Magnetic Excitations In The Iridate Sr_2IrO_4

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13.06.2014

Contents

Motivation

- Iridates contain Iridium embedded in an oxygen complex

Group→ / ↓Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
		*	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
		**	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

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- How and when does a metal-insulator transition occur?
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- Test the Hubbard model as an effective model.
- Calculate the magnetic excitations of $\mathrm{Sr_2IrO_4}$ and relate them to measurements.

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- Strong interaction between electrons
- Strong spin-orbit coupling (SOC)
- Effective spin-$\frac{1}{2}$ states
- Antiferromagnetic ordering
- Weak ferromagnetic moment
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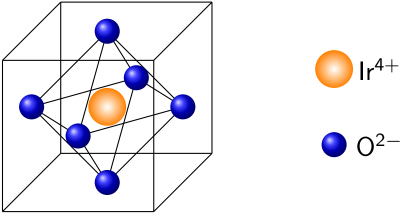
Crystal Field

Building block of iridates:



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- Lifts degeneracy of $5d$ states

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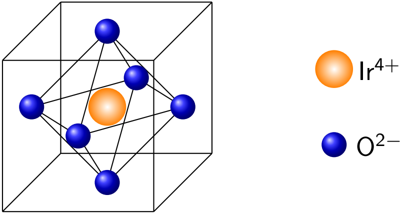

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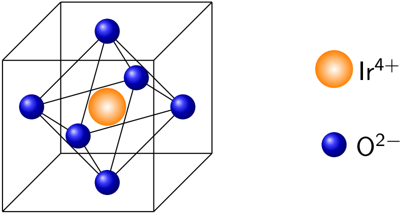

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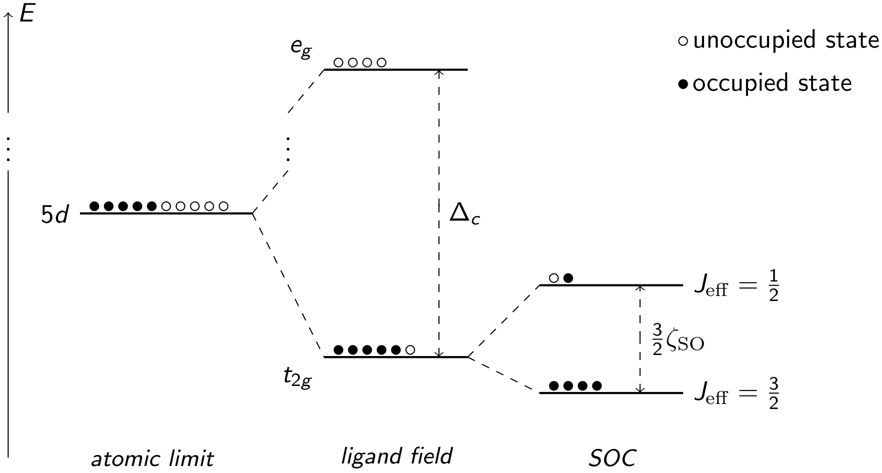
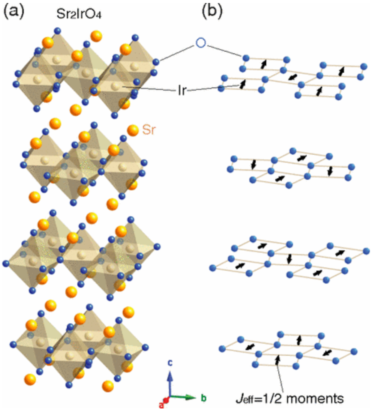
Atomic States



Unit Cell Of Sr_2IrO_4



Graphic taken from Jungho Kim *et al.*, Phys.Rev.Lett. 108:177003.

Crystall structure of Sr_2IrO_4

- Layered
- 2-dimensional square lattice
- One orbital, half filled

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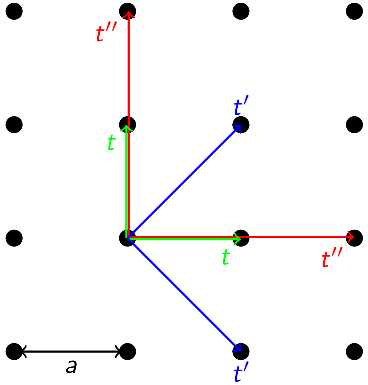
The Hubbard Hamiltonian

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma} \right) - \mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}.$$

- t: hopping term, corresponds to kinetic energy
- U: intra-orbital repulsion between electrons
- $n_\sigma = c^\dagger_{i,\sigma} c_{i,\sigma}$
- sum restricted to nearest neighbour pairs $\langle i, j \rangle$
- fermionic anti-commutation relations
  $\{c^\dagger_{i,\sigma}, c_{j,\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}; \quad \{c^\dagger_{i,\sigma}, c^\dagger_{j,\sigma'}\} = 0$
- μ: chemical potential

The Hubbard Hamiltonian



Momentum space for a square lattice

- Periodic system $\Rightarrow k_i + \frac{2\pi}{a} \sim k_i$.
- Momenta restricted to Brillouin zone $[-\frac{\pi}{a}, \frac{\pi}{a}]^2$.
- Normalize lattice constant a to 1.
- Finite systems with N lattice sites result in N discretized momenta.

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The Hubbard Hamiltonian in momentum space

$$\hat{H} = \sum_{\vec{k},\sigma} \left(\varepsilon_{\vec{k}} - \mu\right) c^{\dagger}_{\vec{k},\sigma} c_{\vec{k},\sigma} + \frac{U}{N} \sum_{\vec{k}\vec{k}'\vec{q}} c^{\dagger}_{\vec{k},\uparrow} c_{\vec{k}-\vec{q},\uparrow} c^{\dagger}_{\vec{k}',\downarrow} c_{\vec{k}'+\vec{q},\downarrow}$$

with the dispersion

$$\varepsilon_{\vec{k}} = -2t\left(\cos k_x + \cos k_y\right) - 4t' \cos k_x \cos k_y - 2t''\left(\cos 2k_x + \cos 2k_y\right)$$

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Heisenberg model

- Stationary spins without a kinetic term.
- Heisenberg Hamiltonian
- Can be derived from the Hubbard model in the large U limit.
- $J \longrightarrow 4\frac{t^2}{U}, \qquad (\frac{t}{U} \rightarrow 0)$
- Long range correlations become more important for lower U.

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\begin{aligned}
U\sum_i n_{i,\uparrow}n_{i,\downarrow} = U\sum_i & (n_{i,\uparrow} - \langle n_{i,\uparrow}\rangle)(n_{i,\downarrow} - \langle n_{i,\downarrow}\rangle) \\
& + n_{i,\uparrow}\langle n_{i,\downarrow}\rangle + n_{i,\downarrow}\langle n_{i,\uparrow}\rangle - \langle n_{i,\uparrow}\rangle\langle n_{i,\downarrow}\rangle
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Mean Field Equations

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$$U \sum_i n_{i,\uparrow} n_{i,\downarrow} \approx U \sum_i n_{i,\uparrow} \langle n_{i,\downarrow} \rangle + n_{i,\downarrow} \langle n_{i,\uparrow} \rangle + \mathrm{const.}$$

Mean field equations

- in momentum space:
$\frac{U}{N}\sum_{\vec{q}}\sum_{\vec{k},\vec{k}',\sigma} c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma} \langle c^\dagger_{\vec{k}'-\vec{q},\sigma} c_{\vec{k}',\sigma}\rangle$
- uniform repulsion for $\vec{q}=0$, $\frac{1}{N}\sum_i \langle c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma}\rangle = n_\sigma$
- staggered magnetic field for $\vec{q}=\vec{Q}\equiv(\pi,\pi)$.
$\frac{1}{N}\sum_{\vec{k}}\langle c^\dagger_{\vec{k},\sigma} c_{\vec{k}+\vec{Q},\sigma}\rangle = \frac{1}{N}\sum_i \langle (-1)^i c^\dagger_{i,\sigma} c_{i,\sigma}\rangle = \frac{s_\sigma}{2} m_s \neq 0$

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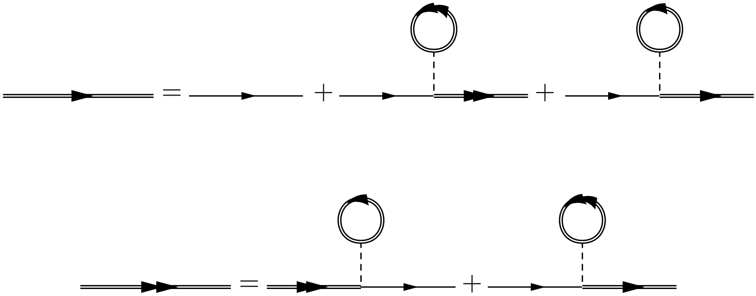
Propagators

$$G_{\vec{k}}(\tau) = \langle c_{\vec{k},\sigma}(\tau) c^{\dagger}_{\vec{k},\sigma}(0) \rangle =$$

$$F_{\vec{k}}(\tau) = \langle c_{\vec{k}+\vec{Q},\sigma}(\tau) c^{\dagger}_{\vec{k},\sigma}(0) \rangle =$$

Mean Field Propagators

Self consistent Dyson equation
Coupled differential equation that can be solved analytically



Propagators

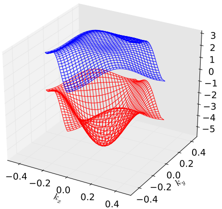
$$G_{\vec{k},\sigma}(\mathrm{i}\omega_n) = \frac{\mathrm{i}\omega_n - \varepsilon_{\vec{k}+\vec{Q}} + \mu - Un_{-\sigma}}{(\mathrm{i}\omega_n - E^{+}_{\vec{k},\sigma})(\mathrm{i}\omega_n - E^{-}_{\vec{k},\sigma})},$$

$$F_{\vec{k},\sigma}(\mathrm{i}\omega_n) = \frac{Um_{s,-\sigma}}{(\mathrm{i}\omega_n - E^{+}_{\vec{k},\sigma})(\mathrm{i}\omega_n - E^{-}_{\vec{k},\sigma})}.$$

with the poles located at

$$E^{\pm}_{\vec{k},\sigma} = \frac{\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{Q}}}{2} - \mu + Un_{-\sigma} \pm \sqrt{\left(\frac{\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{Q}}}{2}\right)^2 + U^2 m^2_{s,-\sigma}}$$

Energy bands $E^{\pm}_{\vec{k},\sigma}$



Dispersion for the t-t'-t''-U-model .

- The $J_{\text{eff}} = \frac{1}{2}$- band is split due to the interaction.
- Explains insulating state.
- Symmetric under translations of $\vec{Q} = (\pi, \pi)$.

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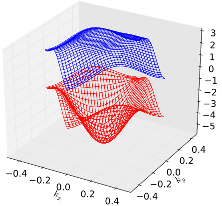

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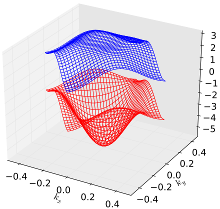

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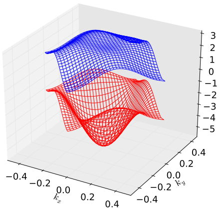

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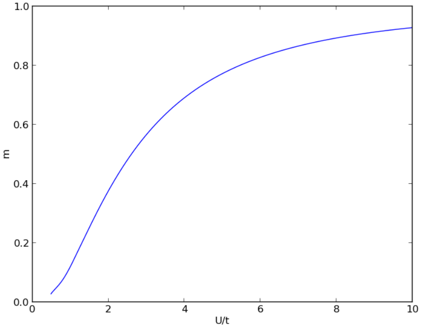
Staggered magnetization



Staggered magnetization as function of $\frac{U}{t}$

Excitations

- study basic magnetic excitations by inelastic scattering: neutron or X-ray (RIXS).
- Differential scattering cross section directly related to dynamic magnetic susceptibility.
- Poles at basic excitations of the system.
- transferred energy and momentum give magnon dispersion.
- Dynamical magnetic susceptibility is a two-point correlation function,

$$\chi^{+-}(\tau, \vec{q}) = \sum_{\vec{k}\vec{k}'} \langle c^{\dagger}_{\vec{k}+\vec{q},\uparrow}(\tau)\, c_{\vec{k},\downarrow}(\tau)\, c^{\dagger}_{\vec{k}',\downarrow}(0)\, c_{\vec{k}'+\vec{q},\uparrow}(0)\, \rangle$$

- Can be expressed in terms of propagators.

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- Can be expressed in terms of propagators.

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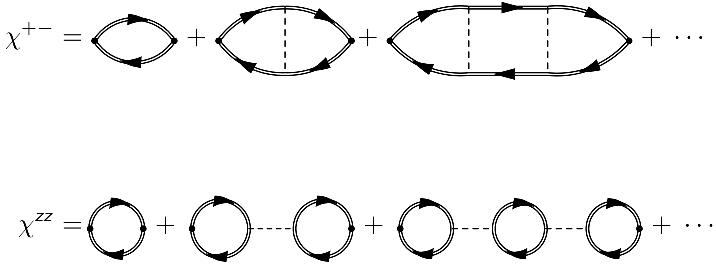
Diagrammatic Expansion



Random Phase Approximation

- Sum subclass of diagrams to infinite order.
- Yields a closed form expression.
- no UV divergence due to periodicity,
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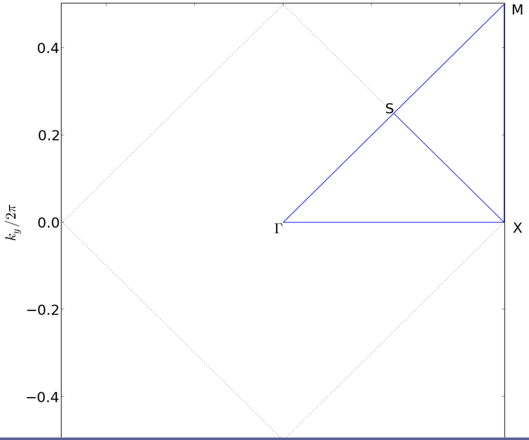
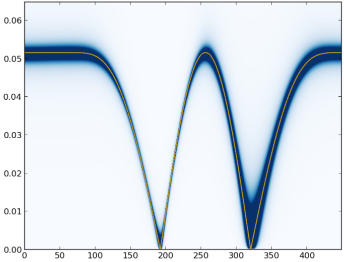
Specifications

- Band structure given
- U as only adjustable parameter
- calculate dispersion along symmetry lines of dispersion

Brillouin zone

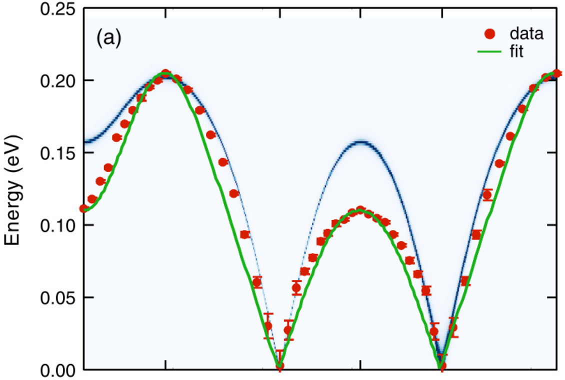


Large U limit



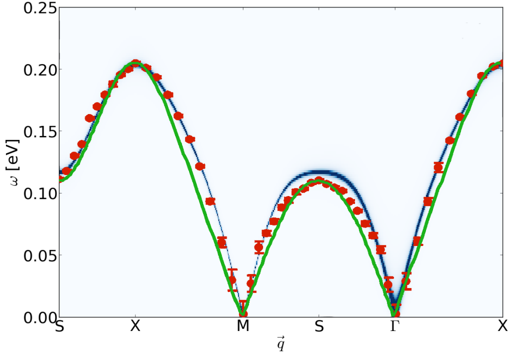
$$U = 40t \quad \omega(\vec{q}) = 4\frac{t^2}{U}\sqrt{1 - \frac{1}{2}(\cos q_x + \cos q_y)}.$$

Results for the t-U-Model



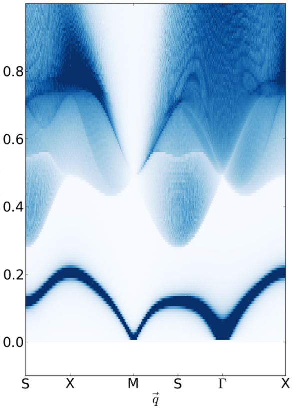
Spin wave dispersion for the t-U-model with $U = 4.7t$

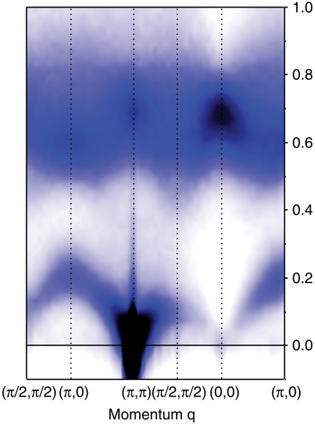
Results for the t-t'-t''-U-Model



Spin wave dispersion for the t-t'-t''-U-model with $U = 4.4t$

Continuous excitations



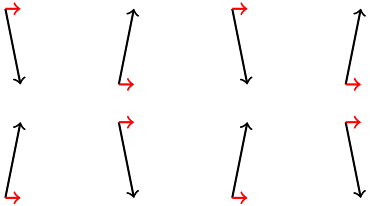


Magnetization

- $U = 4.4t = 1.1$eV
- just above the Metal insulator transition point for a SOC with $\zeta_{\mathrm{SO}} = 0.37$eV
- $m_s = 0.73$
- charge gap $\Delta_{\mathrm{Mott}} = \max(E^{+}_{\vec{k}} - E^{-}_{\vec{k}'}) = 0.47\mathrm{eV}$ (experimentally 0.54eV)

Ferromagnetic moment

- Created by canted structure



- $\frac{M}{M_{\text{local}}} = m_s \sin \Theta = 0.139$
- experimentally $M = 1.14\mu_b$
- $M_{\text{local}} = 1\frac{\mu_b}{\text{Ir}^{4+}}$, as in the atomic limit

Improvements

- Quantum corrections
- Refine Band structure

Further Calculations

- Change filling factor
- Different materials

Thank you for your attention.