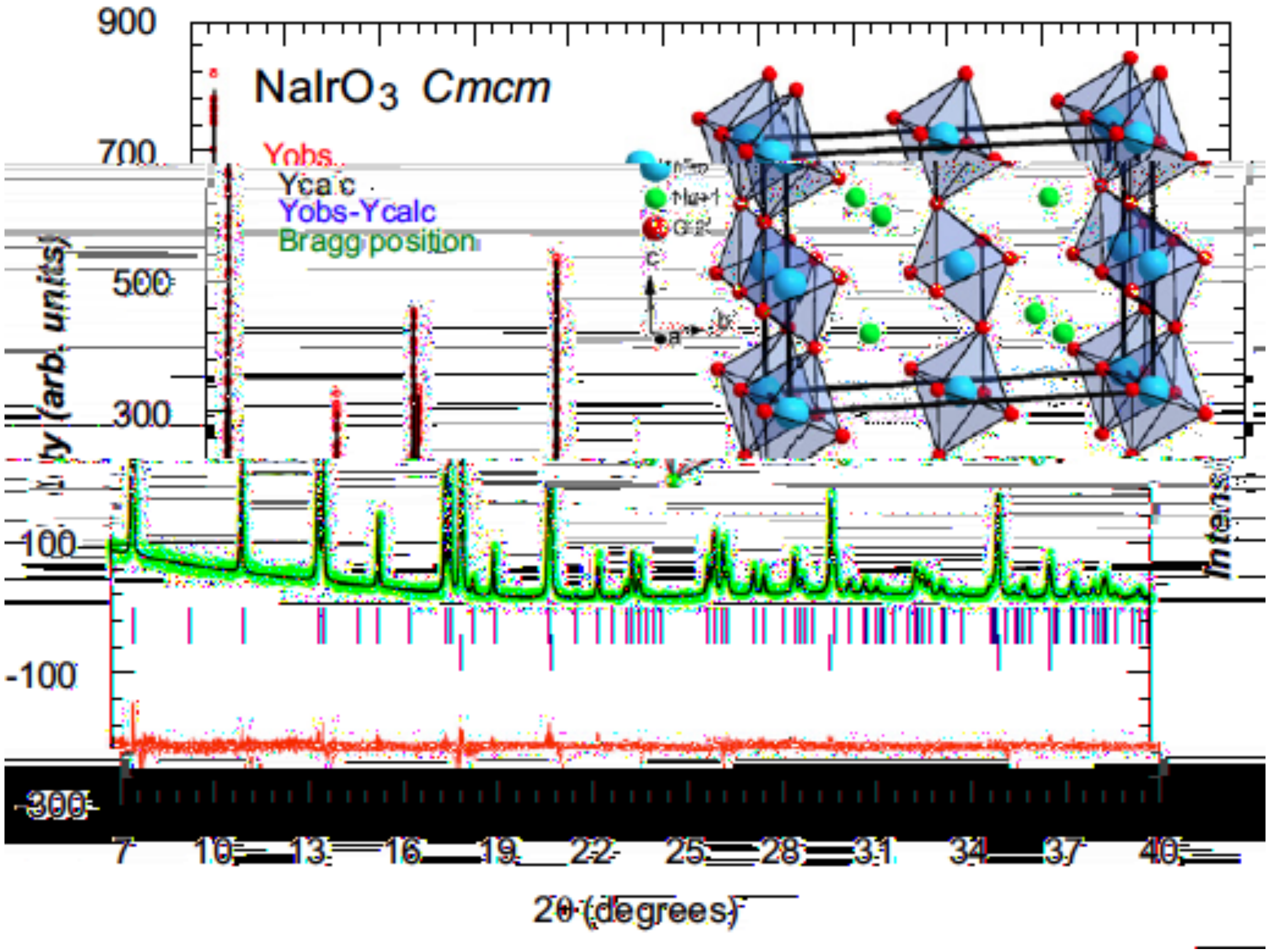

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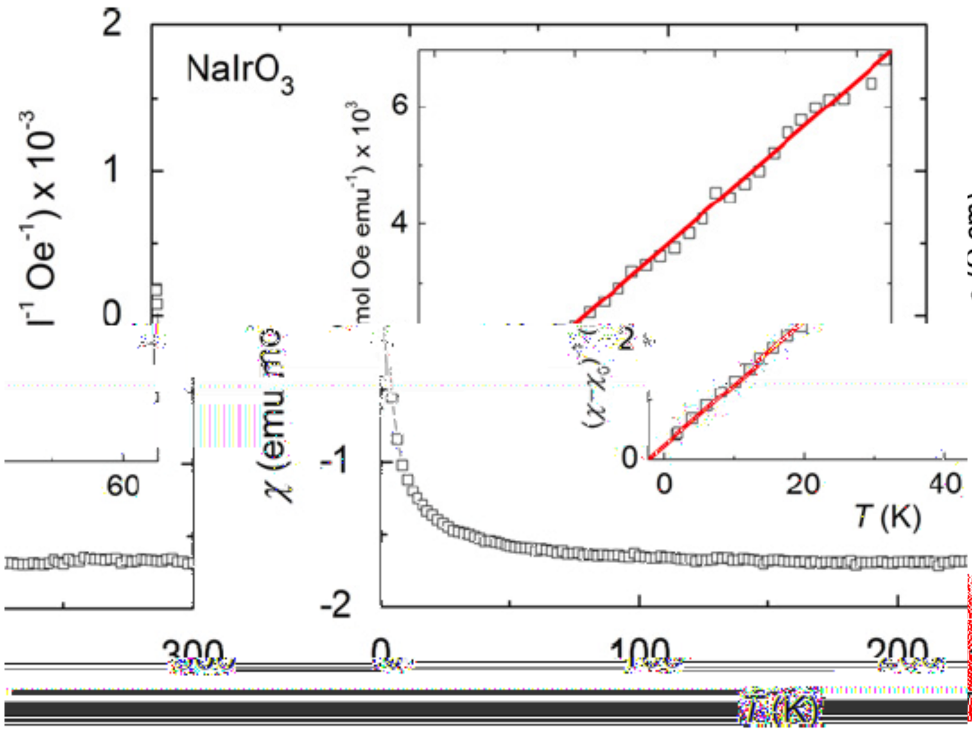

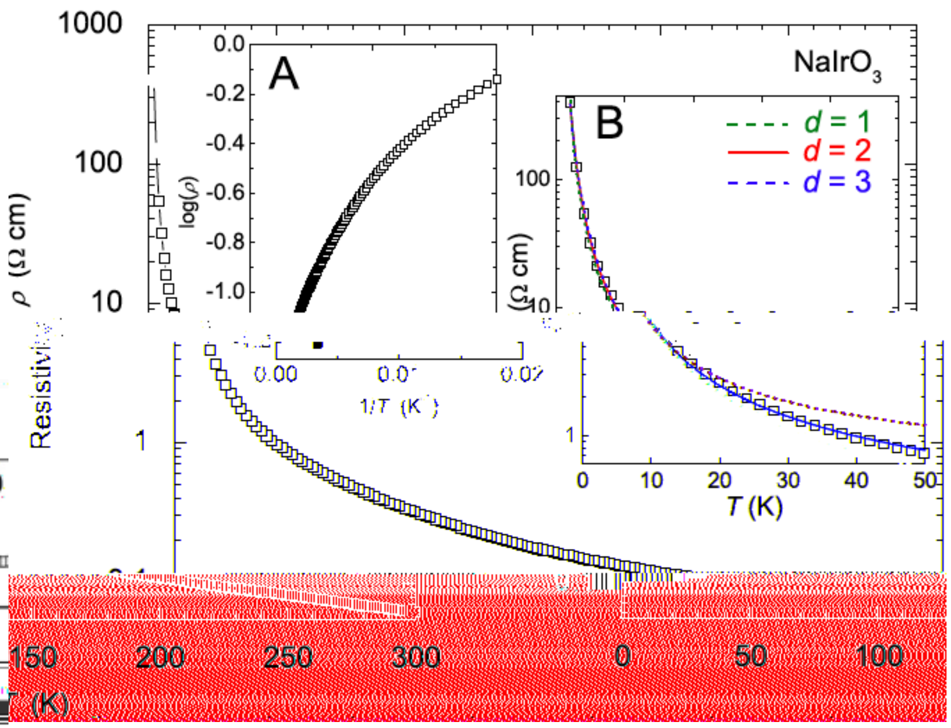

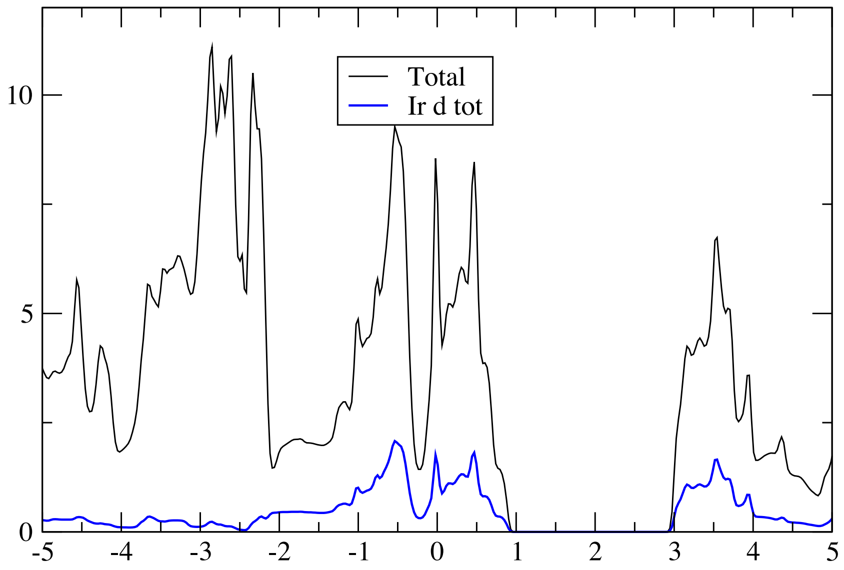
Total
Ir d tot
0
5
10
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-3
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1
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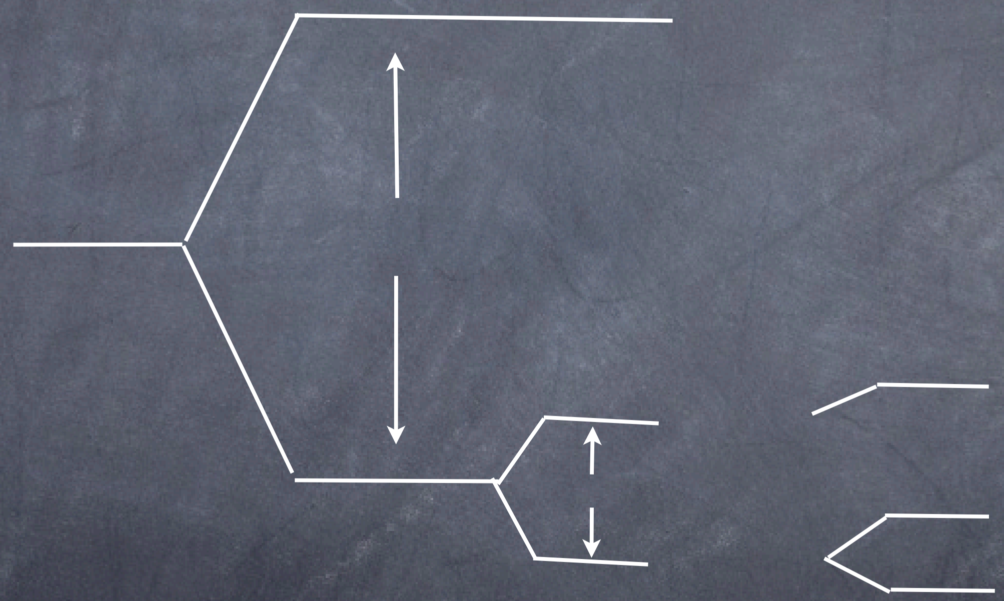
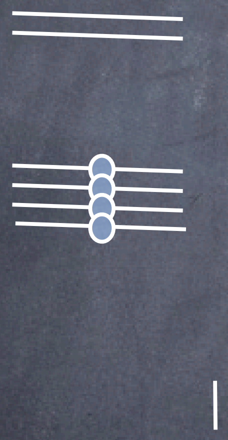
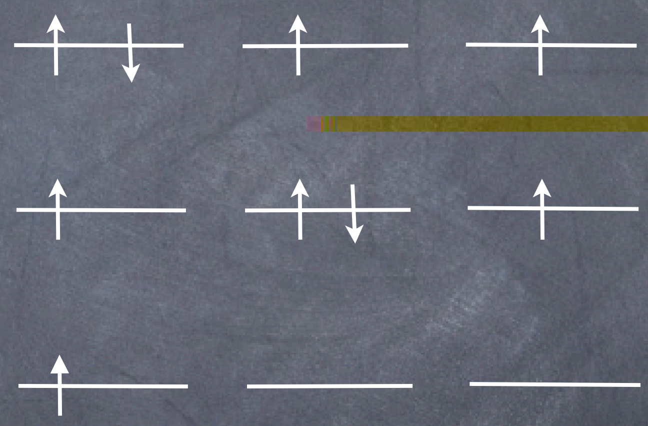






General tight-binding Hamiltonian

Three-band Hubbard Model With SOC:

$$H = H_0 + H_{SO} + H_U$$

Kinetic Energy Terms:

$$H_0 = \sum_{i\neq j,a\sigma} t_{ij}^{a\sigma} d^{\dagger}_{i,a\sigma} d_{j,a\sigma}$$

Spin-Orbit Coupling Terms:

$$H_{SO} = \sum_{a\sigma}\sum_{b\sigma'} \zeta \langle a\sigma | l \quad \ldots \quad {}_x s_x + l_y s_y + l_z s_z | b\sigma' \rangle d^{\dagger}_{a\sigma} d_{b\sigma'}$$

Coulomb Interaction Terms:

$$H_U = U \sum_{a} n_{a,\uparrow} n_{a,\downarrow} + U' \quad \ldots \sum_{a<b,\sigma\sigma'} n_{a,\sigma} n_{b,\sigma'} - J_z \sum_{a<b,\sigma} n_{a,\sigma} n_{b,\sigma}$$

$$- J_{xy} \sum_{a<b} \Big(d^{\dagger}_{a,\uparrow} d_{a,\downarrow} d^{\dagger}_{b,\downarrow} \quad \ldots \quad d_{b,\uparrow} + d^{\dagger}_{a,\uparrow} d^{\dagger}_{a,\downarrow} d_{b,\uparrow} d_{b,\downarrow} + h.c. \Big)$$

M

Rotational Invariant Gutzwiller Approximation

Gutzwiller variational wavefunction:

$$|\Psi_G\rangle = \mathcal{P}|\Psi_0\rangle = \prod_{\mathbf{R}} \mathcal{P}_{\mathbf{R}}|\Psi_0\rangle$$

$$\mathcal{P}_{\mathbf{R}} = \sum_{\Gamma\Gamma'} \lambda(\mathbf{R})_{\Gamma\Gamma'} |\Gamma, \mathbf{R}\rangle\langle\Gamma', \mathbf{R}|$$

$|\Gamma\rangle$: eigenstates of atomic hamiltonian H_U

Ψ_0: [illegible]

$\mathcal{P}_{\mathbf{R}}$: projector operator modify weight of local configuration

Gutzwiller Constraints:

$$\langle\Psi_0|\mathcal{P}^\dagger\mathcal{P}|\Psi_0\rangle = 1$$

$$\langle\Psi_0|\mathcal{P}^\dagger\mathcal{P}n_{i\alpha}|\Psi_0\rangle = \langle\Psi_0|n_{i\alpha}|\Psi_0\rangle$$

Total Energy In Gutzwiller Wavefunction:

$$E^G = E^G_{kin} + E^G_{loc} = \langle \Psi_G | H_0 | \Psi_G \rangle + \langle \Psi_G | (H_U + H_{SO}) | \Psi_G \rangle$$

tional Procedure(Fixed n^0 Algorithm): Gutzwiller varia

$$\frac{\partial E^G}{\partial \langle \Psi_0 |} = \sum_{i \neq j} \sum_{\gamma\delta} \sum_{\alpha\beta} t_{ij}^{\alpha\beta} \mathcal{R}^{\dagger}_{\alpha\gamma} \mathcal{R}_{\delta\beta} c^{\dagger}_{i\gamma} c_{j\delta} | \Psi_0 \rangle - \sum_{i\alpha} \eta_\alpha c^{\dagger}_{i\alpha} c_{i\alpha} | \Psi_0 \rangle = 0$$

$$\frac{\partial E^G}{\partial \lambda_{\Gamma\Gamma'}} = \sum_{\delta\beta} \left(\frac{\partial E_{kin}}{\partial \mathcal{R}_{\delta\beta}} \frac{\partial \mathcal{R}_{\delta\beta}}{\partial \lambda_{\Gamma\Gamma'}} + \frac{\partial E_{kin}}{\partial \mathcal{R}^{\dagger}_{\beta\delta}} \frac{\partial \mathcal{R}^{\dagger}_{\beta\delta}}{\partial \lambda_{\Gamma\Gamma'}} \right) + \frac{\partial E_{loc}}{\partial \lambda_{\Gamma\Gamma'}} + \sum_{\alpha} \eta_\alpha \frac{\partial n^G_\alpha}{\partial \lambda_{\Gamma\Gamma'}} = 0$$

The Lagrange parameters η_α come from Guztwiller Constraint.

$$\mathcal{R}^{\dagger}_{\alpha\gamma} = \frac{\mathrm{Tr}\left(\phi^{\dagger} c^{\dagger}_{\alpha} \phi c_{\gamma} \right)}{\sqrt{n^0_\gamma (1 - n^0_\gamma)}}$$

$$\phi_{II'} = \langle I | \hat{P} | I' \rangle \sqrt{\langle \Psi_0 | I' \rangle \langle I' | \Psi_0 \rangle}$$

Figure: Phase diagram at plane of U and SOC ζ for ... RIGA (b) DMFT (CT-QMC)

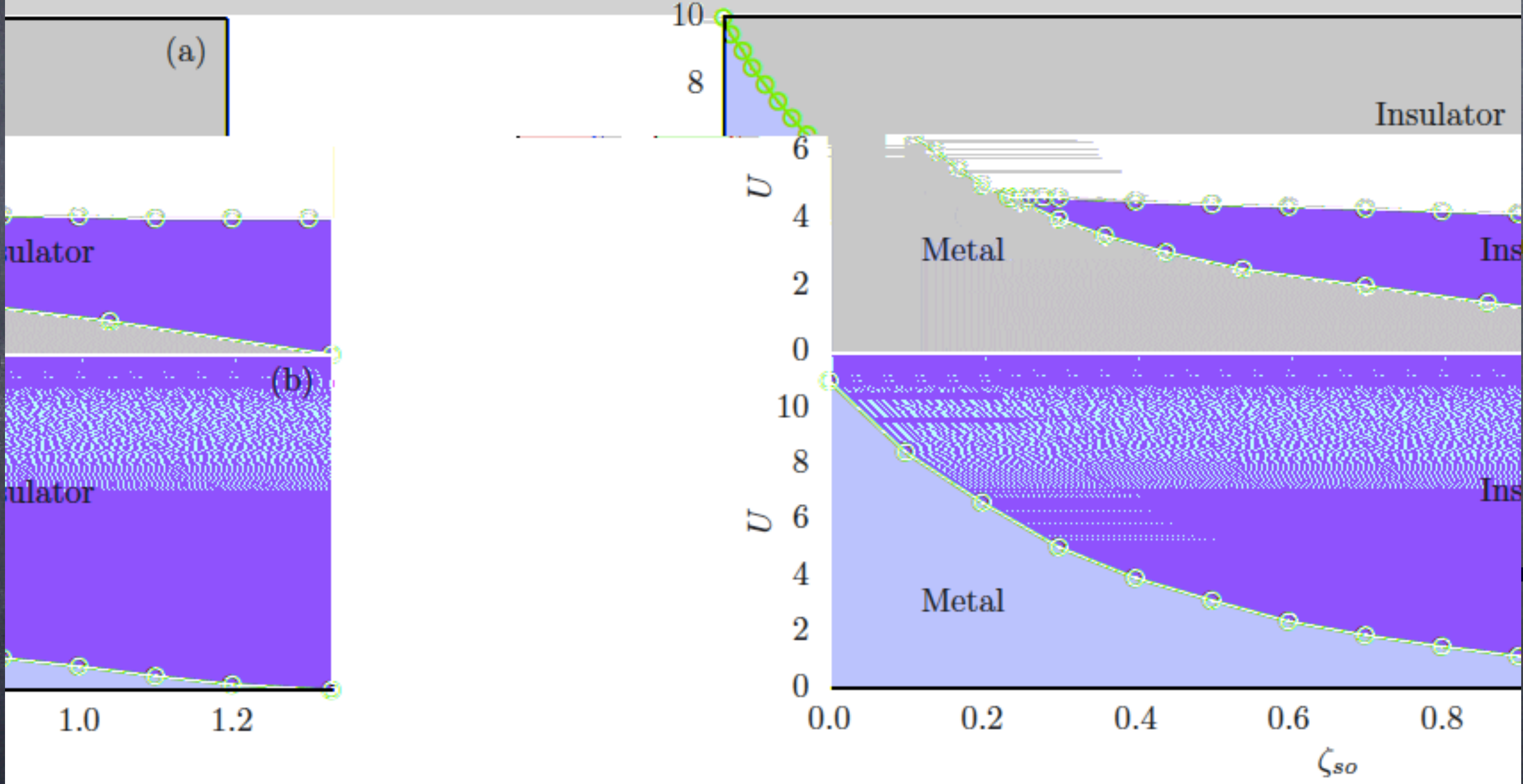


Figure: Energy and Quasiparticle weight as function of $0 \leq \delta n^0 \leq 1$ at

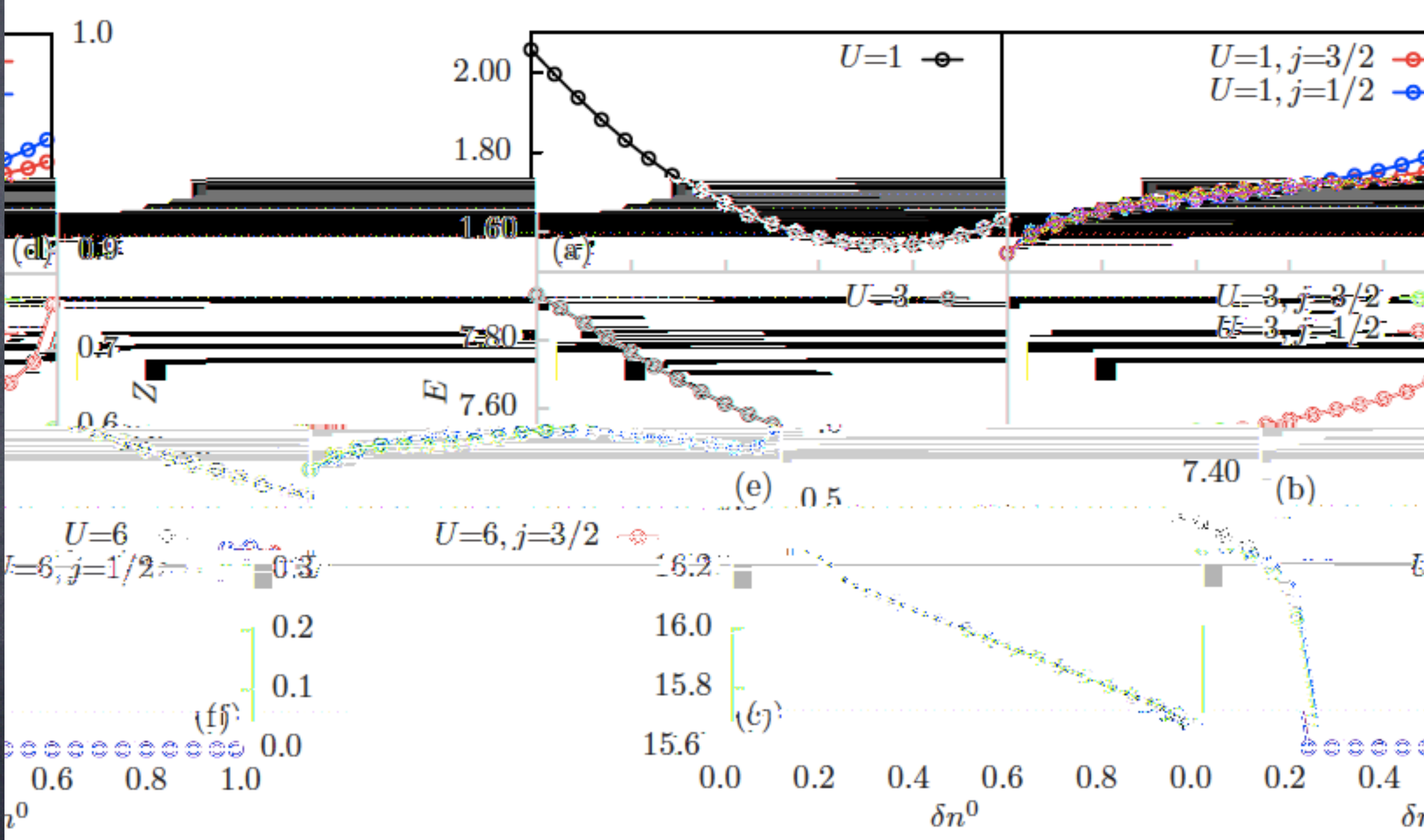


Figure: Expectational Value of L^2, S^2, J^2 as function of U with fix SOC $\zeta = 0.7$, Derived by DMFT+CTQMC

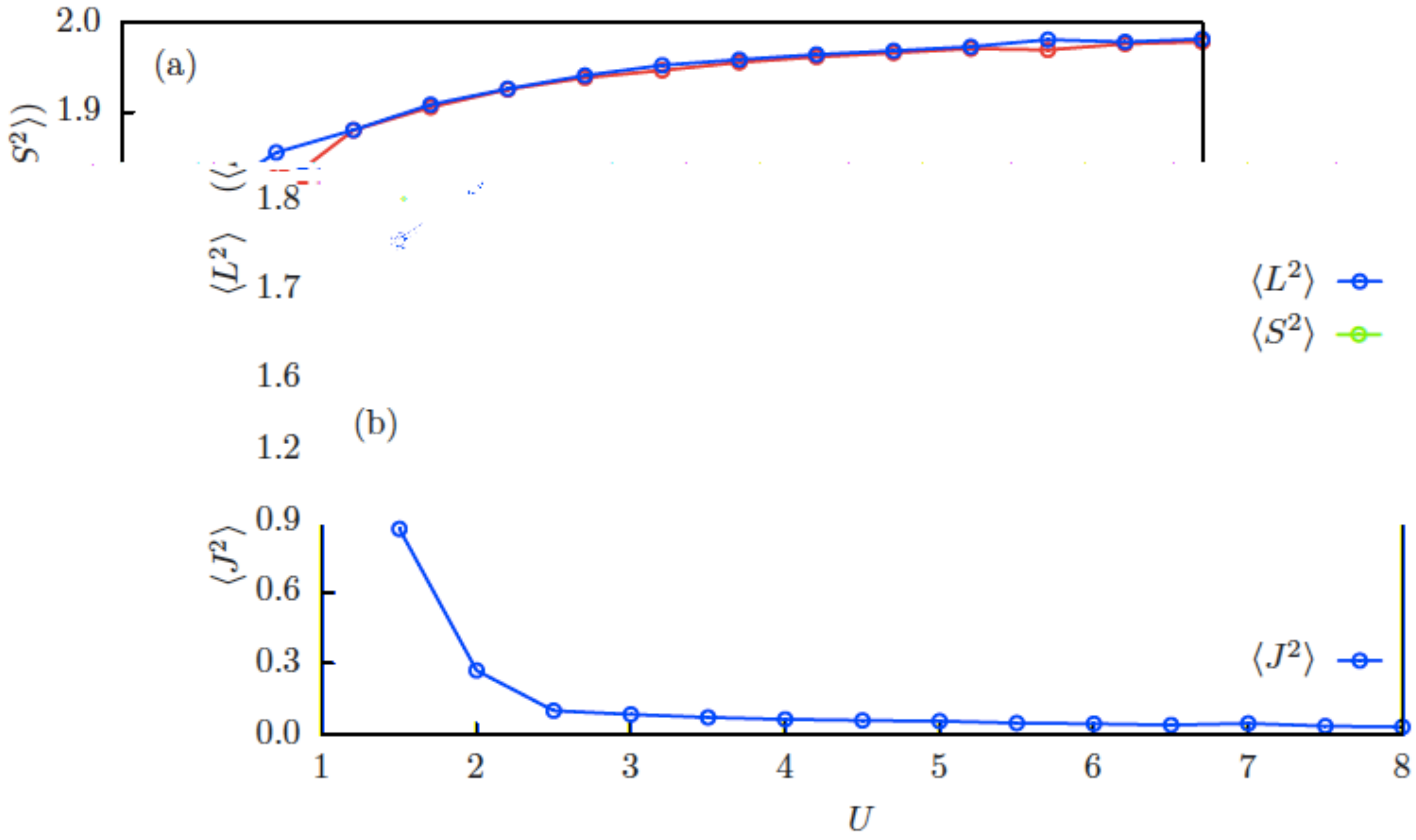
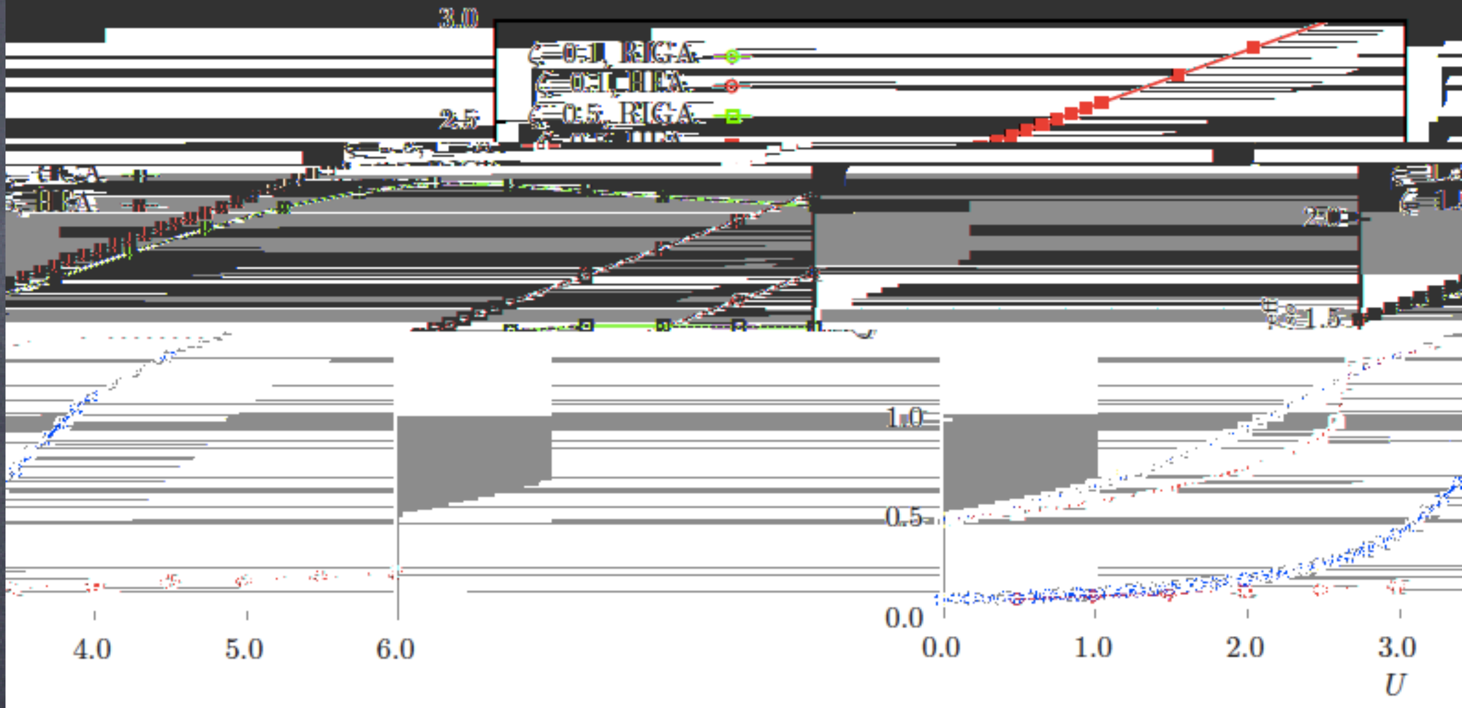
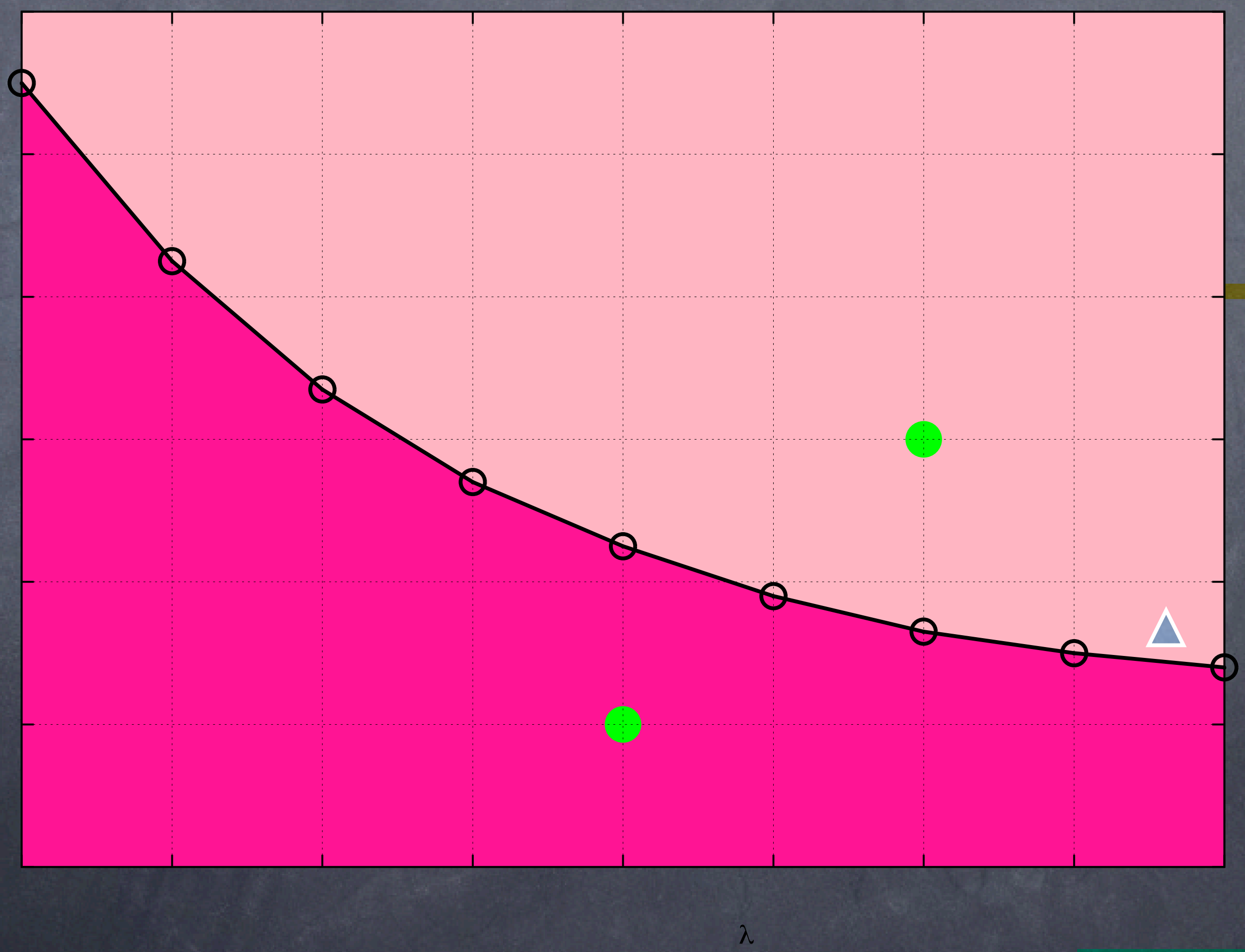


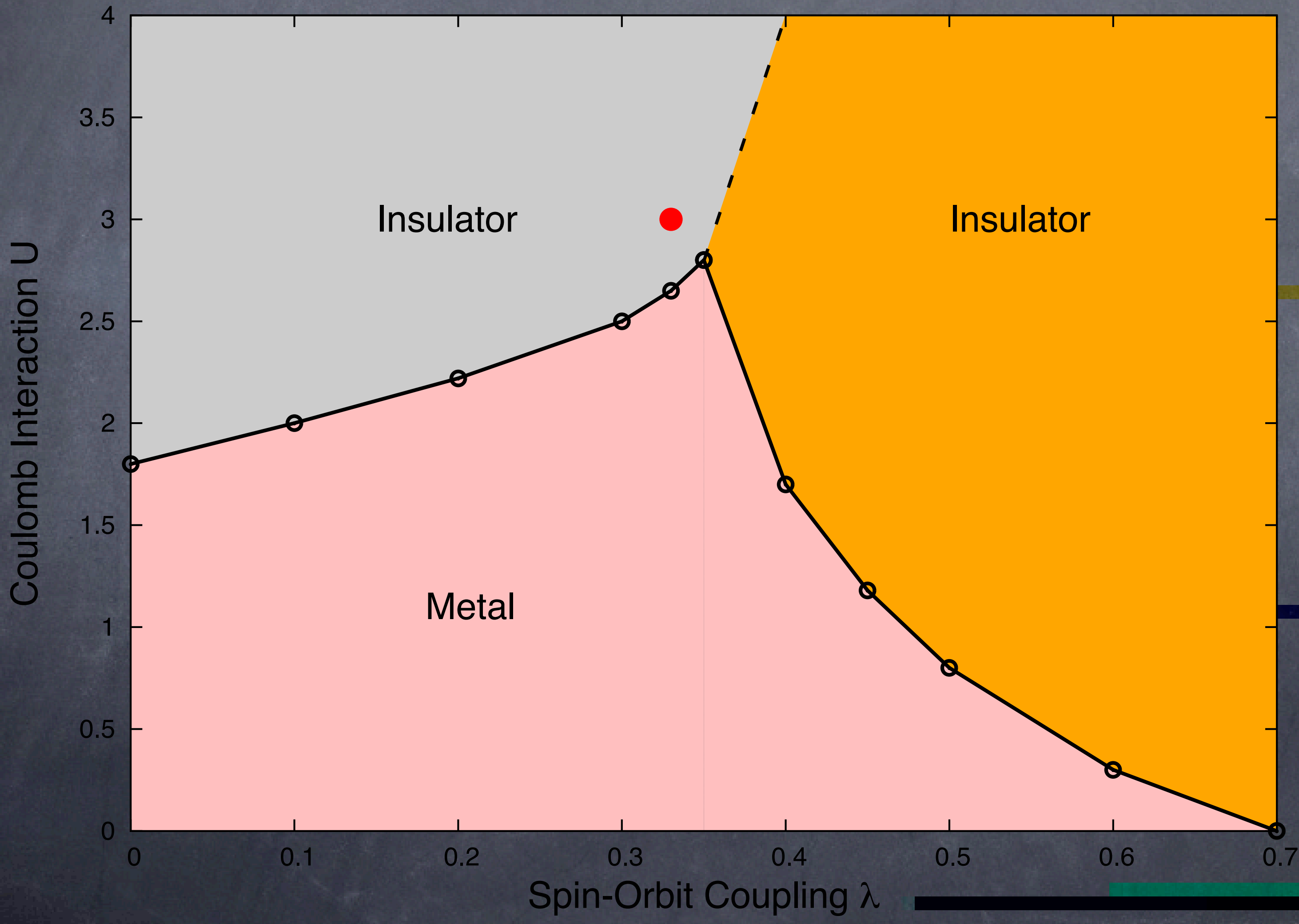
Figure: Effective spin-orbit coupling ζ^{eff} as function U at fixed $\zeta = 0.1, 0.5, 1.5$, derived by HFA and RIGA



$$\lambda_{eff} = \frac{\partial E_{int}}{\partial n^0_{1/2}} - \frac{\partial E_{int}}{\partial n^0_{3/2}}$$



λ


Insulator
Insulator
Metal
Coulomb Interaction U
Spin-Orbit Coupling λ
0
0.5
1
1.5
2
2.5
3
3.5
4
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7