Density matrix renormalization group study of a three-orbital Hubbard model with spin-orbit coupling in one dimension

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Introduction and Motivation

Iron Based Superconductors, Cuprates etc.

Sr_2RhO_4 [d^5], Sr_2RuO_4[d^4], etc.

Sr_2IrO_4[d^5], Ba_2YIrO_6[d^4], etc.

Electron Type	*U(eV)*	*λ(eV)*	*Interactions*
3d	*5-7*	*0.01-0.1*	$U > CF > \lambda$
4d	*0.5-3*	*0.1-0.3*	$U \sim CF > \lambda$
5d	*0.4-2*	*0.1-1*	$U \sim CF \sim \lambda$

Spin-orbit coupling = λ***(L.S)*** *; grows as* Z^2 *for outer shell electrons.*

Gang Cao, Pedro Schlotman, 2018 Rep. Prog. Phys.

Introduction and Motivation

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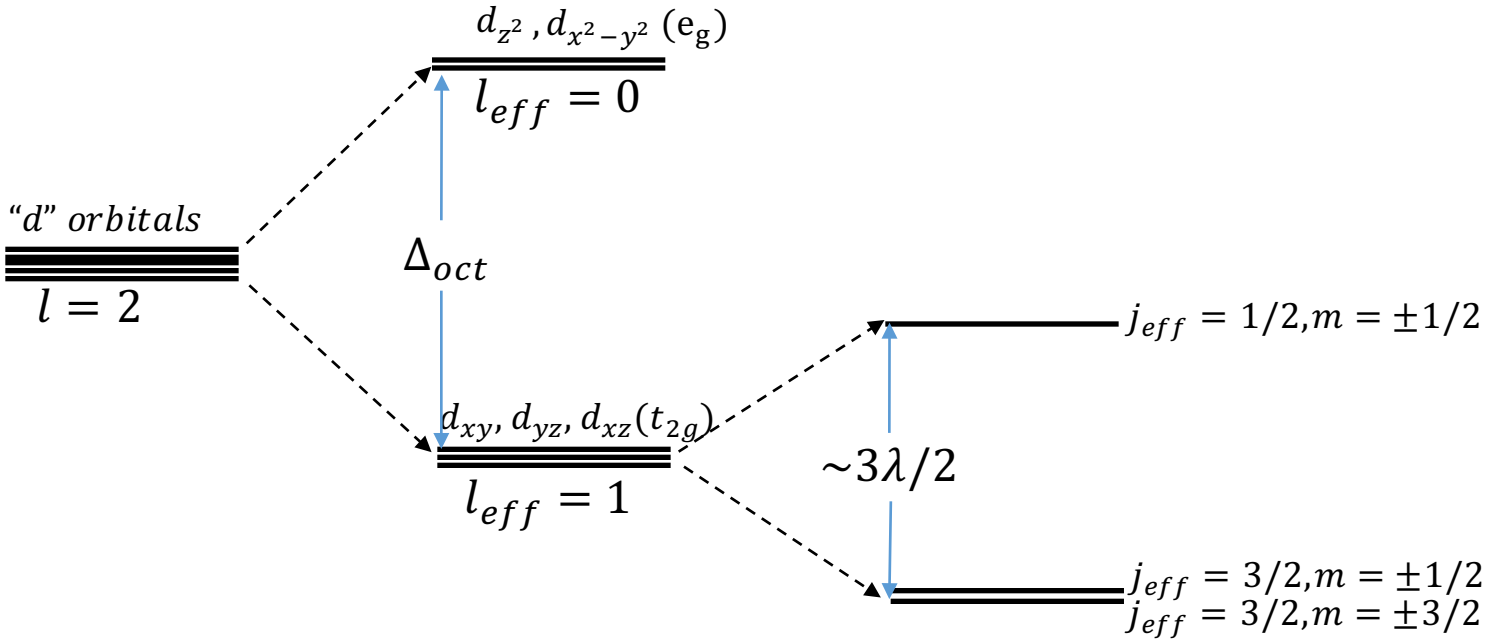
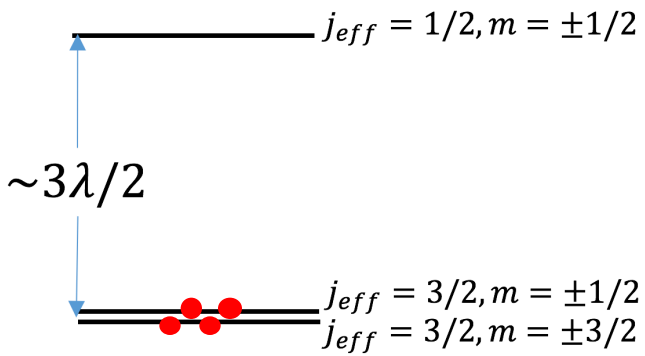
CF(Crystal Field) + Spin orbit coupling:

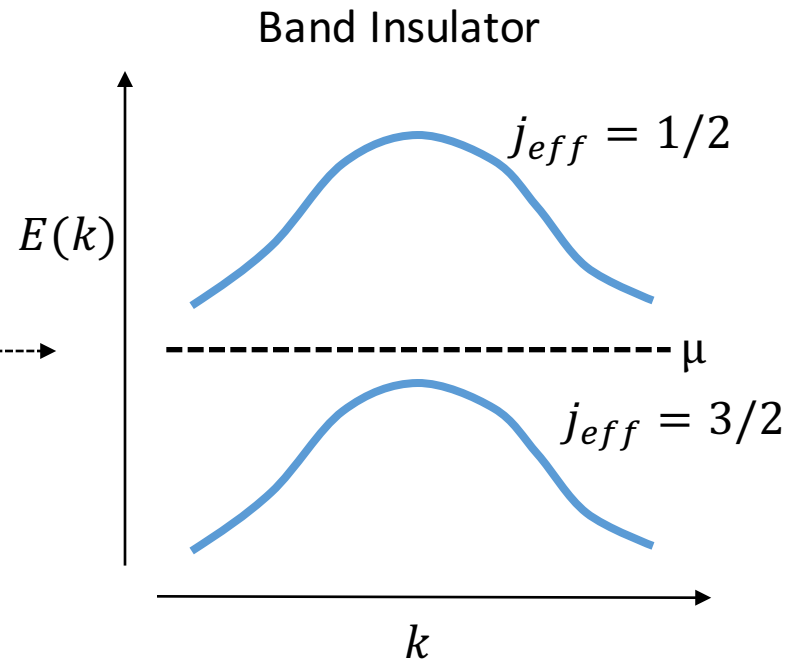


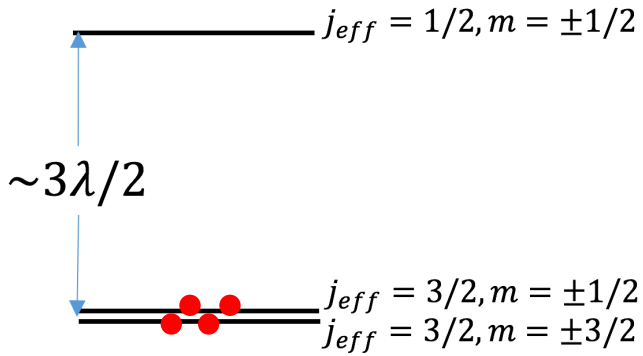
Introduction and Motivation

Case: d^4 [Relevant for materials like Sr_2YIrO_4 , Ba_2YIrO_6]



Turn on the hopping



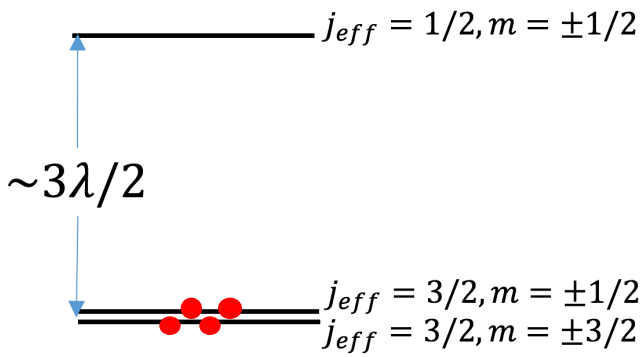


Turn on the hopping+ **Correlation [U]**

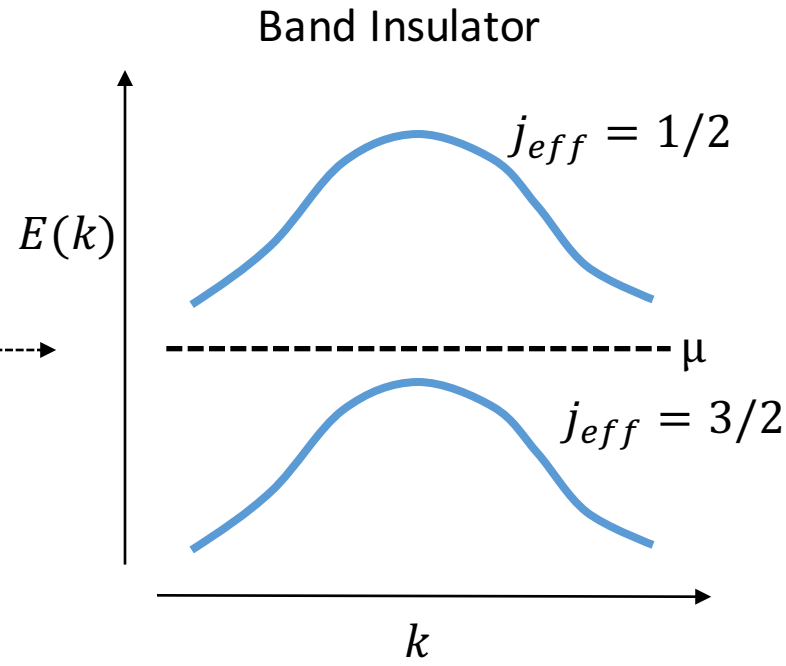
Very limited information ?

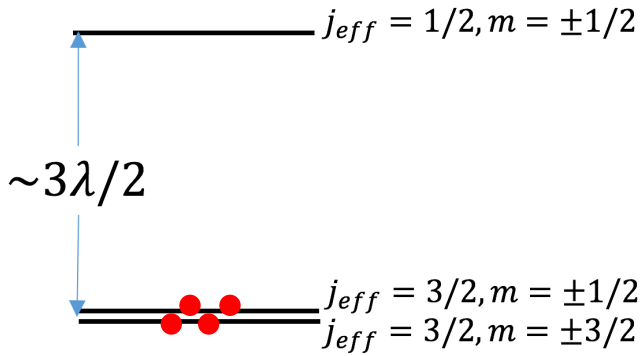
Introduction and Motivation

Case: d^4 [Relevant for materials like Sr_2YIrO_4 , Ba_2YIrO_6]



Turn on the hopping





Turn on the hopping+ **Correlation [U]**

AFM predicted by theory in strong coupling.
Experiments on Sr_2YIrO_6, Ba_2YIrO_6 have also show AFM at $T_N \sim 2K$.

1.*G. Khaliullin, Phys. Rev. Lett. **111**, 197201 (2013)
2.*C. Svoboda et al., Phys. Rev. B **95**, 014409 (2017)
3. G.Cao et al., Phys. Rev. Lett. **112**, 056402 (2014)
4. Q. Chen et al., Phys. Rev. B **96**, 144423 (2017)

Focus of the work:

Creating a "λ vs U" phase diagram for n=4 case. We aim to understand the phases emerging from SOC and U competition.

Why is this important?

Because ours is the first numerically exact study of SOC+U effects. Previous work relied on static and dynamical mean field theory.*

Numerical Technique used:

Density Matrix Renormalization Group technique is used to solve one-dimensional multi(3)-orbital Hubbard model in presence of spin-orbit coupling.

*T. Sato et al., Phys. Rev. B **91**, 125122 (2015)
T. Sato et al., arXiv:1603.01800

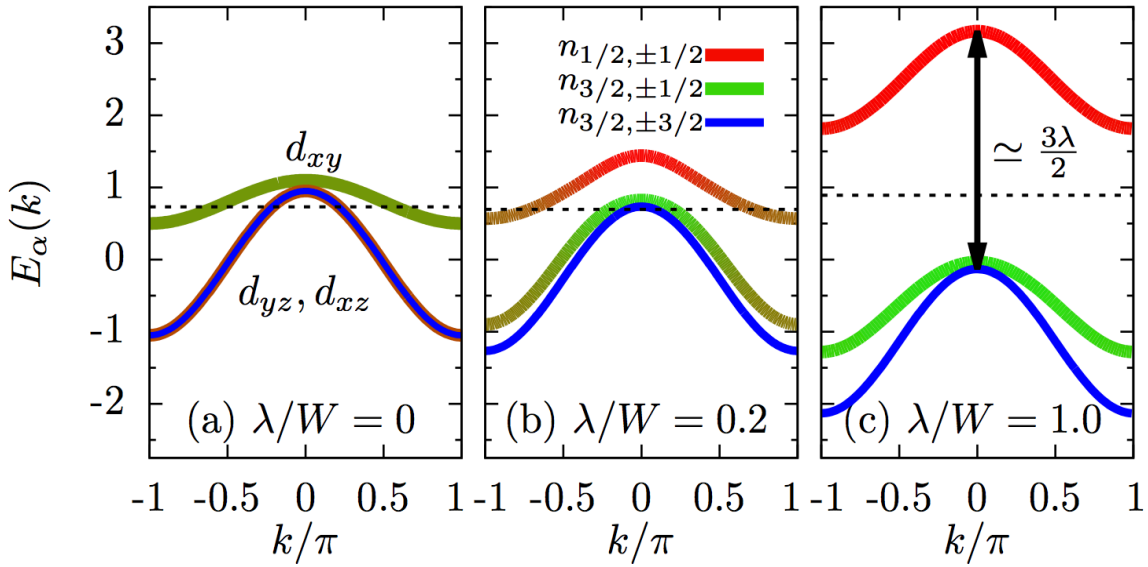
Model

$$H_{\mathrm{t}} = -\sum_{\mathrm{i}\sigma\gamma\gamma'} t_{\gamma\gamma'}(c^{\dagger}_{\mathrm{i}\sigma\gamma} c_{\mathrm{i+1}\sigma\gamma'} + \mathrm{h.c.}) + \sum_{\mathrm{i}\sigma\gamma} \Delta_{\gamma} n_{\mathrm{i}\sigma\gamma}$$

$$H_{\mathrm{SO}} = \lambda \sum_{\gamma,\delta,\sigma,\sigma'} A^{\gamma,\delta}_{\sigma,\sigma'} c^{\dagger}_{\gamma\sigma} c_{\delta,\sigma'}$$

Where, $A^{\gamma,\delta}_{\sigma,\sigma'} = < \gamma|\mathbf{L}|\delta > . < \sigma|\mathbf{S}|\sigma' >$

Increasing λ, for Non-interacting case



Metal ⟶ Band-insulator

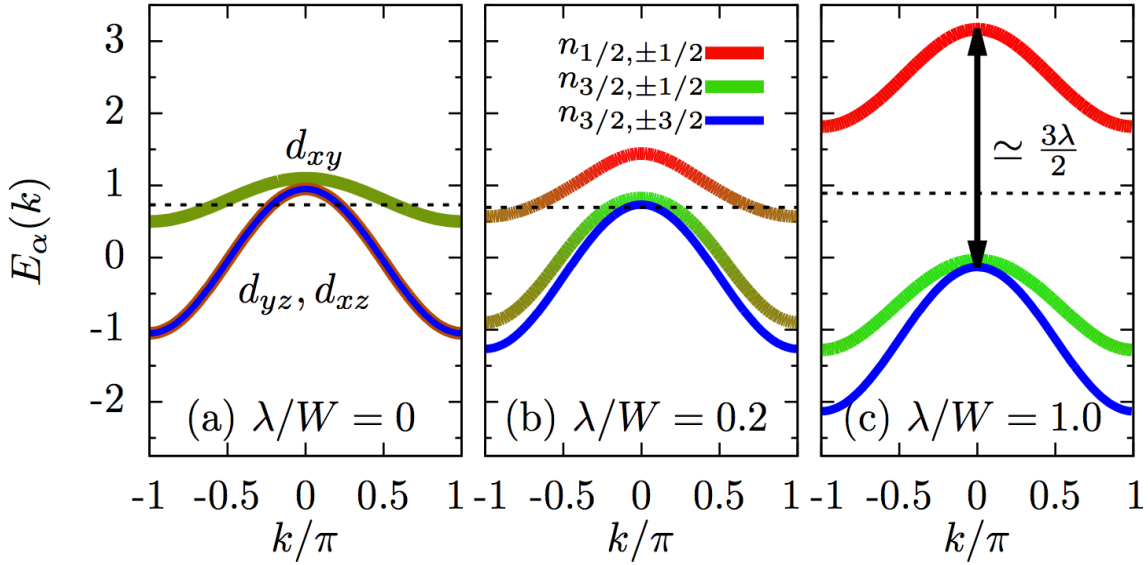
Model

$$H_{\rm t} = -\sum_{{\rm i}\sigma\gamma\gamma'} t_{\gamma\gamma'}(c^{\dagger}_{{\rm i}\sigma\gamma}c_{{\rm i+1}\sigma\gamma'} + {\rm h.c.}) + \sum_{{\rm i}\sigma\gamma}\Delta_{\gamma}n_{{\rm i}\sigma\gamma}$$

$$H_{\rm SO} = \lambda \sum_{\gamma,\delta,\sigma,\sigma'} A^{\gamma,\delta}_{\sigma,\sigma'} c^{\dagger}_{\gamma\sigma}c_{\delta,\sigma'}$$

Where, $A^{\gamma,\delta}_{\sigma,\sigma'} = <\gamma|\mathbf{L}|\delta> . <\sigma|\mathbf{S}|\sigma'>$

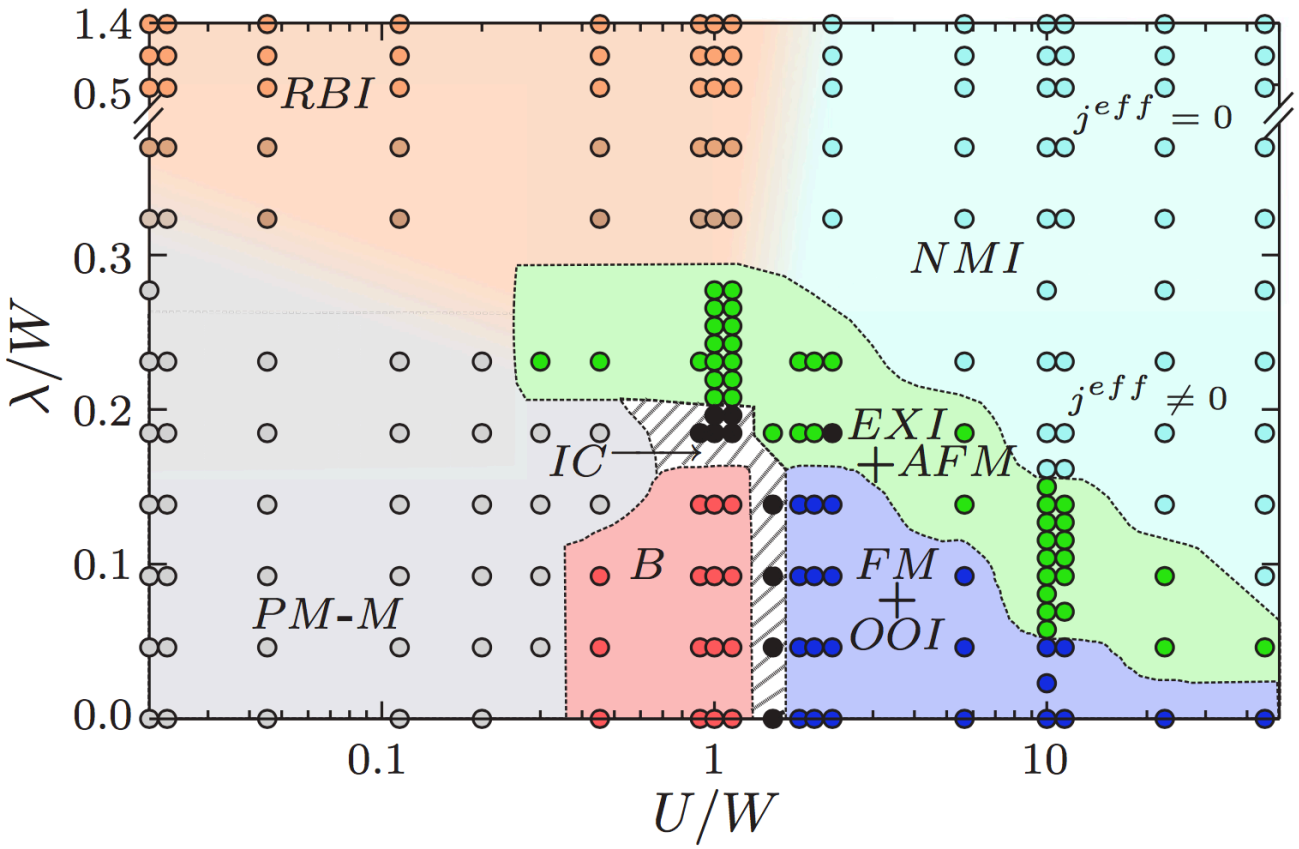
Increasing λ, for Non-interacting case



Metal ⟶ Band-insulator

$$H_{\rm Coul} = U\sum_{{\rm i}\gamma} n_{{\rm i}\uparrow\gamma}n_{{\rm i}\downarrow\gamma} + (U' - J_H/2)\sum_{{\rm i}\gamma<\gamma'} n_{{\rm i}\gamma}n_{{\rm i}\gamma'}$$
$$- 2J_H \sum_{{\rm i}\gamma<\gamma'} \mathbf{S}_{{\rm i}\gamma}\cdot\mathbf{S}_{{\rm i}\gamma'} + J_H\sum_{{\rm i}\gamma<\gamma'}\left(P^{+}_{{\rm i}\gamma}P_{{\rm i}\gamma'} + {\rm h.c.}\right)$$

Phase Diagram [U vs λ] for n=4

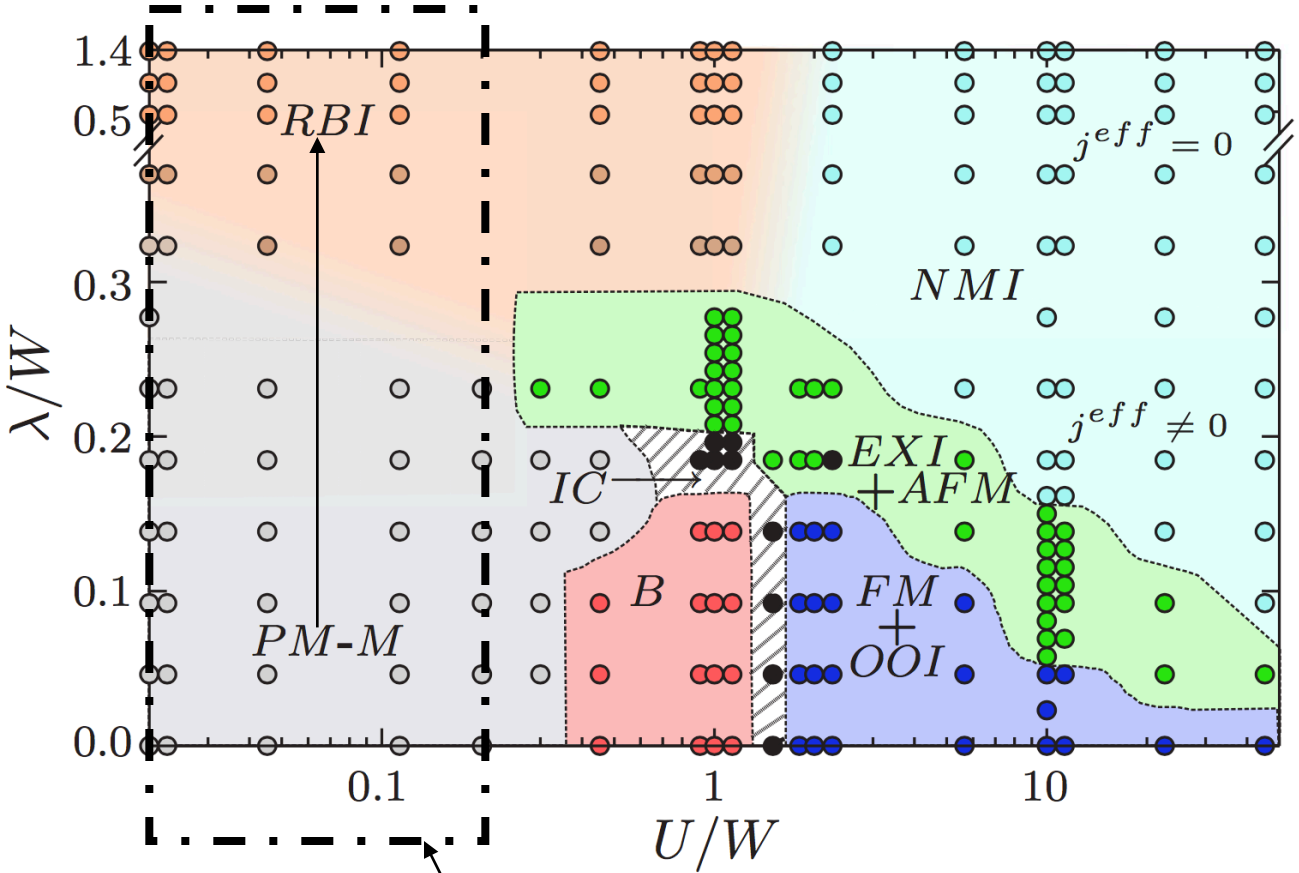


Calculations are performed for L=16 [upto L=32] sites.

$$\frac{J_H}{U} = \frac{1}{4}$$

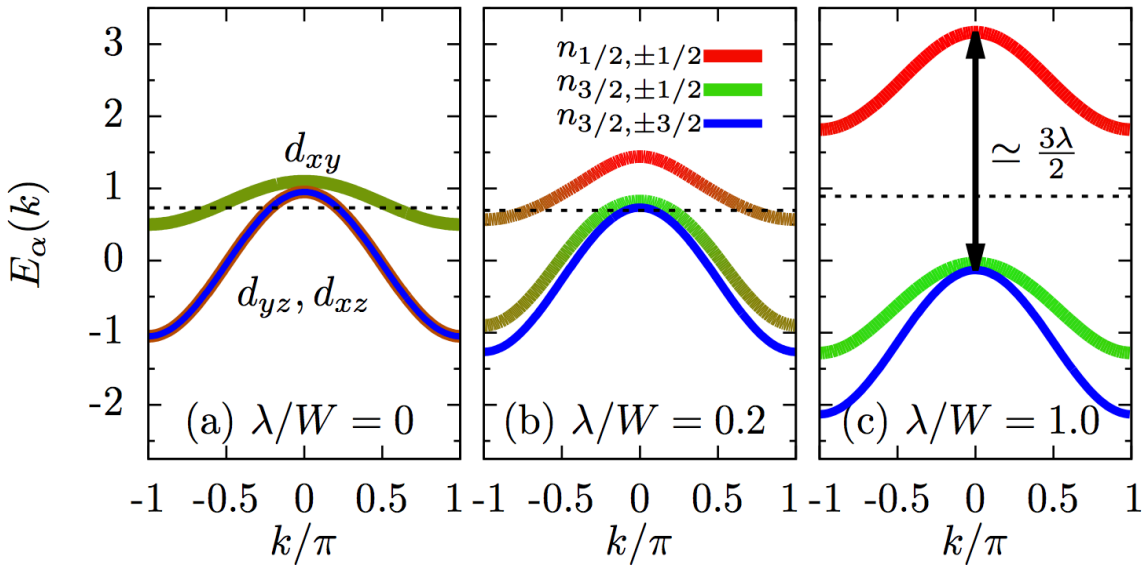
N. Kaushal et al., Phys. Rev. B **96**, 155111 (2017).

Phase Diagram [U vs λ] for n=4



Weak coupling limit:
Metal to Relativistic Band Insulator transition

Increasing λ, for Non-interacting case



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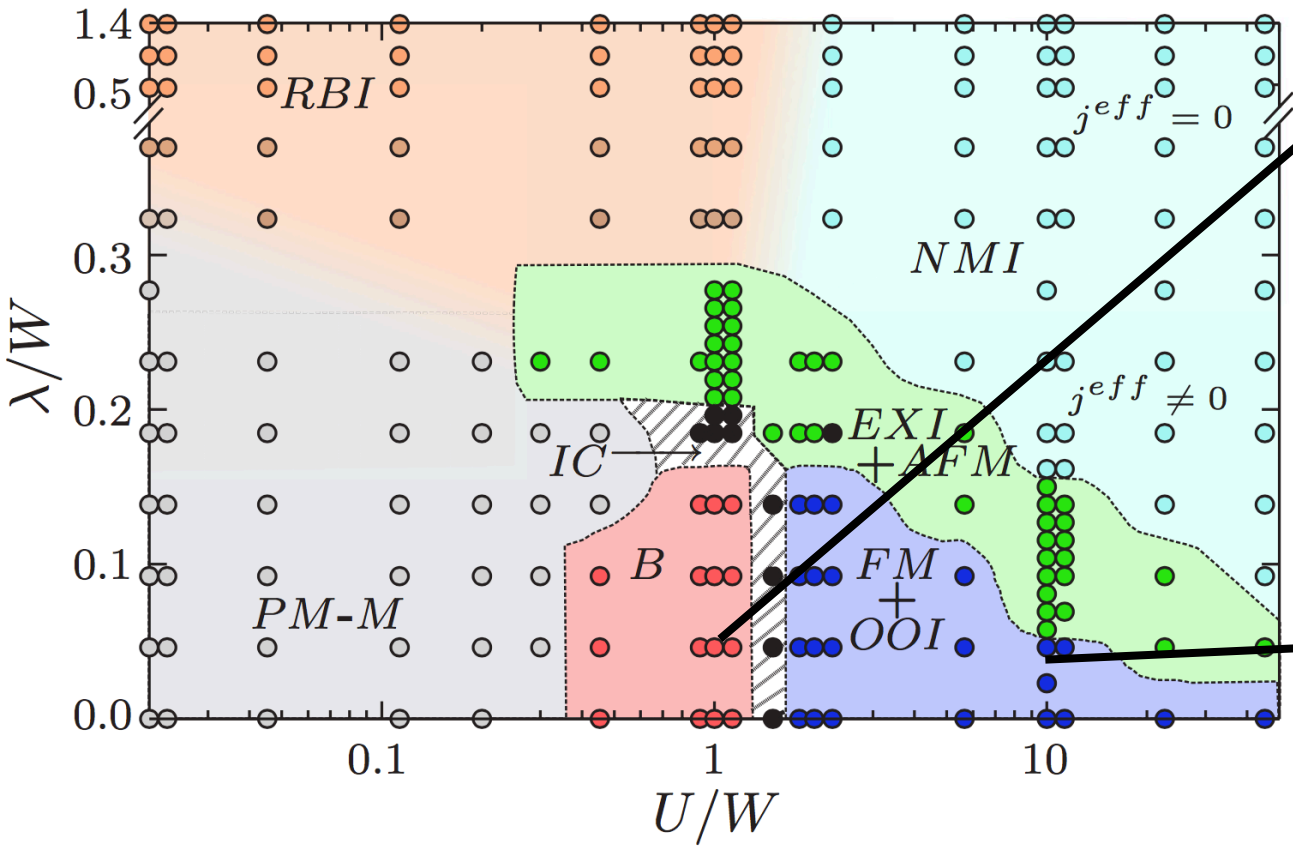
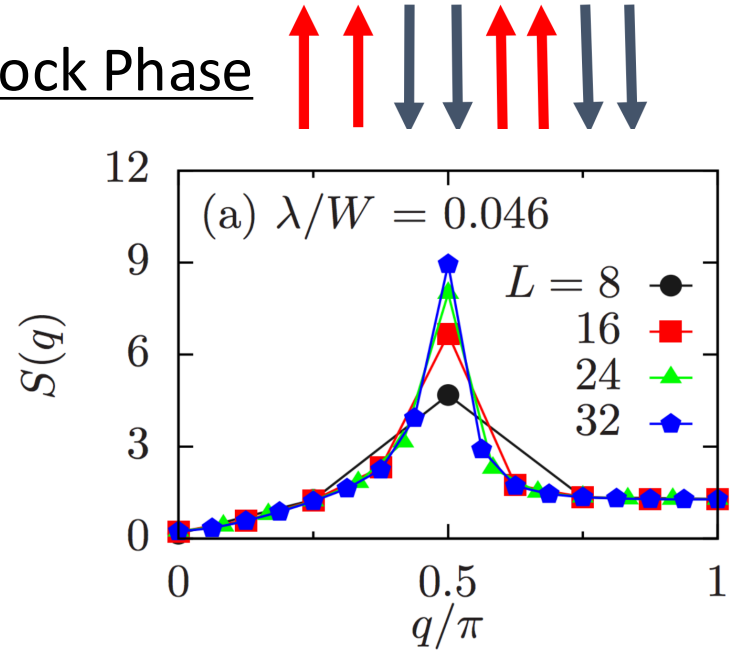
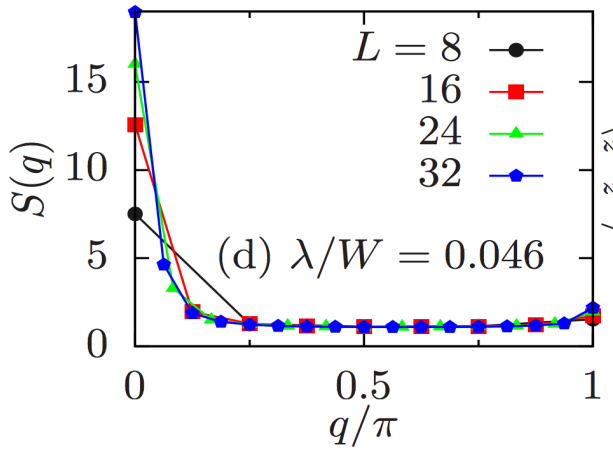
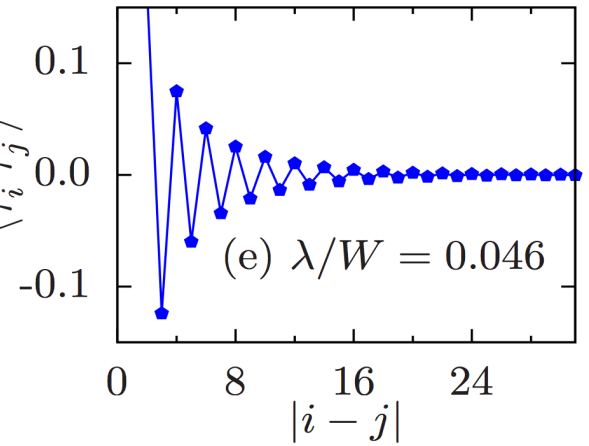


Block Phase



Ferromagnetic + Orbital Ordering





where $\tau_z(i) = n_{iyz} - n_{ixz}$

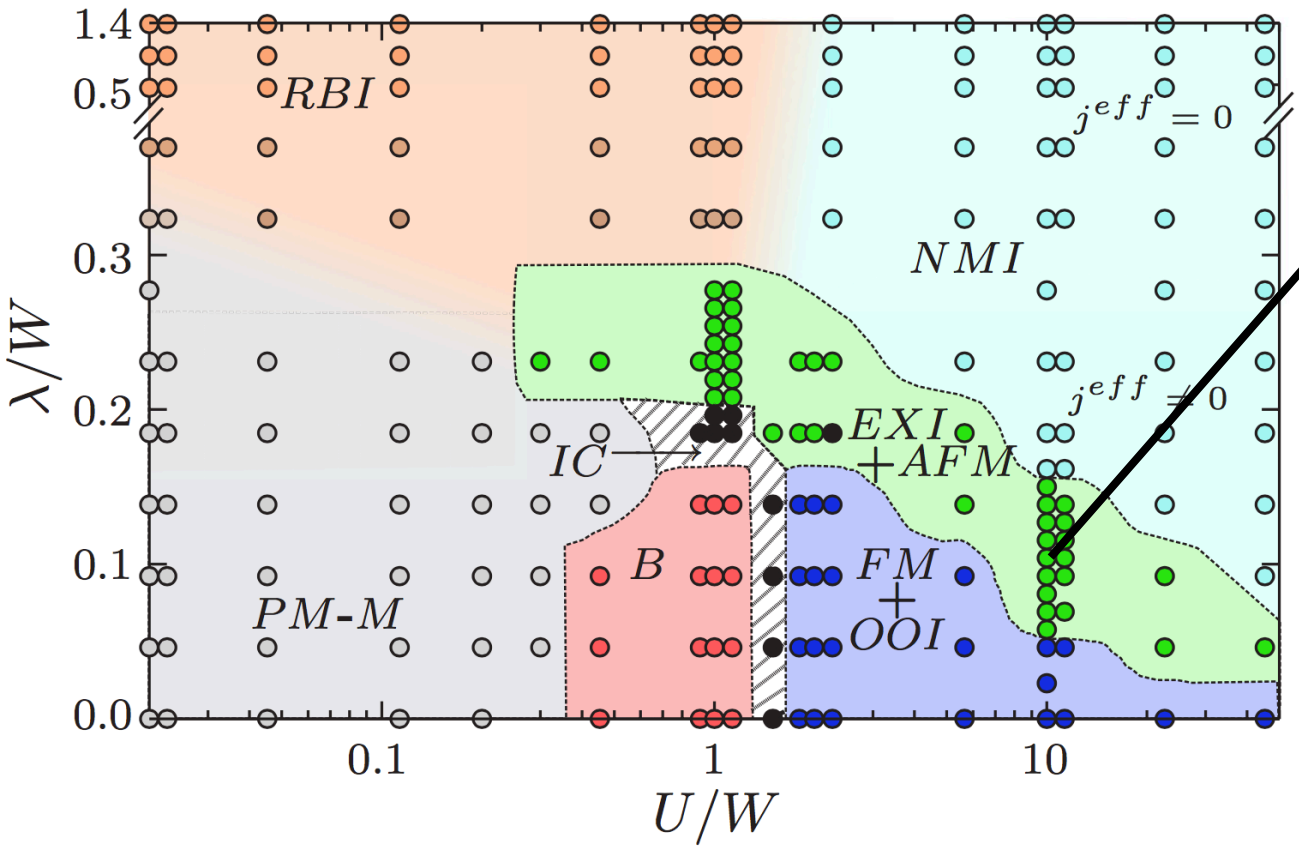
Both phases are well studied in literature on the same model:

J. Rincon et al., Phys. Rev. Lett. **112**, 106405 (2014)

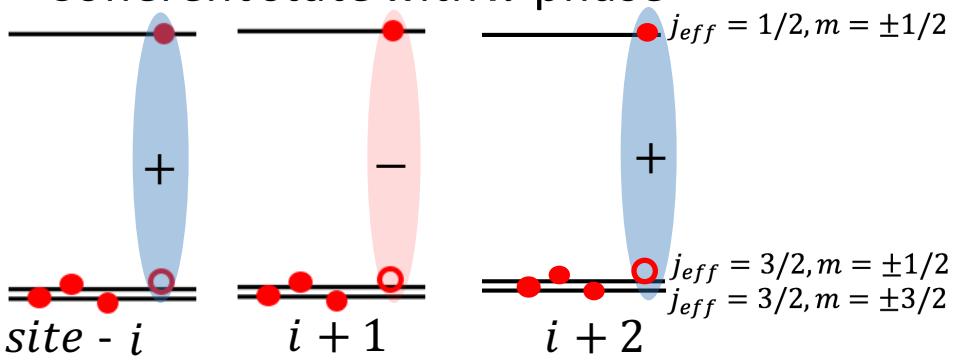
G. Liu et al., Phys. Rev. E **93**, 063313 (2016)

S. Li et al., Phys. Rev. B. **94**, 235126 (2016)

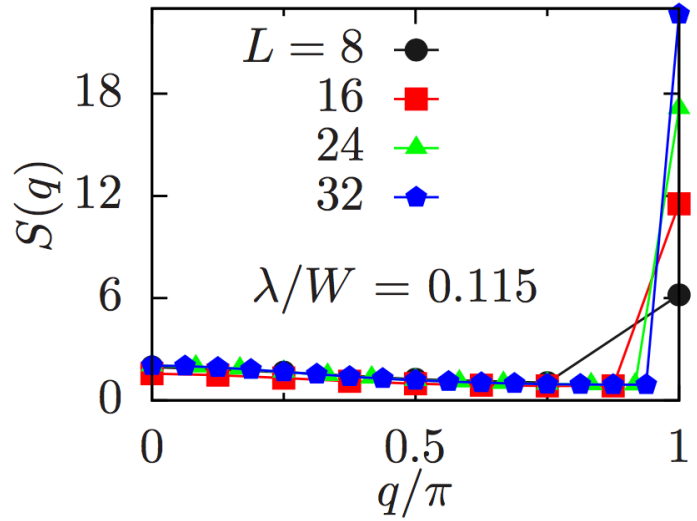
Phase Diagram [U vs λ] for n=4

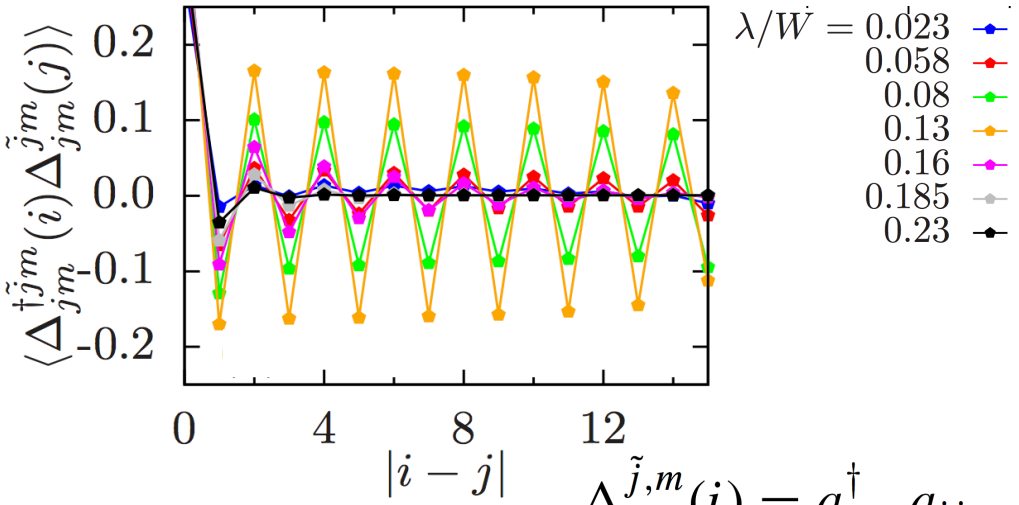


Coherent state with π phase



Antiferromagnetism + Excitons



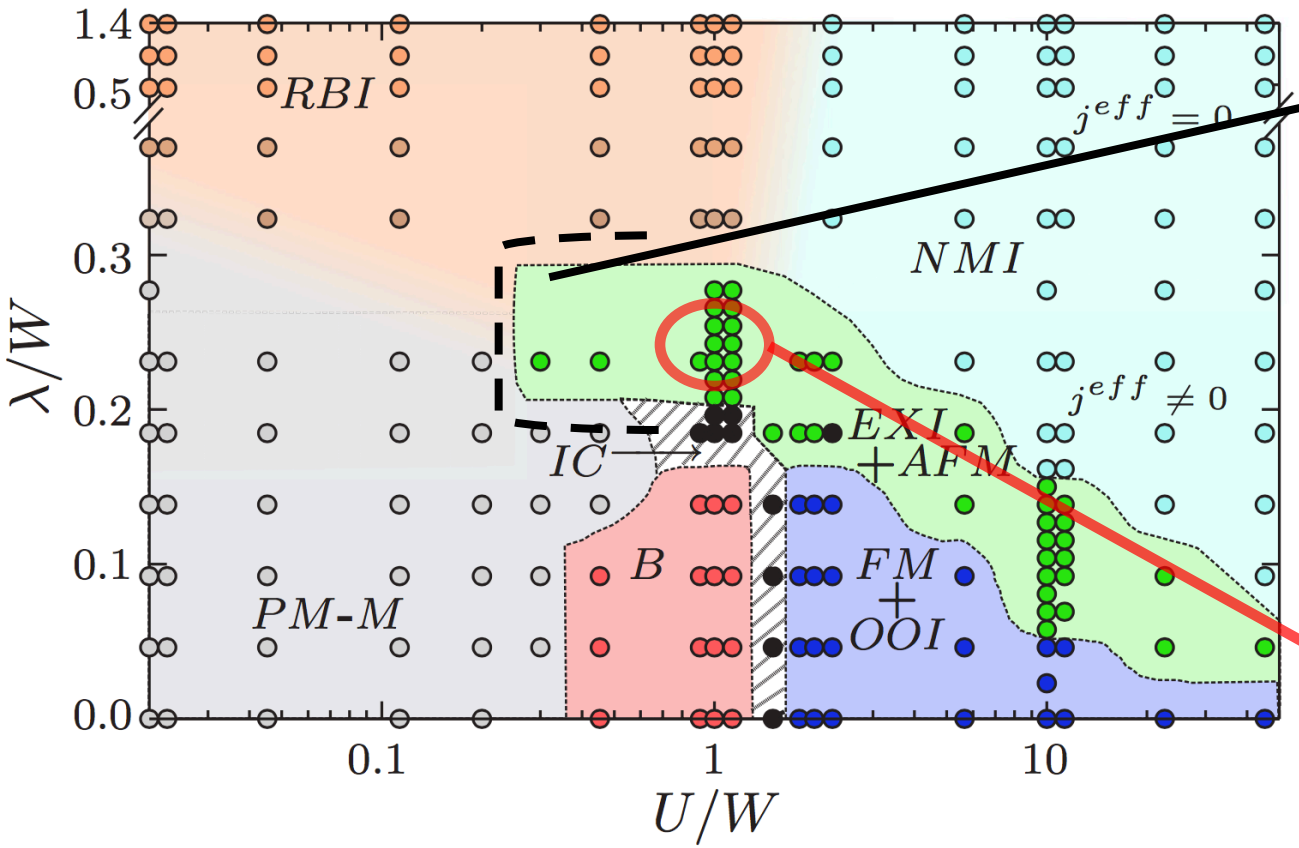


$$\Delta^{\tilde{j},m}_{j,m}(i)=a^{\dagger}_{i\,\tilde{j}m}a_{ijm}$$

$\tilde{j}=1/2, j=3/2$

$m=\pm 1/2$

Phase Diagram [U vs λ] for n=4



Antiferromagnetism + Excitons

- Present for U/W > 0.2
- Intermediate coupling is sufficient for Excitonic condensate.
- **"4d, 5d materials have small $U \sim W$"**

$\underline{Sr_2YIrO_4\ (d^4)}$

$$\frac{U}{W_{t_{2g}}} \sim 1.0, \frac{\lambda}{W_{t_{2g}}} \sim 0.23, W_{t_{2g}} \sim 2eV$$

S. Bhowal et al., Phys. Rev. B **92**, 121113(R)

Conclusion and importance of this work:

- First DMRG study on multiorbital Hubbard model with spin-orbit coupling.
- Full "$U\ vs\ \lambda$" phase diagram presented. We found excitonic magnetism in intermediate coupling region, within the physical region for 5d materials.

Future Directions:

- Although doping 4d/5d materials is difficult experimentally, in numerical studies we can predict phases that may emerge from doping with both U and SOC.

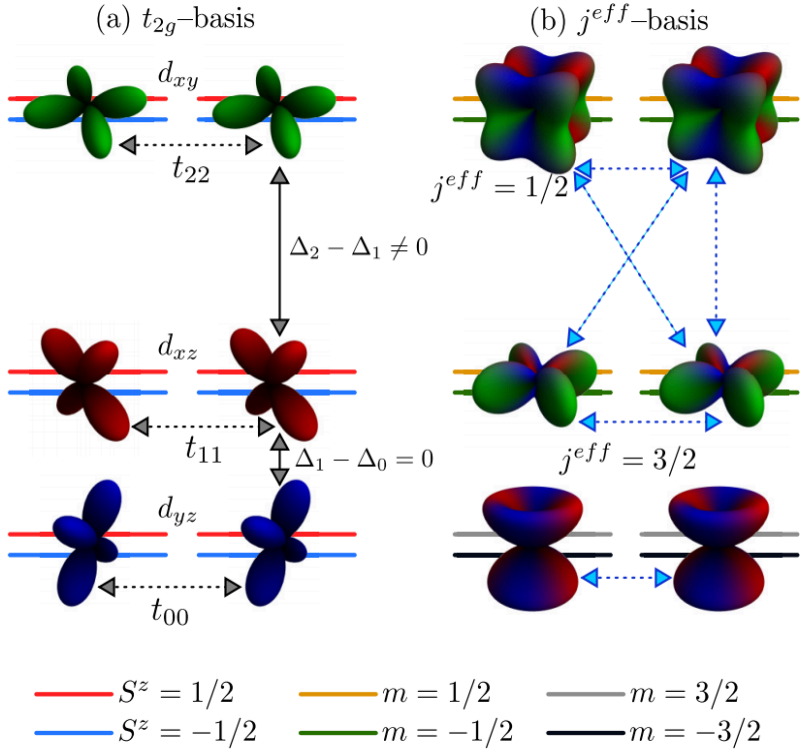
THANK YOU!!

EXTRA SLIDES:

CF + hopping in (j_{eff}, m) basis:

$$H = \sum_{\langle u' \rangle} \begin{bmatrix} a^\dagger_{l,\frac{3}{2},\frac{3}{2}} & a^\dagger_{l,\frac{3}{2},-\frac{1}{2}} & a^\dagger_{l,\frac{1}{2},-\frac{1}{2}} & a^\dagger_{l,\frac{3}{2},-\frac{3}{2}} & a^\dagger_{l,\frac{3}{2},\frac{1}{2}} & a^\dagger_{l,\frac{1}{2},\frac{1}{2}} \end{bmatrix} \begin{bmatrix} \frac{t_{00}+t_{11}}{2} & \frac{it_{00}-it_{11}+2t_{01}}{2\sqrt{3}} & \frac{-it_{00}+it_{11}-2t_{01}}{\sqrt{6}} & 0 & \frac{t_{12}+it_{02}}{\sqrt{3}} & \frac{t_{12}+it_{02}}{\sqrt{6}} \\ \frac{-it_{00}+it_{11}+2t_{01}}{2\sqrt{3}} & \frac{t_{00}+t_{11}+4t_{22}}{6} & \frac{-t_{00}-t_{11}+2t_{22}}{3\sqrt{2}} & \frac{t_{12}+it_{02}}{\sqrt{3}} & 0 & \frac{t_{02}+it_{12}}{\sqrt{2}} \\ \frac{it_{00}-it_{11}-2t_{01}}{\sqrt{6}} & \frac{-t_{00}-t_{11}+2t_{22}}{3\sqrt{2}} & \frac{t_{00}+t_{11}+t_{22}}{3} & \frac{t_{12}+it_{02}}{\sqrt{6}} & \frac{-t_{02}-it_{12}}{\sqrt{2}} & 0 \\ 0 & \frac{t_{12}-it_{02}}{\sqrt{3}} & \frac{t_{12}-it_{02}}{\sqrt{6}} & \frac{t_{00}+t_{11}}{2} & \frac{it_{00}-it_{11}-2t_{01}}{2\sqrt{3}} & \frac{-it_{00}+it_{11}+2t_{01}}{\sqrt{6}} \\ \frac{t_{12}-it_{02}}{\sqrt{3}} & 0 & \frac{-t_{02}-it_{12}}{\sqrt{2}} & \frac{-it_{00}+it_{11}-2t_{01}}{2\sqrt{3}} & \frac{t_{00}+t_{11}+4t_{22}}{6} & \frac{-t_{00}-t_{11}+2t_{22}}{3\sqrt{2}} \\ \frac{t_{12}-it_{02}}{\sqrt{6}} & \frac{t_{02}-it_{12}}{\sqrt{2}} & 0 & \frac{it_{00}-it_{11}+2t_{01}}{\sqrt{6}} & \frac{-t_{00}-t_{11}+2t_{22}}{3\sqrt{2}} & \frac{t_{00}+t_{11}+t_{22}}{3} \end{bmatrix} \begin{bmatrix} a_{l',\frac{3}{2},\frac{3}{2}} \\ a_{l',\frac{3}{2},-\frac{1}{2}} \\ a_{l',\frac{1}{2},-\frac{1}{2}} \\ a_{l',\frac{3}{2},-\frac{3}{2}} \\ a_{l',\frac{3}{2},\frac{1}{2}} \\ a_{l',\frac{1}{2},\frac{1}{2}} \end{bmatrix}$$

$$+ \sum_{l} \begin{bmatrix} a^\dagger_{l,\frac{3}{2},\frac{3}{2}} & a^\dagger_{l,\frac{3}{2},-\frac{1}{2}} & a^\dagger_{l,\frac{1}{2},-\frac{1}{2}} & a^\dagger_{l,\frac{3}{2},-\frac{3}{2}} & a^\dagger_{l,\frac{3}{2},\frac{1}{2}} & a^\dagger_{l,\frac{1}{2},\frac{1}{2}} \end{bmatrix} \begin{bmatrix} \frac{\Delta_0+\Delta_1}{2} & \frac{i\Delta_0-i\Delta_1}{2\sqrt{3}} & \frac{-i\Delta_0+i\Delta_1}{\sqrt{6}} & 0 & 0 & 0 \\ \frac{-i\Delta_0+i\Delta_1}{2\sqrt{3}} & \frac{\Delta_0+\Delta_1+4\Delta_2}{6} & \frac{-\Delta_0-\Delta_1+2\Delta_2}{3\sqrt{2}} & 0 & 0 & 0 \\ \frac{i\Delta_0-i\Delta_1}{\sqrt{6}} & \frac{-\Delta_0-\Delta_1+2\Delta_2}{3\sqrt{2}} & \frac{\Delta_0+\Delta_1+\Delta_2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\Delta_0+\Delta_1}{2} & \frac{i\Delta_0-i\Delta_1}{2\sqrt{3}} & \frac{-i\Delta_0+i\Delta_1}{\sqrt{6}} \\ 0 & 0 & 0 & \frac{-i\Delta_0+i\Delta_1}{2\sqrt{3}} & \frac{\Delta_0+\Delta_1+4\Delta_2}{6} & \frac{-\Delta_0-\Delta_1+2\Delta_2}{3\sqrt{2}} \\ 0 & 0 & 0 & \frac{i\Delta_0-i\Delta_1}{\sqrt{6}} & \frac{-\Delta_0-\Delta_1+2\Delta_2}{3\sqrt{2}} & \frac{\Delta_0+\Delta_1+\Delta_2}{3} \end{bmatrix} \begin{bmatrix} a_{l,\frac{3}{2},\frac{3}{2}} \\ a_{l,\frac{3}{2},-\frac{1}{2}} \\ a_{l,\frac{1}{2},-\frac{1}{2}} \\ a_{l,\frac{3}{2},-\frac{3}{2}} \\ a_{l,\frac{3}{2},\frac{1}{2}} \\ a_{l,\frac{1}{2},\frac{1}{2}} \end{bmatrix}.$$



To have $[H_K, J_z^{\text{eff}}] = 0$

$$J_z^{\text{eff}} = \sum_{ijm} (m) n_{i,j,m}.$$

(i) $t_{\gamma\gamma'} = 0 \; \forall \; \gamma \neq \gamma'$, i.e., no interorbital hopping;

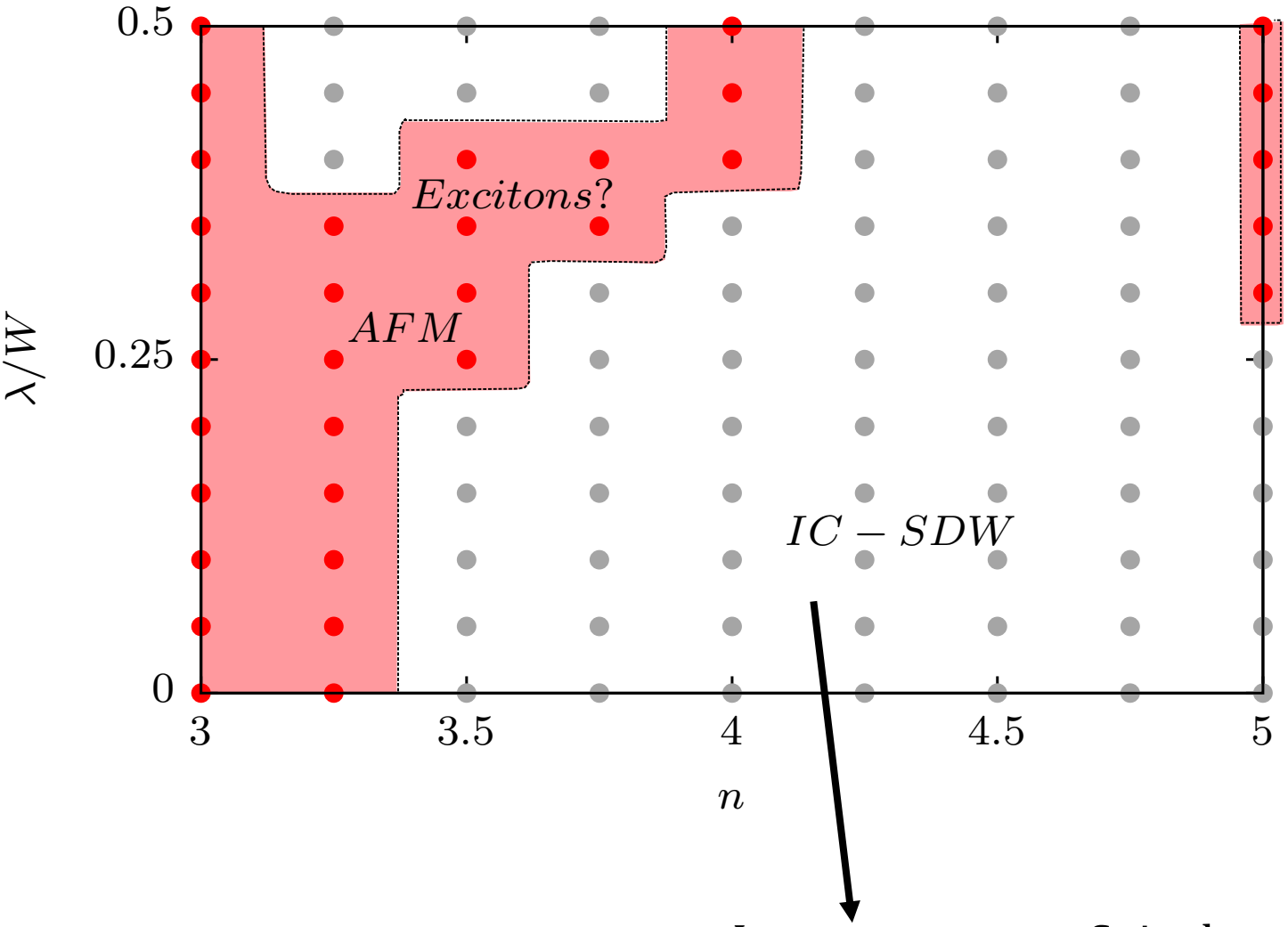
(ii) $t_{00} = t_{11}$, namely the hopping amplitudes of the d_{xz} and d_{yz} orbitals must be equal;

(iii) $\Delta_0 = \Delta_1$, namely the crystal-field splittings for the d_{xz} and d_{yz} orbitals must be equal.

Current Work

Effect of different filling (n)?

Phase Diagram [n vs λ] for U/W=1.0



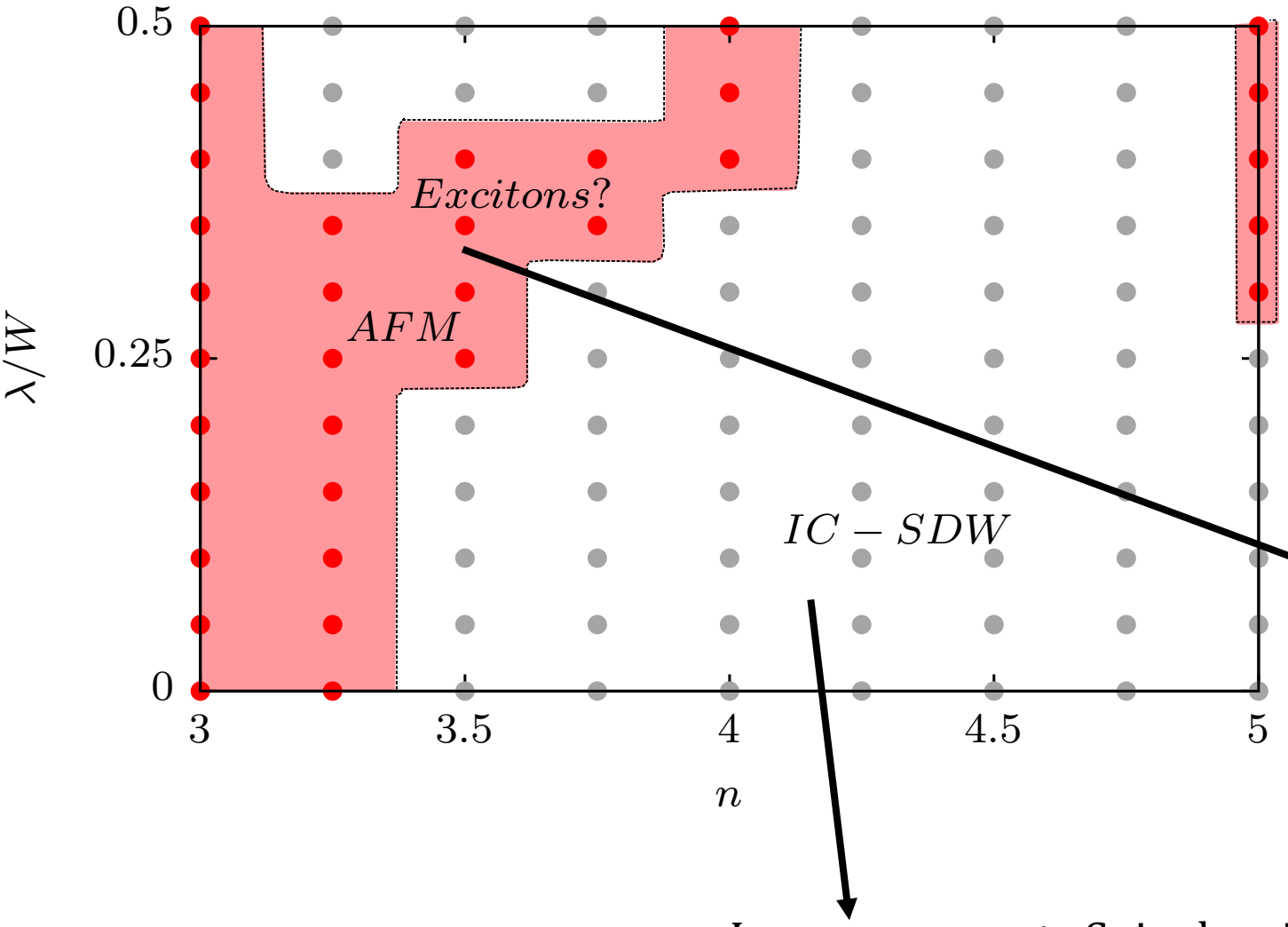
Model:

- Degenerate t_{2g} bands are used.
- Relevant for materials with nearly octahedral crystal field splitting.

Incommensurate Spin density wave coming from nesting in bands.

N. Kaushal et al. Unpublished (Under Progress)

Phase Diagram [n vs λ] for U/W=1.0



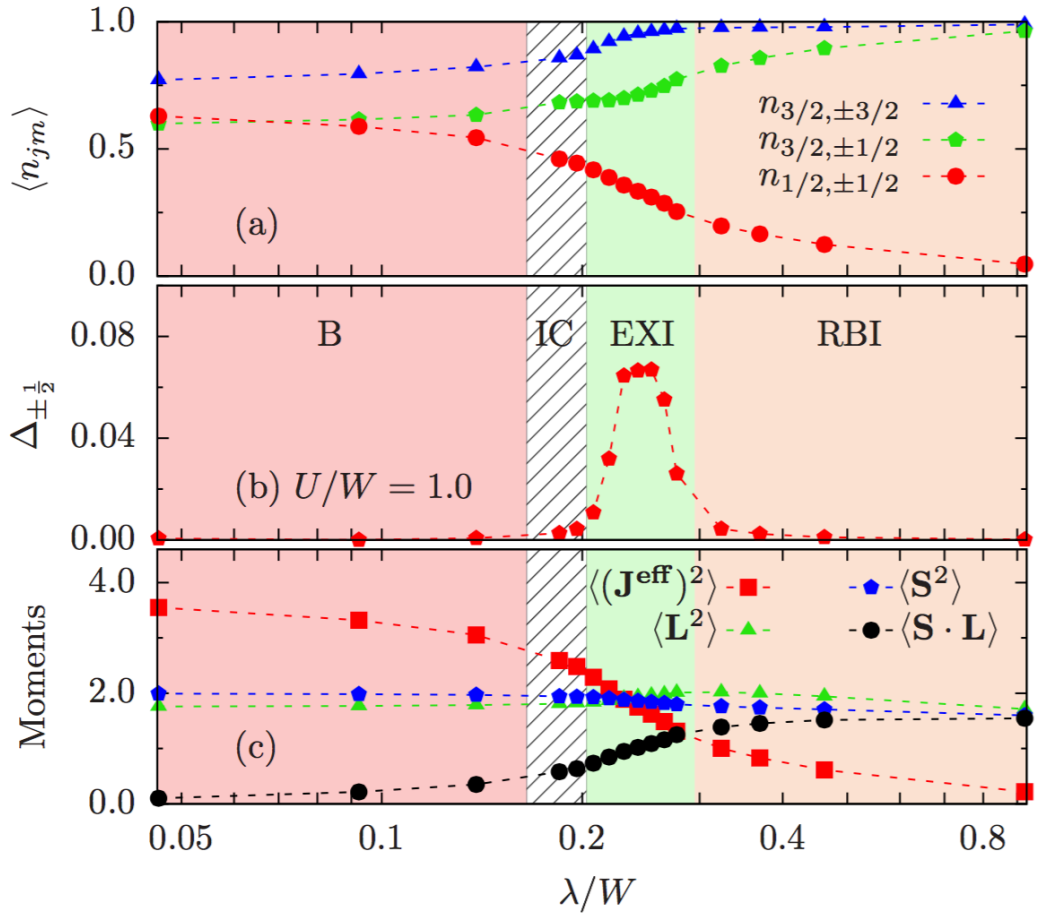
Model:

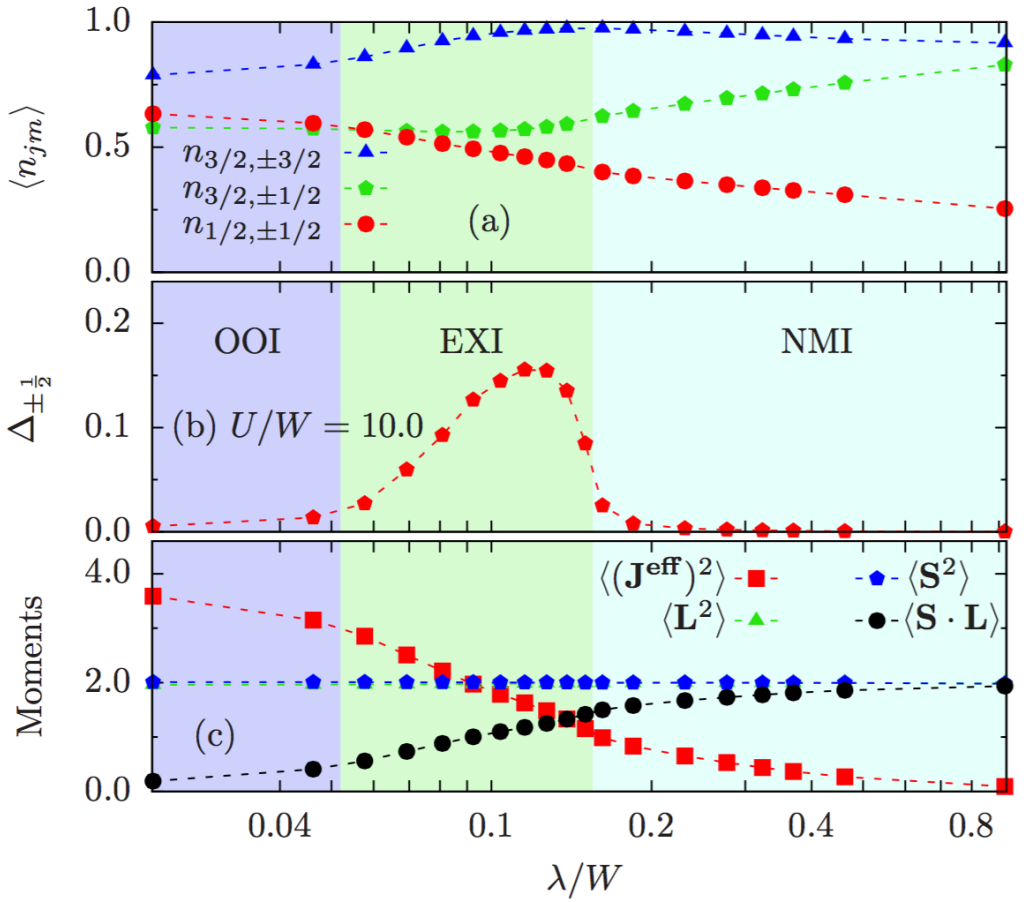
- Degenerate t_{2g} bands are used.
- Relevant for materials with nearly octahedral crystal field splitting.

Antiferromagnetic ordering is found for $n < 4$ as well. Promising region to look for Excitonic condensate?

Incommensurate Spin density wave coming from nesting in bands.

N. Kaushal et al. Unpublished (Under Progress)



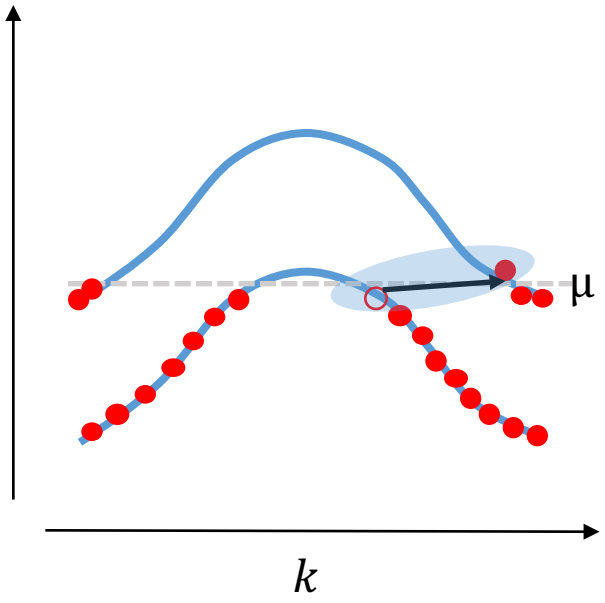


DMRG results obtained at $U/W = 1$ (intermediate coupling) and using a $L = 16$ system. (a) shows occupation number in the (j^{eff},m) bands while (b) shows the excitonic parameter Δ_m defined in Eq. (8) varying λ/W. (c) shows the three local moment strengths as well as $\langle \mathbf{S}.\mathbf{L} \rangle$.

$$\Delta_m = \frac{1}{L^2} \sum_{|i-i'|>0} (-1)^{|i-i'|} \left\langle \Delta^{\dagger \tilde{j}m}_{jm}(i) \Delta^{\tilde{j}m}_{jm}(i') \right\rangle.$$

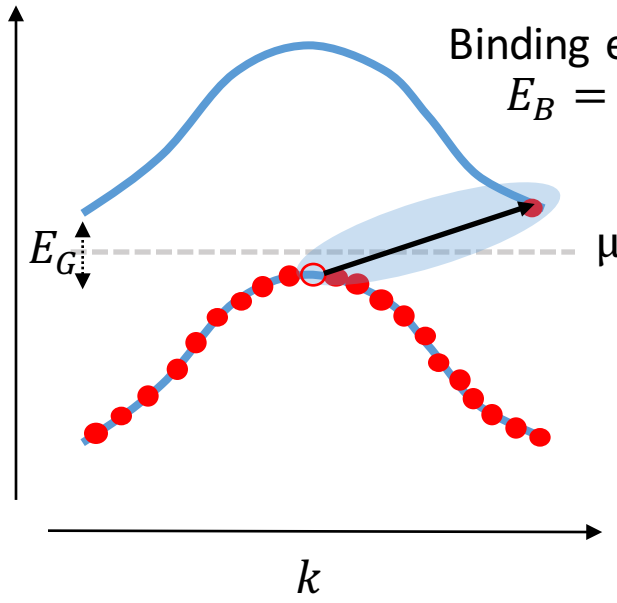
Excitons at Metal –Insulator transition [In Intermediate coupling limit]:

Semi-metal



Small no of carriers
→ Unscreened coloumb replusion
→electron-hole pairs

Semiconductor

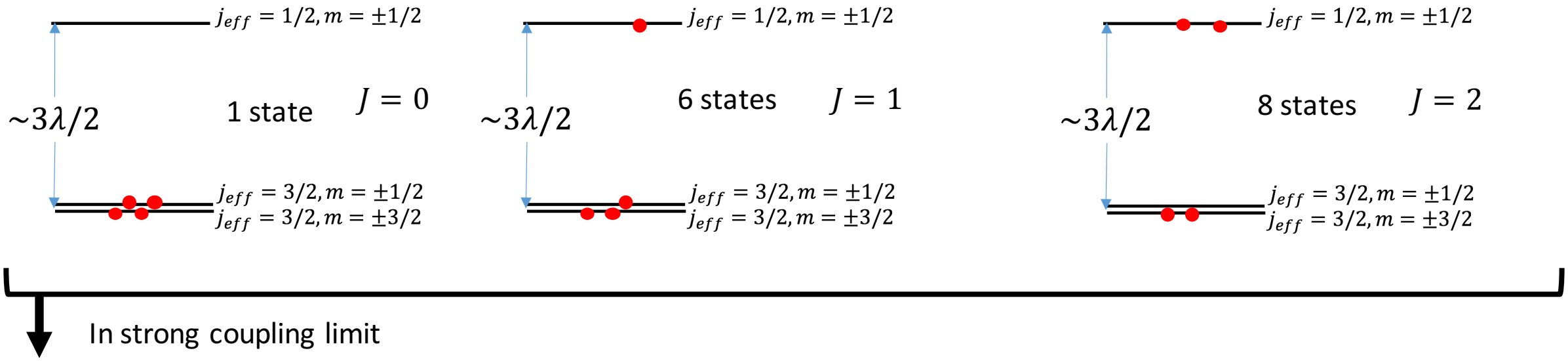


Energy to create Exciton = $E_G - E_B$

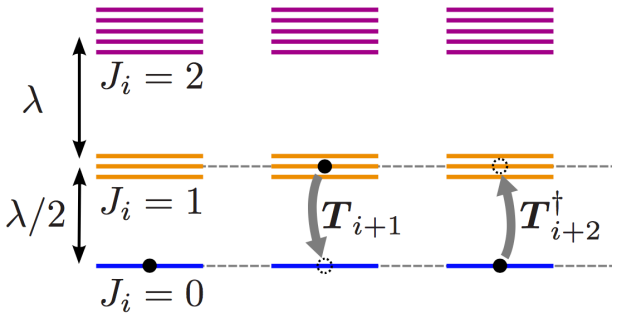
If $E_G < E_B$ → Spontaneous formation of Excitons

B. Halperin and T. M. Rice, REVIEWS OF MODERN PHYSICS, VOLUME 40, No. 4, 1968

Excitons as Singlet-Triplet Excitations [In Strong coupling limit]:



In strong coupling limit



$$\sim J_{exc}(\boldsymbol{T}_i^{\dagger} \cdot \boldsymbol{T}_j + \text{H.c.})$$

Giniyat Khaliullin, PRL 111, 197201 (2013)

Christopher Svoboda et al., PHYSICAL REVIEW B **95**, 014409 (2017)

L^2_{eff} *in* t_{2g} *and* e_g *sectors*:

In t_{2g}:

In unquenched t_{2g} orbitals, **L** becomes following,

$$L_z = \begin{bmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, L_+ = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & i \\ -1 & -i & 0 \end{bmatrix}, L_- = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & i \\ 1 & -i & 0 \end{bmatrix} \quad \text{and} \quad L^2 = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

in the basis $|yz\rangle, |xz\rangle$, and $|xy\rangle$ (same sequence is followed while writing above matrices), where

$$|yz\rangle = \frac{i}{\sqrt{2}}(|1\rangle + |-1\rangle), |xz\rangle = \frac{1}{\sqrt{2}}(-|1\rangle + |-1\rangle), |xy\rangle = \frac{-i}{\sqrt{2}}(-|-2\rangle + |2\rangle)$$

- $|1\rangle_{eff} = -i|-1\rangle$
- $|-1\rangle_{eff} = i|1\rangle$
- $|0\rangle_{eff} = |xy\rangle$
- $\mathbf{L}^{l=1} \equiv -\mathbf{L}^{t_{2g}}$

SOC term:

The transformation between the t_{2g} orbitals and the j^{eff} basis is given by (dropping site i index)

$$\begin{bmatrix} a_{\frac{3}{2},\frac{3s}{2}} \\ a_{\frac{3}{2},-\frac{s}{2}} \\ a_{\frac{1}{2},-\frac{s}{2}} \end{bmatrix} = \begin{bmatrix} \frac{is}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{s}{\sqrt{6}} & \frac{i}{\sqrt{6}} & \frac{2}{\sqrt{6}} \\ \frac{-s}{\sqrt{3}} & \frac{-i}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{bmatrix} \begin{bmatrix} c_{\sigma yz} \\ c_{\sigma xz} \\ c_{\bar{\sigma} xy} \end{bmatrix},$$

where s is $1(-1)$ when σ is $\uparrow$ $(\downarrow)$ and $\bar{\sigma} = -\sigma$. The H_{SOC} term in the j^{eff} basis becomes

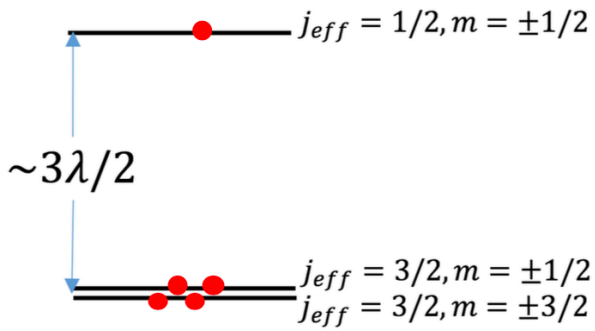
$$\begin{aligned} H_{\text{SOC}} = \sum_i \frac{\lambda}{2} \big(& - a^\dagger_{i,\frac{3}{2},\frac{3}{2}} a_{i,\frac{3}{2},\frac{3}{2}} - a^\dagger_{i,\frac{3}{2},-\frac{1}{2}} a_{i,\frac{3}{2},-\frac{1}{2}} \\ & - a^\dagger_{i,\frac{3}{2},-\frac{3}{2}} a_{i,\frac{3}{2},-\frac{3}{2}} - a^\dagger_{i,\frac{3}{2},\frac{1}{2}} a_{i,\frac{3}{2},\frac{1}{2}} \\ & + 2a^\dagger_{i,\frac{1}{2},\frac{1}{2}} a_{i,\frac{1}{2},\frac{1}{2}} + 2a^\dagger_{i,\frac{1}{2},-\frac{1}{2}} a_{i,\frac{1}{2},-\frac{1}{2}} \big). \end{aligned}$$

$$H_{\text{SO}} = \lambda \sum_{\gamma,\delta,\sigma,\sigma'} A^{\gamma,\delta}_{\sigma,\sigma'} c^\dagger_{\gamma\sigma} c_{\delta,\sigma'}$$

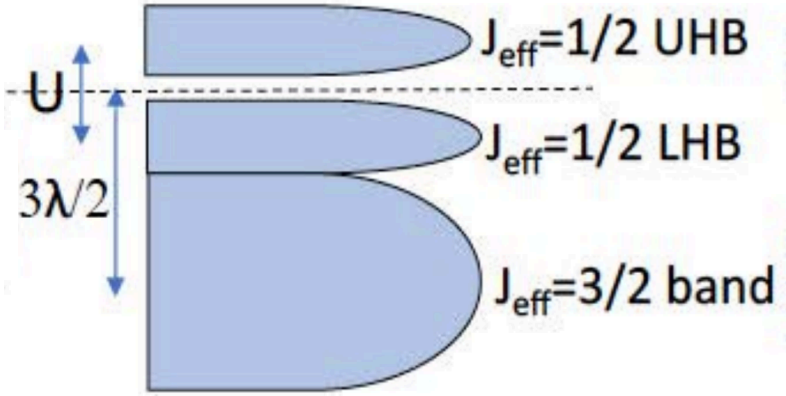
Where, $A^{\gamma,\delta}_{\sigma,\sigma'} = < \gamma | \mathbf{L} | \delta > . < \sigma | \mathbf{S} | \sigma' >$

Introduction and Motivation

Case: d^5

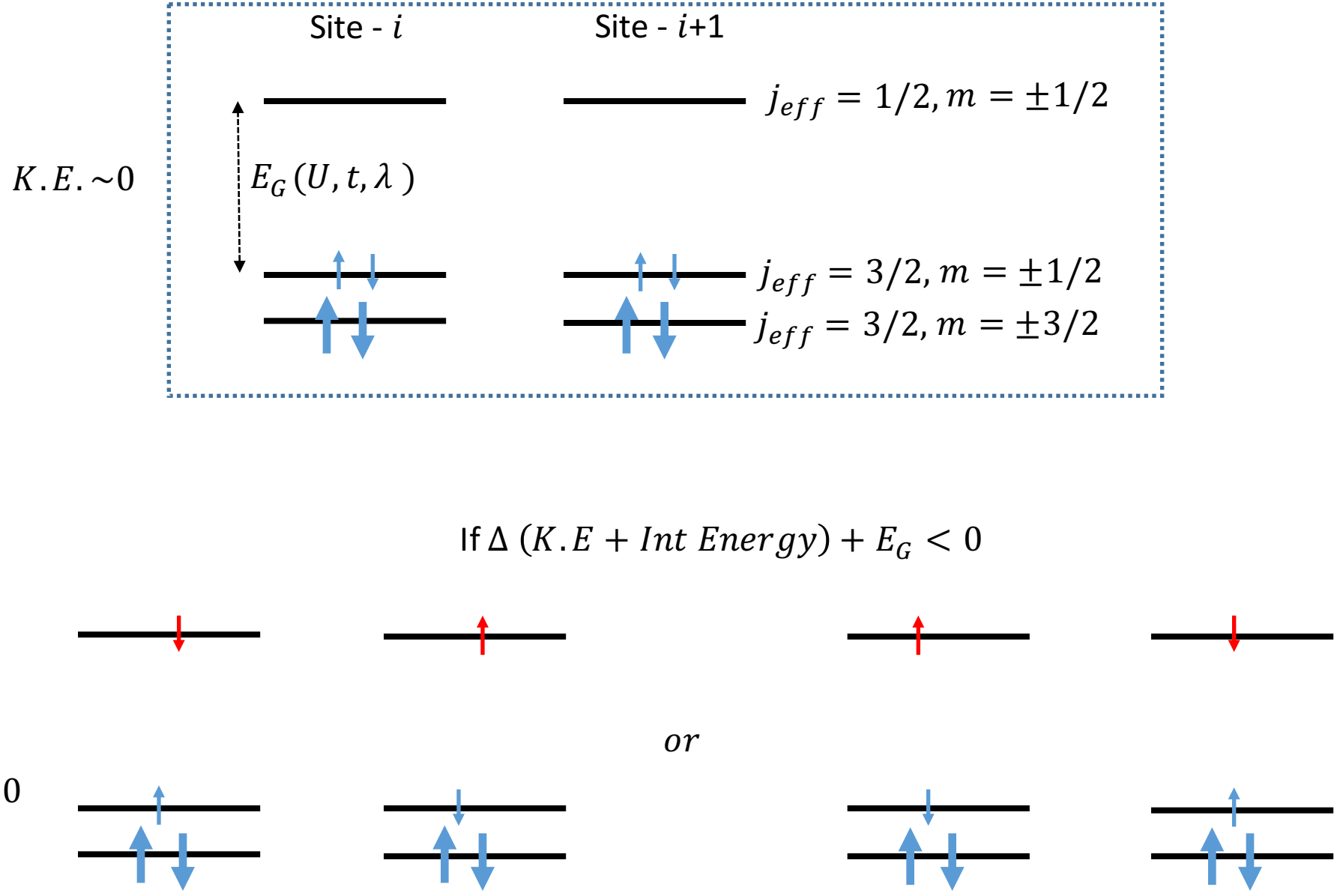


Half-filled;
In presence of e-e correlations and hopping, a Mott insulator is stabilized [opens a gap in $j_{eff} = 1/2$ band]



Explain why materials like $Sr_2IrO_4[d^{5]*}$, $Ba_2IrO_4[d^5]$ shows Mott insulating behavior.

*B J Kim et al., Phys. Rev. Lett. **101**, 076402 (2008)


Site - i
Site - i+1
$j_{eff} = 1/2, m = \pm 1/2$
$K.E. \sim 0$
$E_G(U, t, \lambda)$
$j_{eff} = 3/2, m = \pm 1/2$
$j_{eff} = 3/2, m = \pm 3/2$
If $\Delta\ (K.E + Int\ Energy) + E_G < 0$
$Cost \sim E_G$
$K.E < 0$
$\Delta(Int.Energy) < 0$
or