多自由度相関系の動的構造物性

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TOHOKU UNIVERSITY

Orbital excitation “Orbiton”

revisited

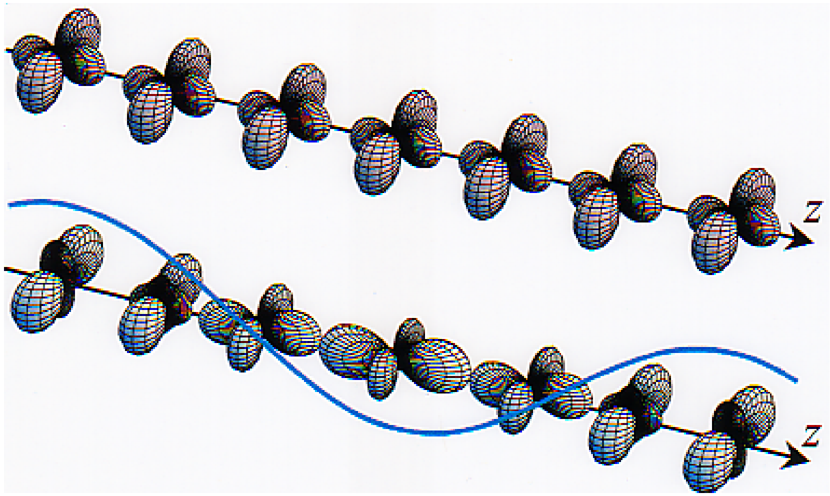
Orbiton

Orbital wave (orbiton)

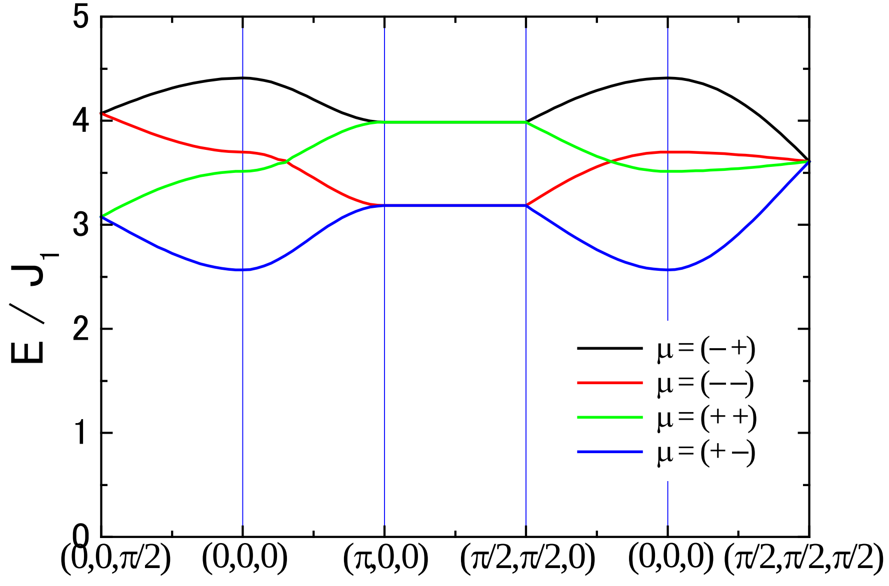
Collective excitation in orbital ordered state

3d transition-metal compounds

Quadrupole order in 4f electron systems



LaMnO$_3$



M. Cyrot and C. Lyon-Caen, J. Phys. (Paris) 36, 253 (1975)

S. Ishihara, J. Inoue, S. Maekawa Phys. Rev. B 55, 8280 ('97).

tal + Dynamical

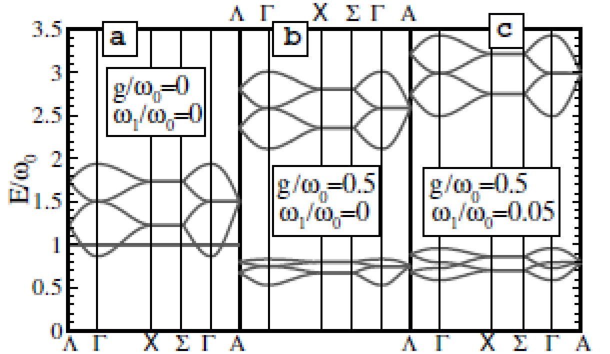


FIG. 2. Orbiton and phonon dispersion, neglecting dynamical effects due to the *e*-*p* coupling; (a) without *e*-*p* coupling *g* and without bare phonon dispersion, (b) $g/\omega_0 = 1/2$, no bare phonon dispersion, and (c) $g/\omega_0 = 1/2$, finite bare phonon dispersion. The points of high symmetry in the Brillouin zone correspond to those of Ref. [13].

Effects of

JT coupling

mics (Dynamical JT,

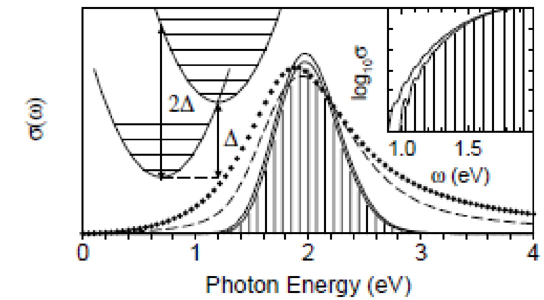
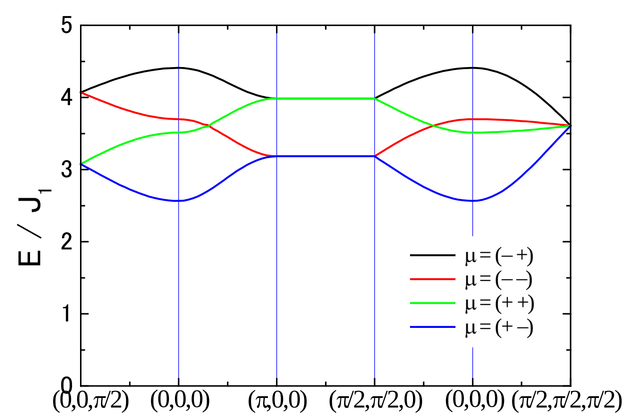


FIG. 2. Optical conductivity of $LaMnO_3$. The points are the lowest Lorentzian oscillator fit by Jung *et al.* [16] to their data. The dashed curve is a $T = 0$ sum of convolved Lorentzians centered at the vibrational replicas shown as vertical bars; the solid curves are $T = 0$ (lower) and $T = 300$ K (upper) sums of convolved Gaussians, also shown in the inset on a logarithmic scale. Tick marks in the inset denote decades.

Vibronic excitation (cooperative JT problem)

SI et al. Phys. Rev. B 62, 2338 ('00)
Frozen JT distortion



V. Pere … 118 (01)
Orbital e … ange int.)

Fu … ics

Orbital – Lattice coupling

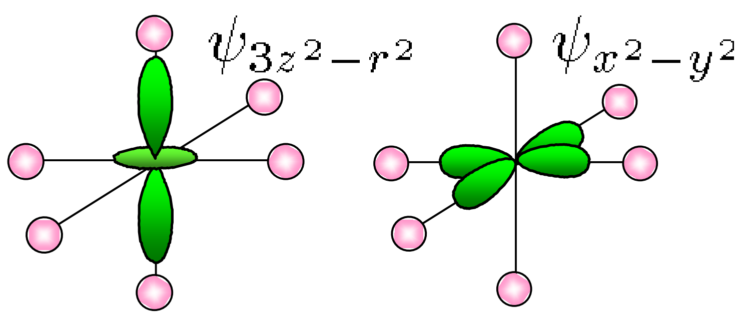
$$
\begin{aligned}
H_J &= -2J_1 \sum_{\langle ij \rangle} \left(\frac{3}{4} + \vec{S}_i \cdot \vec{S}_j \right) \left(\frac{1}{4} - \tau_i^l \tau_j^l \right) \\
&\quad -2J_2 \sum_{\langle ij \rangle} \left(\frac{1}{4} - \vec{S}_i \cdot \vec{S}_j \right) \left(\frac{3}{4} + \tau_i^l \tau_j^l + \tau_i^l + \tau_j^l \right)
\end{aligned}
$$

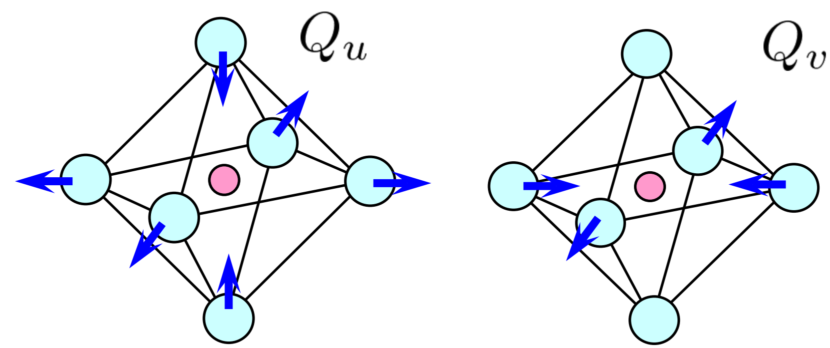
Exchange interaction

$$\vec{S}_i \cdot \vec{S}_j \rightarrow \langle \vec{S}_i \cdot \vec{S}_j \rangle$$

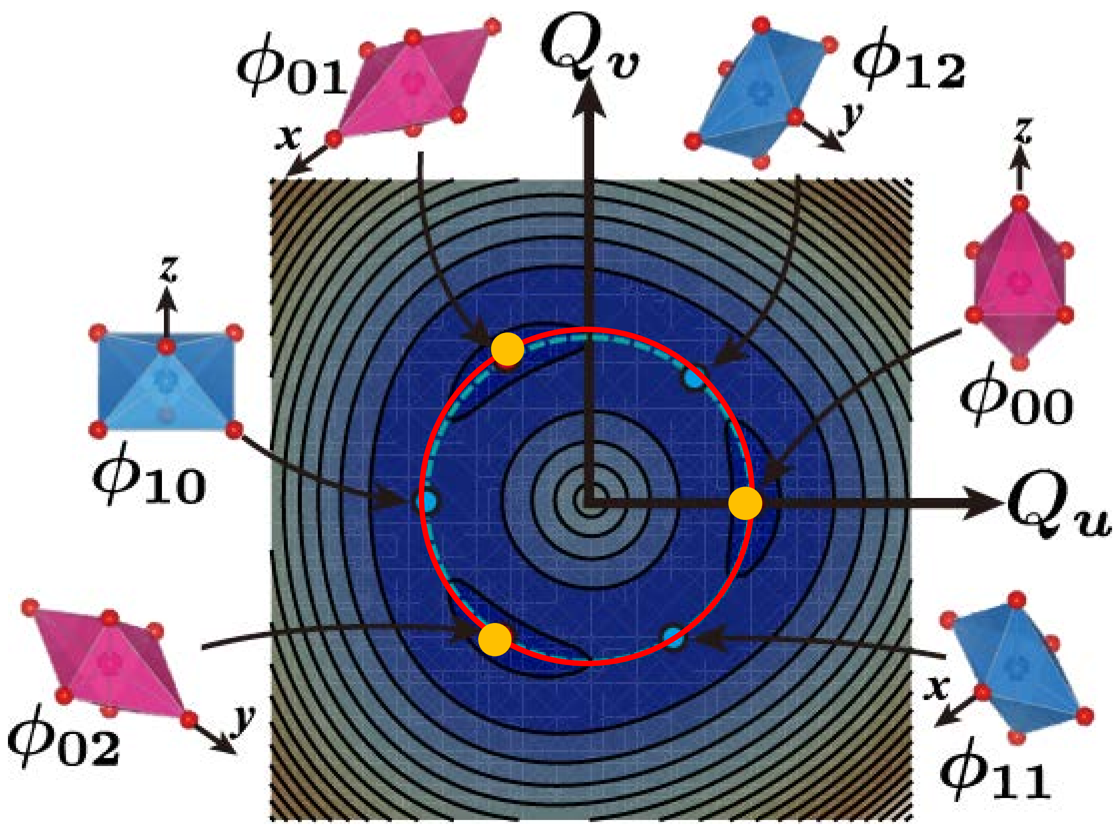
$$H_{\mathrm{JT}} = -\frac{\hbar^2}{2M} \left(\frac{\partial^2}{\partial Q_u^2} + \frac{\partial^2}{\partial Q_v^2} \right) + \frac{M\omega^2}{2} (Q_u^2 + Q_v^2) + A(\sigma^x Q_v - \sigma^z Q_u)$$

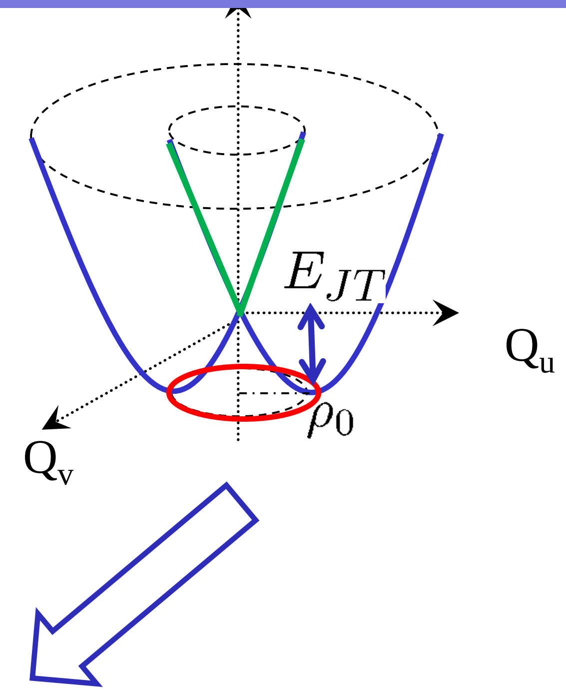
Kinetic | Lattice potential | JT interaction



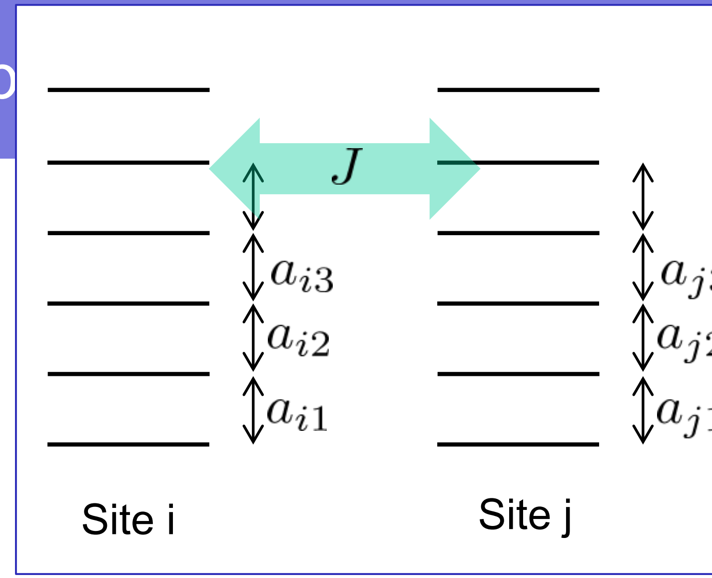


Dynamical Jahn-Teller effect





Generalized spin wave app



1) MF approximation for the exchange term

$$T_i^z = \langle T^z \rangle + \delta T_i^z$$

$$\mathcal{H} = -\sum_{\langle ij \rangle} (J_z \delta T_i^z \delta T_j^z + J_x T_i^x T_j^x) + \sum_i \mathcal{H}_i^{\mathrm{MF}}.$$

2) Diagonalization for on-site Hamiltonian

Local eigen state : $\{|\Phi_n\rangle\}$

Local eigen energy : $\{E_n\}$

up to $\mathcal{N}(\geq n)$

3) Boson operator for Local excitations

$$T_i^x = \sum_{m,n=0}^{\mathcal{N}} (T^x)_{mn} X_i^{mn}, \quad \delta T_i^z = \sum_{m,n=0}^{\mathcal{N}} (\delta T^z)_{mn} X_i^{mn},$$

$$X_i^{mn} = a_{in}^\dagger a_{im}, \qquad X_i^{n0} = a_{in}^\dagger \left(M - \sum_{m=1}^{\mathcal{N}} a_{im}^\dagger a_{im} \right)^{1/2}$$

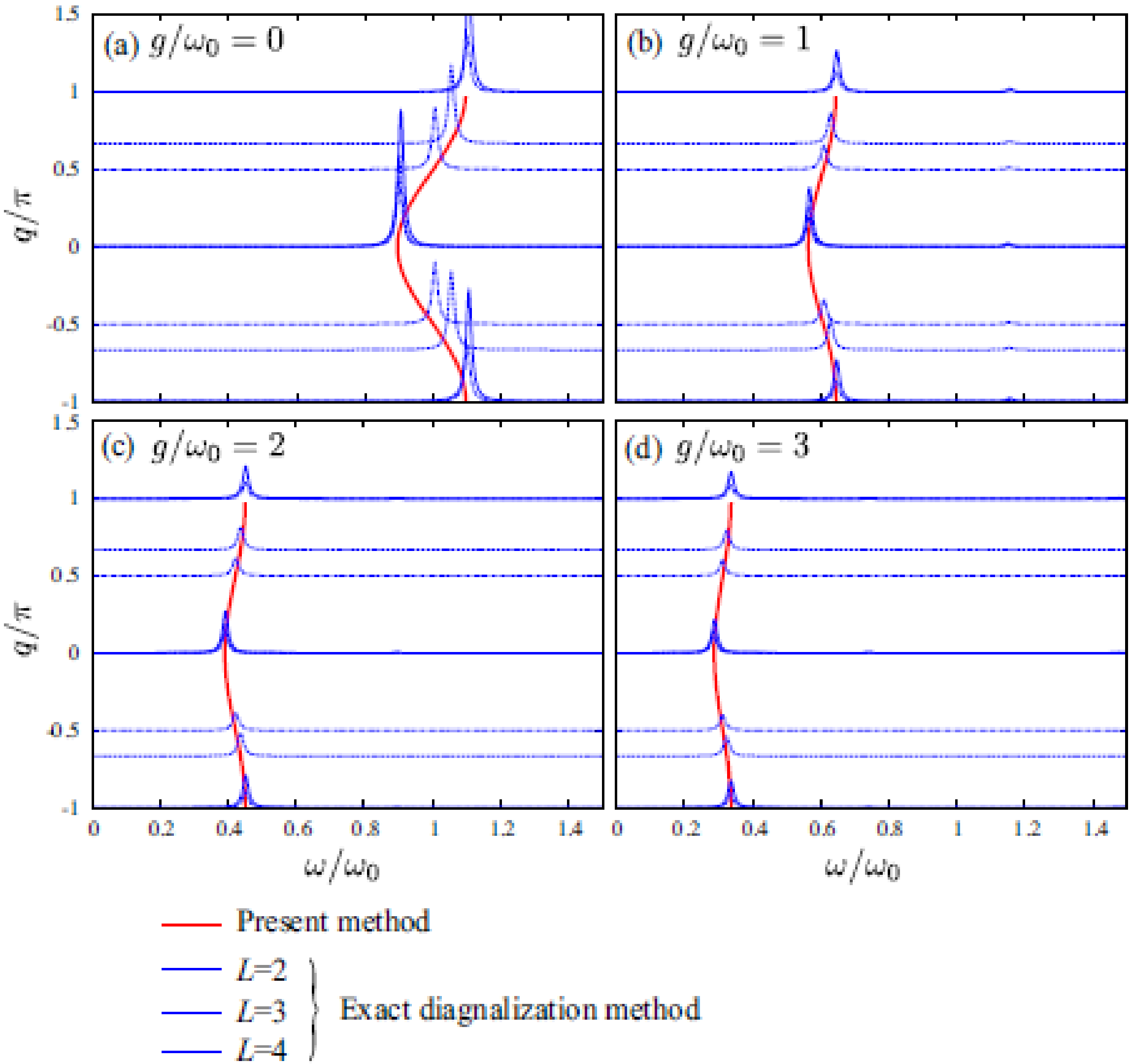
N. Papanicolaou,
Nucl. Phys. B 305, 367 (1988)
R. Shiina, H. Shiba, et al.
JPSJ. 72, 1216 (2003)
H. Kusunose and Y. Kuramoto
JPSJ 70, 3076 (2001)

4) Inter-site interaction written by boson

$$\mathcal{H} = \sum_{\boldsymbol{q}} \sum_{m,n}^{(\mathrm{even})} \left[(\Delta E_n \delta_{mn} - z\gamma_{\boldsymbol{q}} J_z v_m^z v_n^z) a_{\boldsymbol{q}m}^\dagger a_{\boldsymbol{q}n} - \frac{z\gamma_{\boldsymbol{q}} J_z}{2} v_m^z v_n^z (a_{\boldsymbol{q}m}^\dagger a_{-\boldsymbol{q}n}^\dagger + h.c) \right]$$

$$- \frac{z\gamma_{\boldsymbol{q}} J_z}{2} v_m^z v_n^z (a_{\boldsymbol{q}m}^\dagger a_{-\boldsymbol{q}n}^\dagger + h.c)] \qquad + \sum_{\boldsymbol{q}} \sum_{m,n}^{(\mathrm{odd})} [(\Delta E_n \delta_{mn} - z\gamma_{\boldsymbol{q}} J_x v_m^x v_n^x) a_{\boldsymbol{q}}^\dagger$$

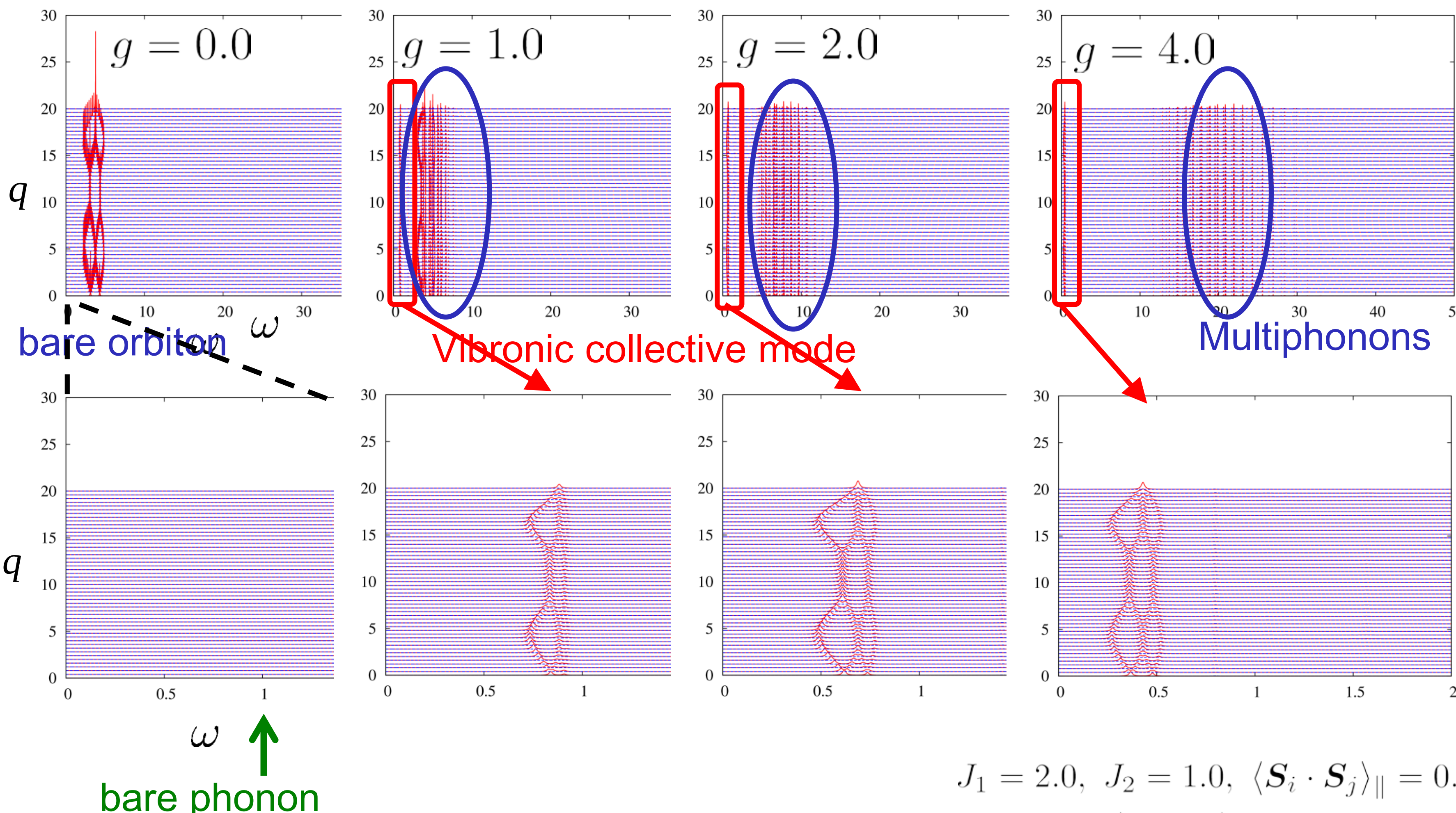
Comparison with exact diagonalization



Valid from weak to strong JT coupling regimes

Orbital spectra

$$\tilde{\chi}^{ll'}_{\Lambda\Lambda'}(\omega) = i\int_0^\infty \langle \delta\tilde{T}^l_{-\boldsymbol{q}\Lambda}(t)\delta\tilde{T}^{l'}_{\boldsymbol{q}\Lambda'}\rangle e^{i\omega t-\eta t}$$



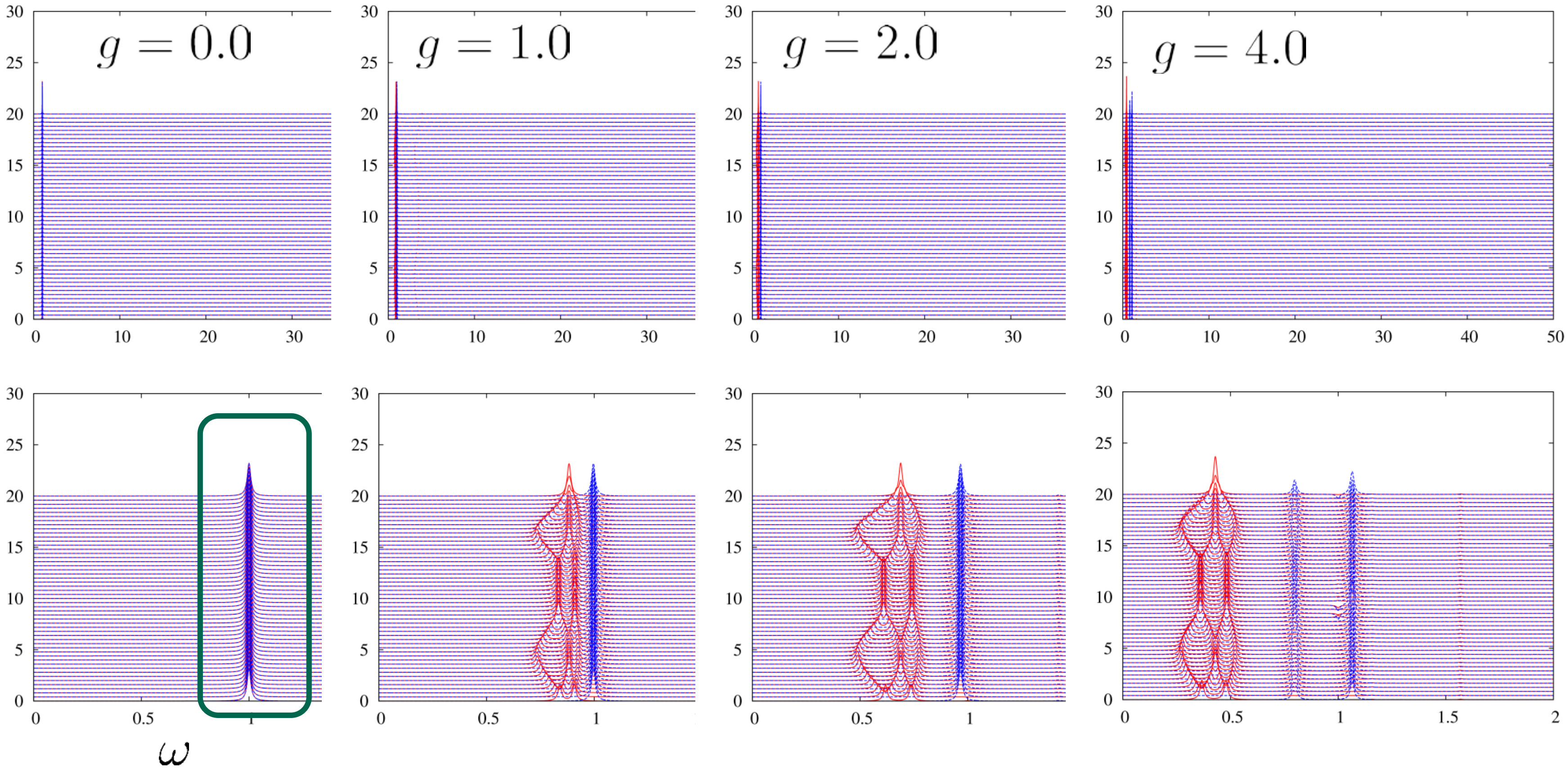
$J_1 = 2.0,\ J_2 = 1.0,\ \langle \boldsymbol{S}_i\cdot\boldsymbol{S}_j\rangle_{\parallel} = 0.0,$
$\langle \boldsymbol{S}_i\cdot\boldsymbol{S}_j\rangle_z = -0.2,\ \omega_0 = 1$

Phonon spectra

$$\tilde{D}^{ll'}_{\Lambda\Lambda'}(\omega) = i\int_0^\infty \langle \tilde{b}^l_{\boldsymbol{q}\Lambda}(t)\tilde{b}^{\dagger l'}_{\boldsymbol{q}\Lambda'}\rangle e^{i\omega t-\eta t}$$

$-\frac{1}{\pi}\mathrm{Im}\tilde{D}^{vv}_{AA}(\omega)$

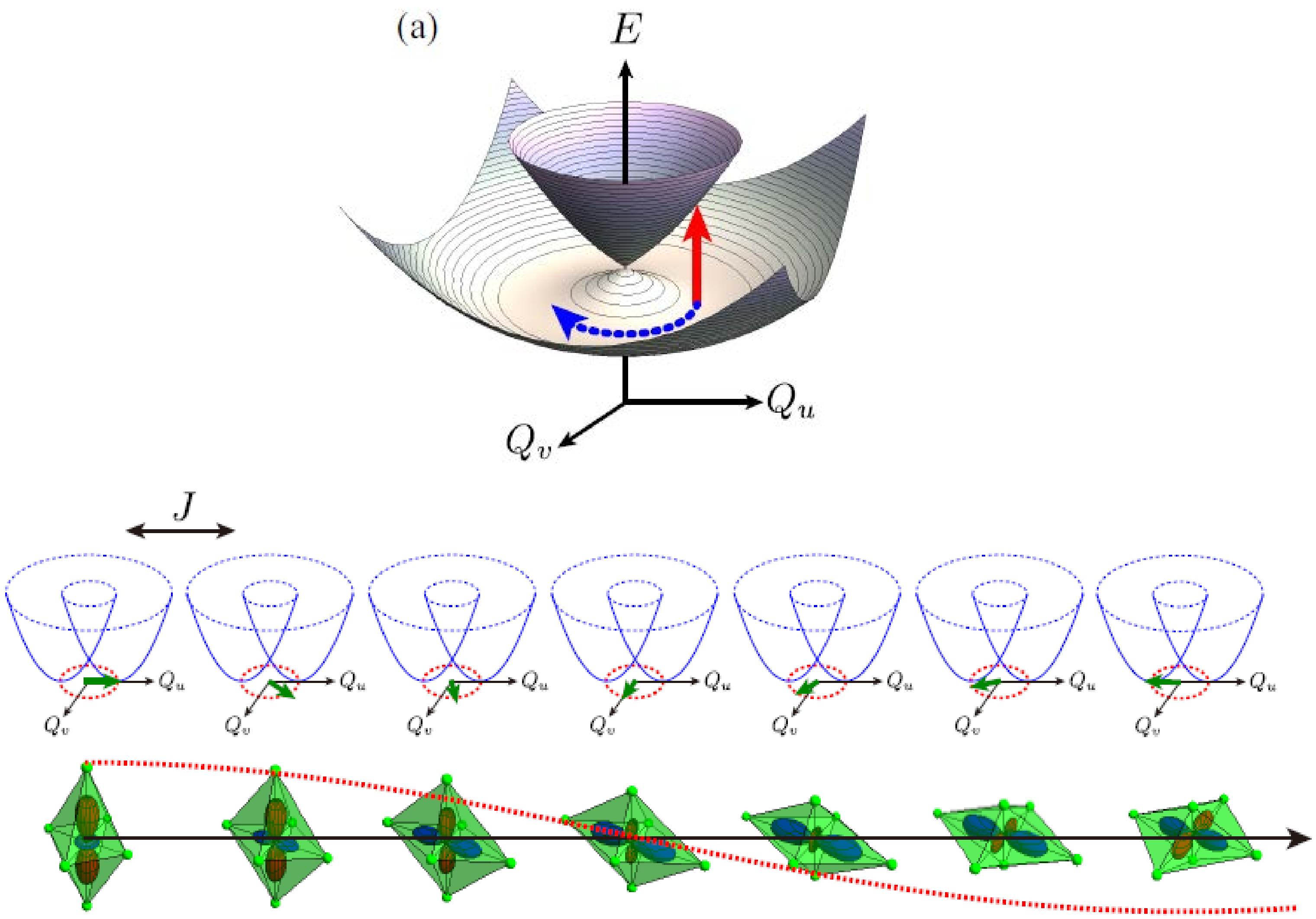
$-\frac{1}{\pi}\mathrm{Im}\tilde{D}^{uu}_{AA}(\omega)$



bare phonon

Vibronic collective mode

Vibronic collective mode



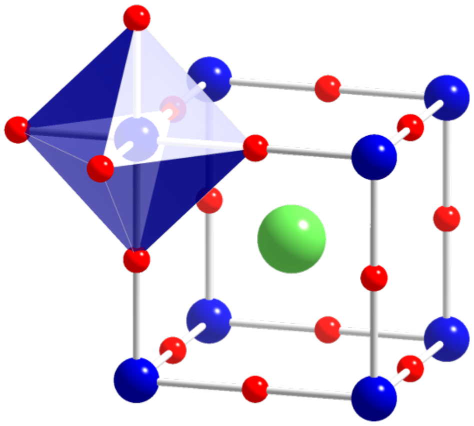
J. Nasu & SI, Phys. Rev. B 88, 205110 (2013) (Editor's suggestion paper)

Excitonic Insulator
and
Collective mode

Perovskite cobaltites

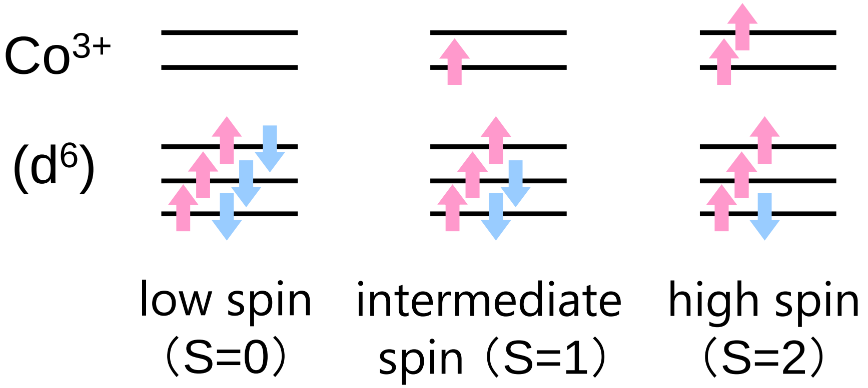
$R_{1-x}A_xCoO_3$ (R:La A: Ca, Sr, Ba)

as another target



perovskite

Spin state degree of freedom



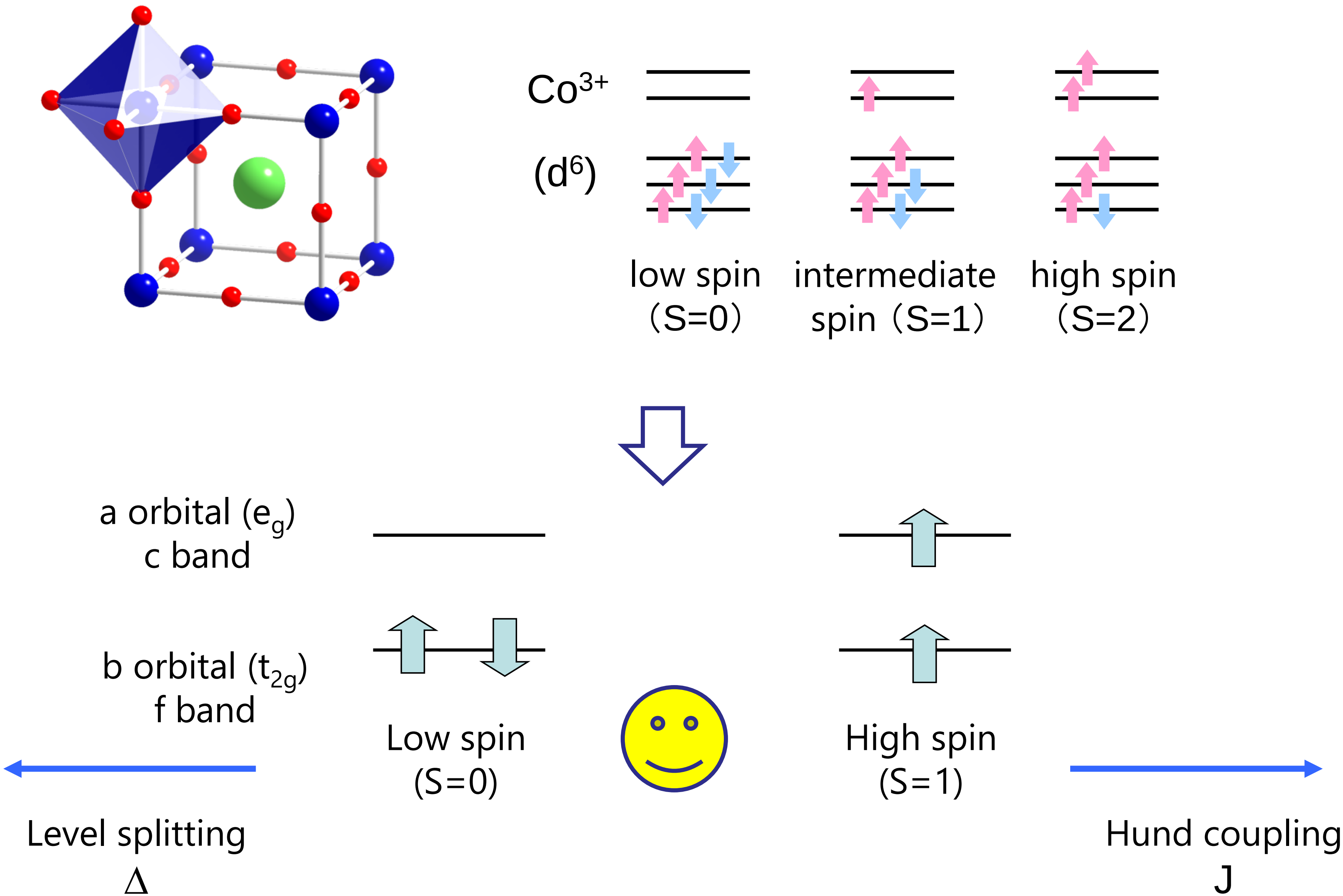
$Pr_{0.5}Ca_{0.5}CoO_3$

J. Kuneš and P. Augustinský PRB 89, 115134 (2014)
J. Kuneš and P. Augustinský PRB 90, 235112 (2014)

Strong coupling approaches

C. D. Batista, PRL 89, 166403 (2002)
L. Balents, PRB 62 2346 (2000)

Perovskite cobaltites



Two band Hubbard model

$$\mathcal{H}_0 = \Delta \sum_i n_{ia}$$

Energy difference

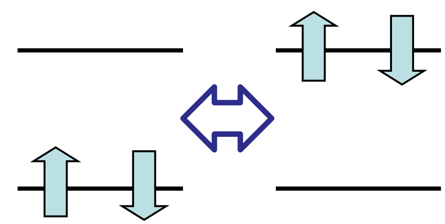
$$+U \sum_{i\gamma} n_{i\gamma\uparrow} n_{i\gamma\downarrow} + U' \sum_i n_{ia} n_{ib}$$

Intra/inter band Coulomb

$$+J \sum_{i\sigma\sigma'} c^\dagger_{ia\sigma} c^\dagger_{ib\sigma'} c_{ia\sigma'} c_{ib\sigma} + I \sum_{i\gamma=\gamma'} c^\dagger_{i\gamma\uparrow} c^\dagger_{i\gamma\downarrow} c_{i\gamma'\downarrow} c_{i\gamma'\uparrow}$$

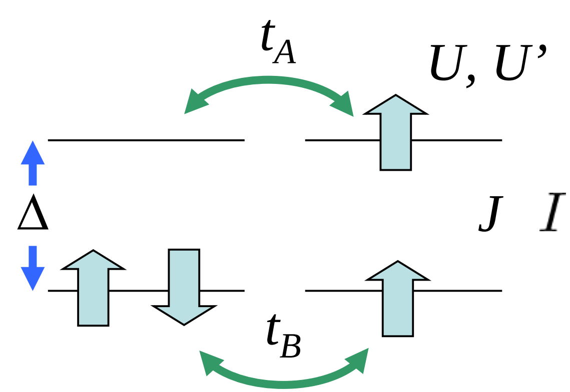
Hund coupling

Pair hopping



$$\mathcal{H}_t = - \sum_{<ij>\gamma\sigma} t_\gamma \left(c^\dagger_{i\gamma\sigma} c_{j\gamma\sigma} + H.c. \right)$$

Transfer



Summary

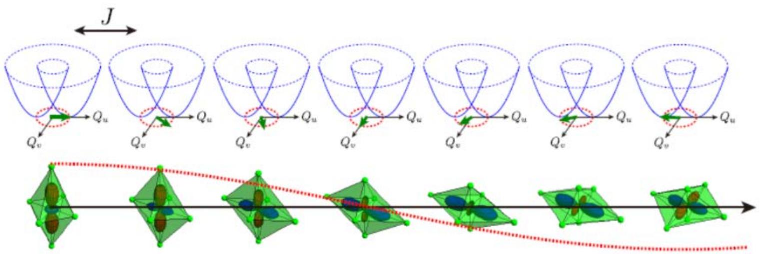
■ Orbiton

Orbiton under dynamical JT coupling

Low-lying collective vibronic mode + multiphonon

Electronic & lattice contributions
by X-ray & Neutron, respectively

J. Nasu & SI, Phys. Rev. B 88, 205110 (2013)
(Editor's suggestion paper)



■ Excitonic Insulator

Two excitonic insulating phases LS-EI(LS)-LS/HS-EI(HS)-HS
Breaking Z2 symmetry in EI phase
(In no-pair hopping, breaking U(1))