

1. QSGW(quasiparticle self-consistent GW)法のGPU化(with M.Obata, T.Oda Kanazawa-u). ecaljパッケージ
 2. QSGW1000(データベースにある物質に一括適用)
 3. 自動モデル化(MTO基底をもとに自動的にTBモデルにする)
 4. スピンゆらぎ計算(今回の発表)、SOCなど
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5. DOSNETをもうすこし改良したい(with K.Sato osaka-u)
 6. 生成AIで結晶を組み立てたい(結晶データベースで第二隣接ぐらいまでのクラスタデータを生成しておく。これらをパズルピースとして結晶がつかれるはず)。MatterGenはまだまだ幼い

時間依存交換相互作用

Harunori Okumura (NIMS)

Takao Kotani (Torino Univ. ,CSRN)

Kazunori Sato (Osaka Univ, CSRN)

1. 高解像度のスピンゆらぎ計算
2. $J(t-t')$ の求め方
3. QSGW法の基底状態を用いた場合のスピンゆらぎ

JPSJ90,094710(2021)

KAKEN: 22K04909

Spin fluctuation

3/19



(a) spin configuration of ferromagnet (0 K)

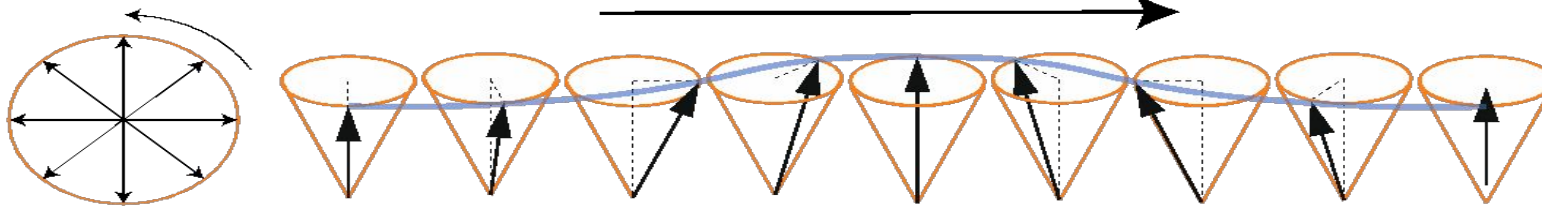
$$H = -J \sum_{\langle i, j \rangle} S_i \cdot S_j$$

Heisenberg model

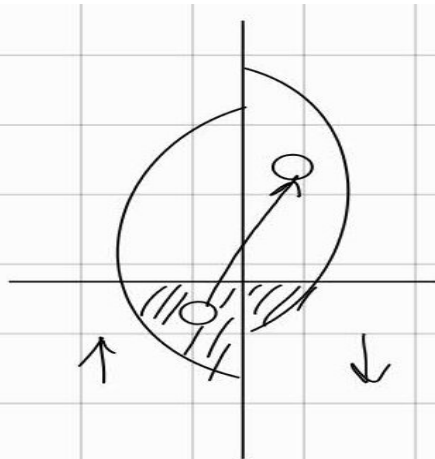
Linear approximation \rightarrow
Equation of motion of spin

energy $\omega(\mathbf{q})$

wave vector \mathbf{q}

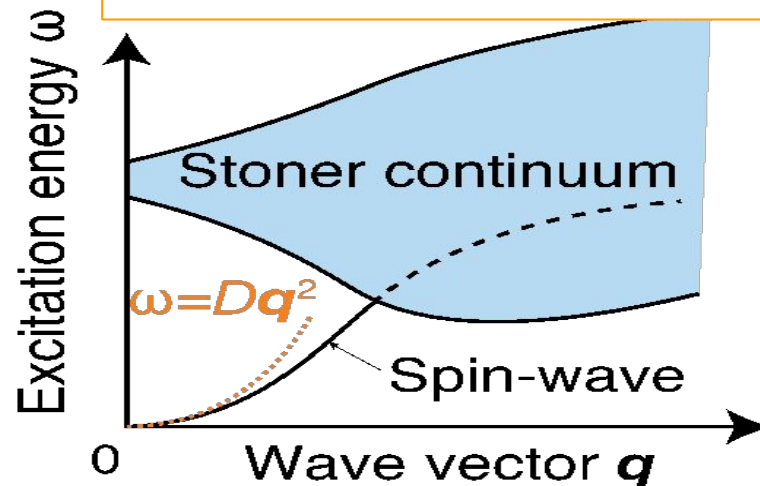


spin-wave



Stoner excitation

Spin fluctuation spectrum = $\text{Im}(\chi^{+-})$



H.Okumura, K.Sato, T.Kotani, (2019) PhysRevB.100.054419

有効場的な近似方法(はしご近似)

外部磁場 B_0 をサイト0に加える

$\Rightarrow K(=X_{0+-})$: 外部磁場 B_0 \rightarrow スピン回転@サイト1

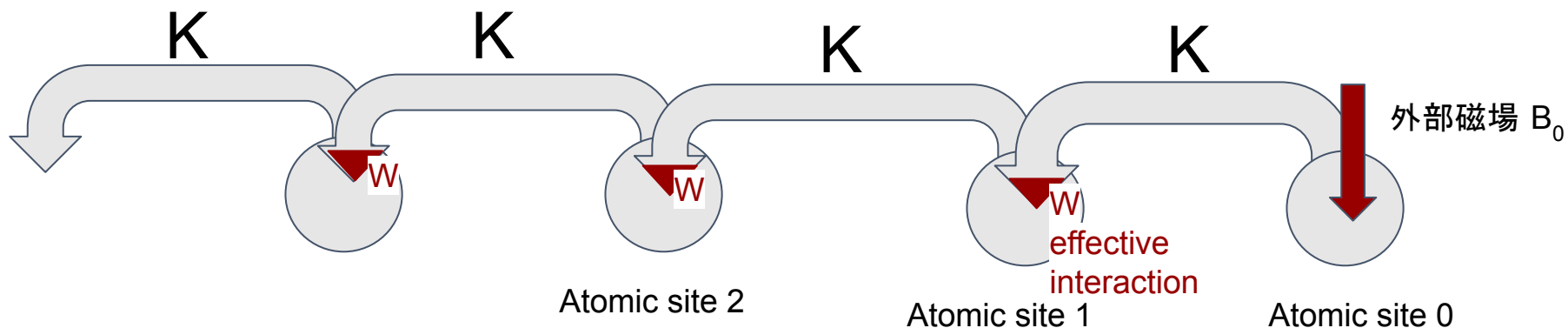
$\Rightarrow W$ (オンサイト): スピン回転@サイト1 \rightarrow 有効磁場 B_1 @サイト1

$\Rightarrow K(=X_{0+-})$: 有効磁場 B_1 @サイト1 \rightarrow スピン回転@サイト2

...

\Rightarrow 有効磁場 = 外部磁場 + 誘起された磁場

(すべての経路を加算する)

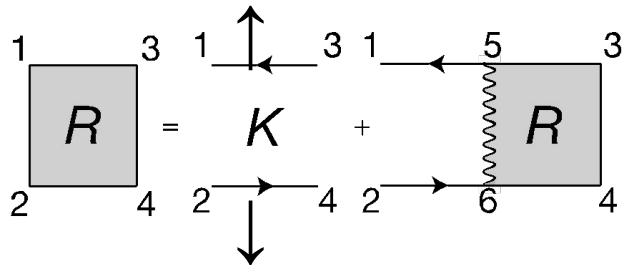


スピン横ゆらぎの線形応答による計算 (R_{+-} means χ_{+-})

$$\langle \delta S_{\mathbf{R}m}^+(t) \rangle = \sum_{\mathbf{R}'m'} \int_{-\infty}^{\infty} dt' R_{\mathbf{R}m\mathbf{R}'m'}^{+-}(t-t') B_{\mathbf{R}'m'}^+(t')$$

$\langle S^+ \rangle$: spin moment, B : external magnetic field

ラダー近似



$W(\mathbf{q}=0, \omega=0)$: Onsite screened Coulomb interaction is calculated in advance.

E. Şaşıoğlu, *et. al.*, *Phys. Rev. B* **81**, 054434 (2010).
C.Friedrich M.C Muller, S.Blugel (2018)

$$R = K + KWK + KWKWK + \dots = \frac{K}{1 - WK}$$

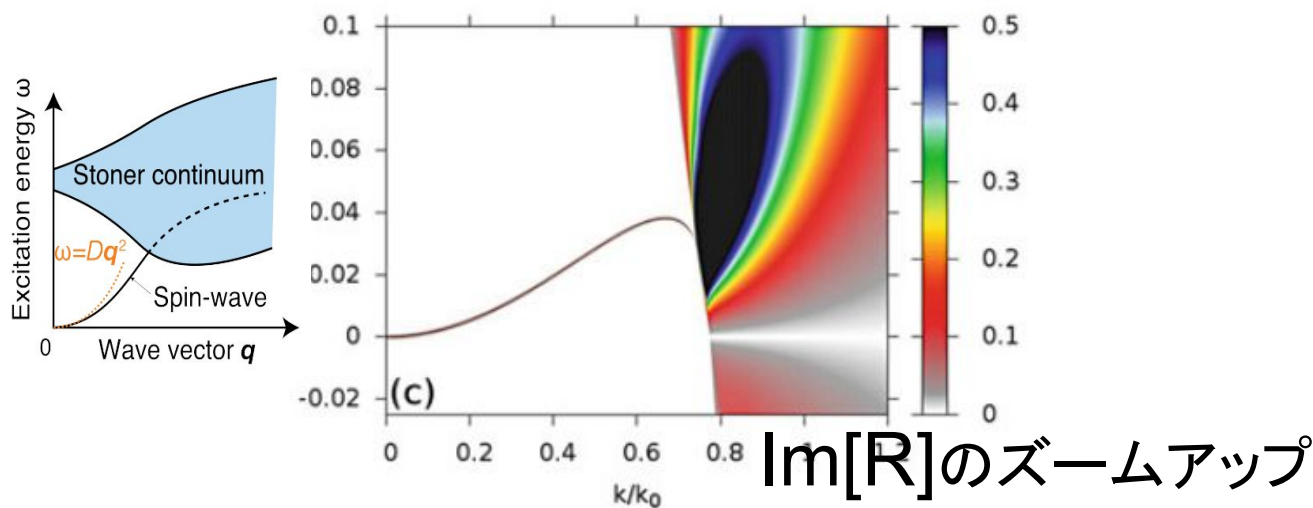
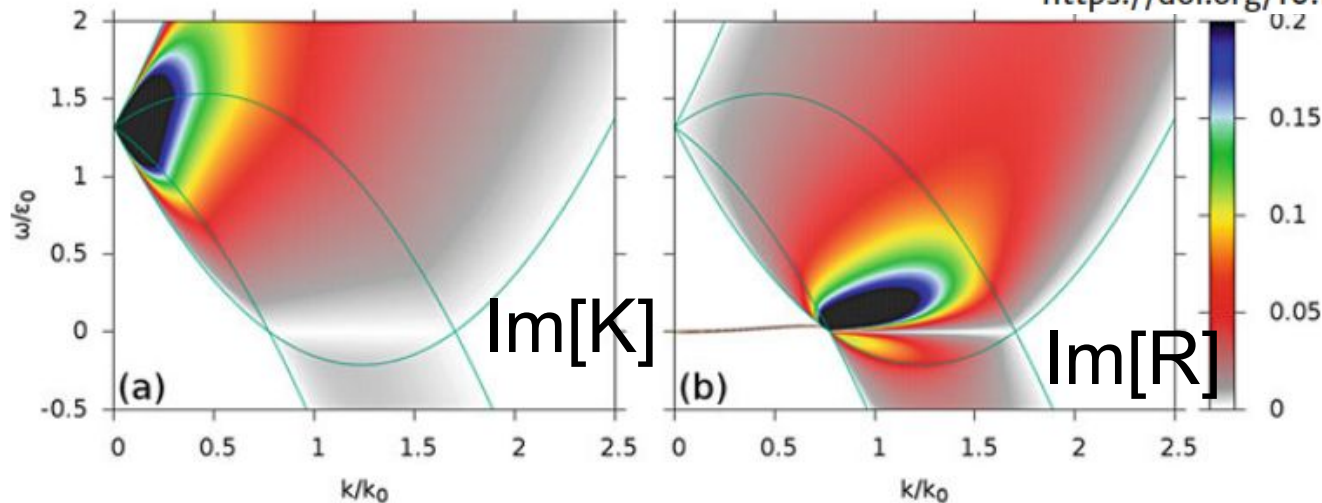
$K(\mathbf{q}, \omega)$: Stoner excitation calculated band structure

$W(\mathbf{q}, 0)$: RPA from band structure

$$R_{\mathbf{R}m\mathbf{R}'m'}^{+-}(t-t') = K(1-WK)^{-1}$$

Spin Excitations in Solid from Many-Body Perturbation Theory

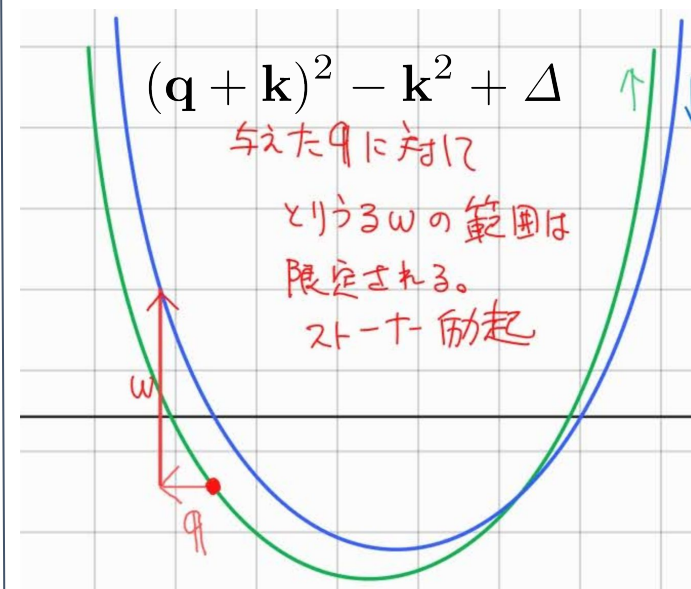
Friedrich, C., Müller, M.C.T.D., Blügel, S. (2018). Spin Excitations in Solid from Many-Body Perturbation Theory. In: Andreoni, W., Yip, S. (eds) Handbook of Materials Modeling. Springer, Cham. https://doi.org/10.1007/978-3-319-42913-7_74-1



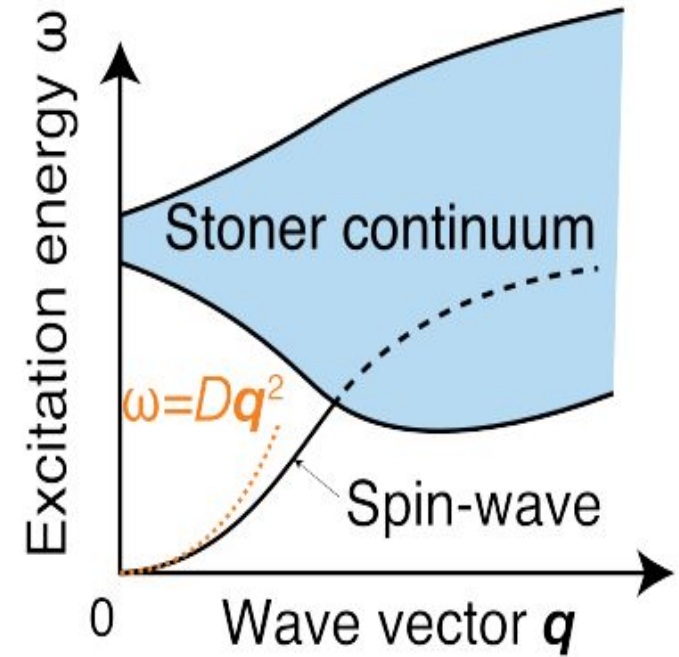
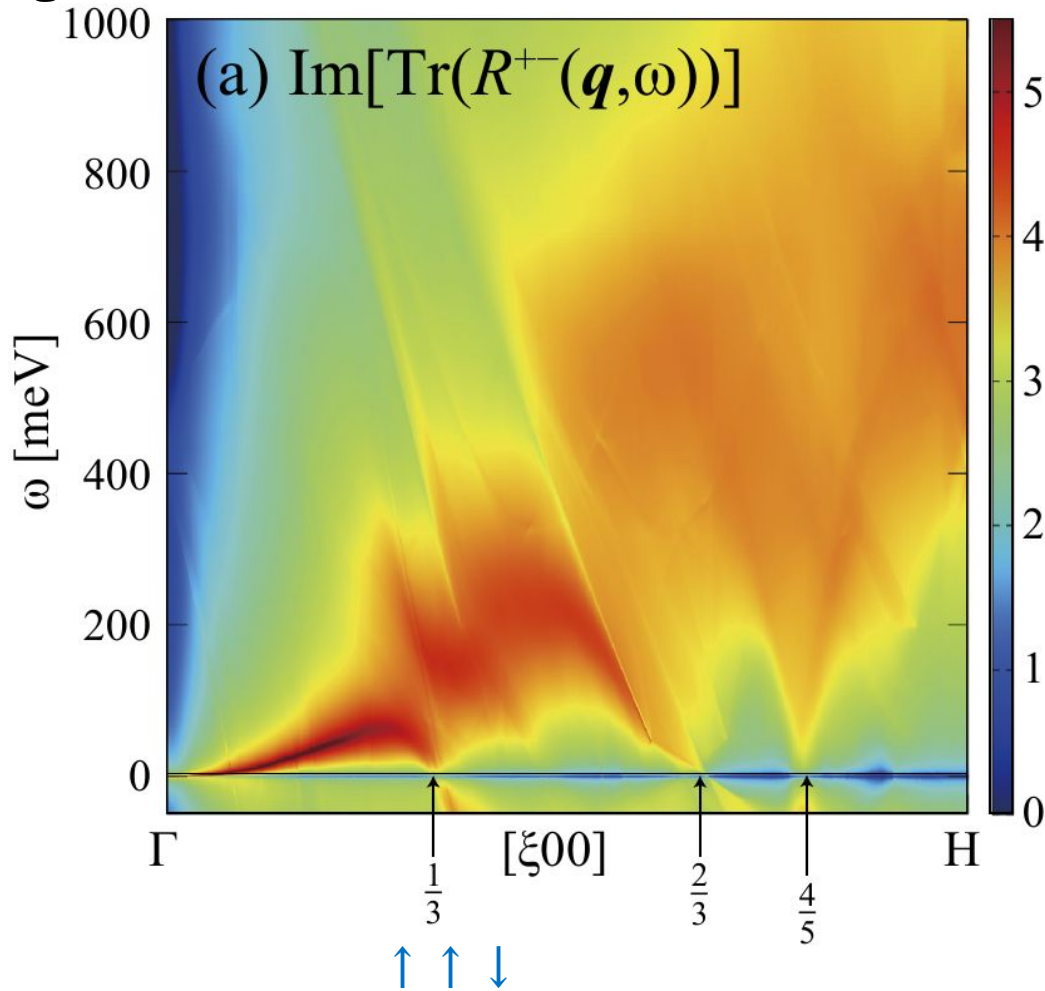
ストーナー境界は

$$q^2 \pm 2qk_{F\uparrow} + \Delta \text{ for } \omega > 0$$

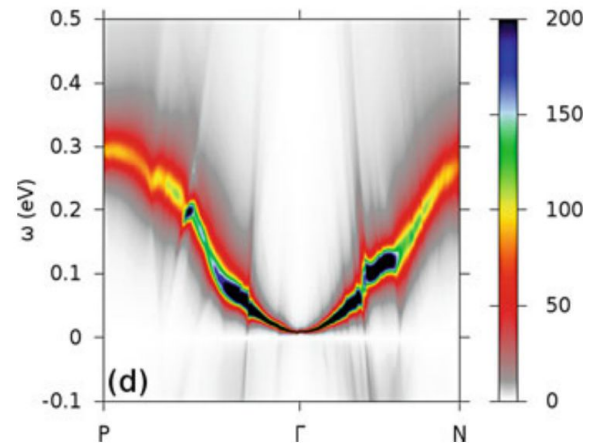
$$-q^2 \pm 2qk_{F\downarrow} + \Delta \text{ for } \omega < 0$$



High resolution!

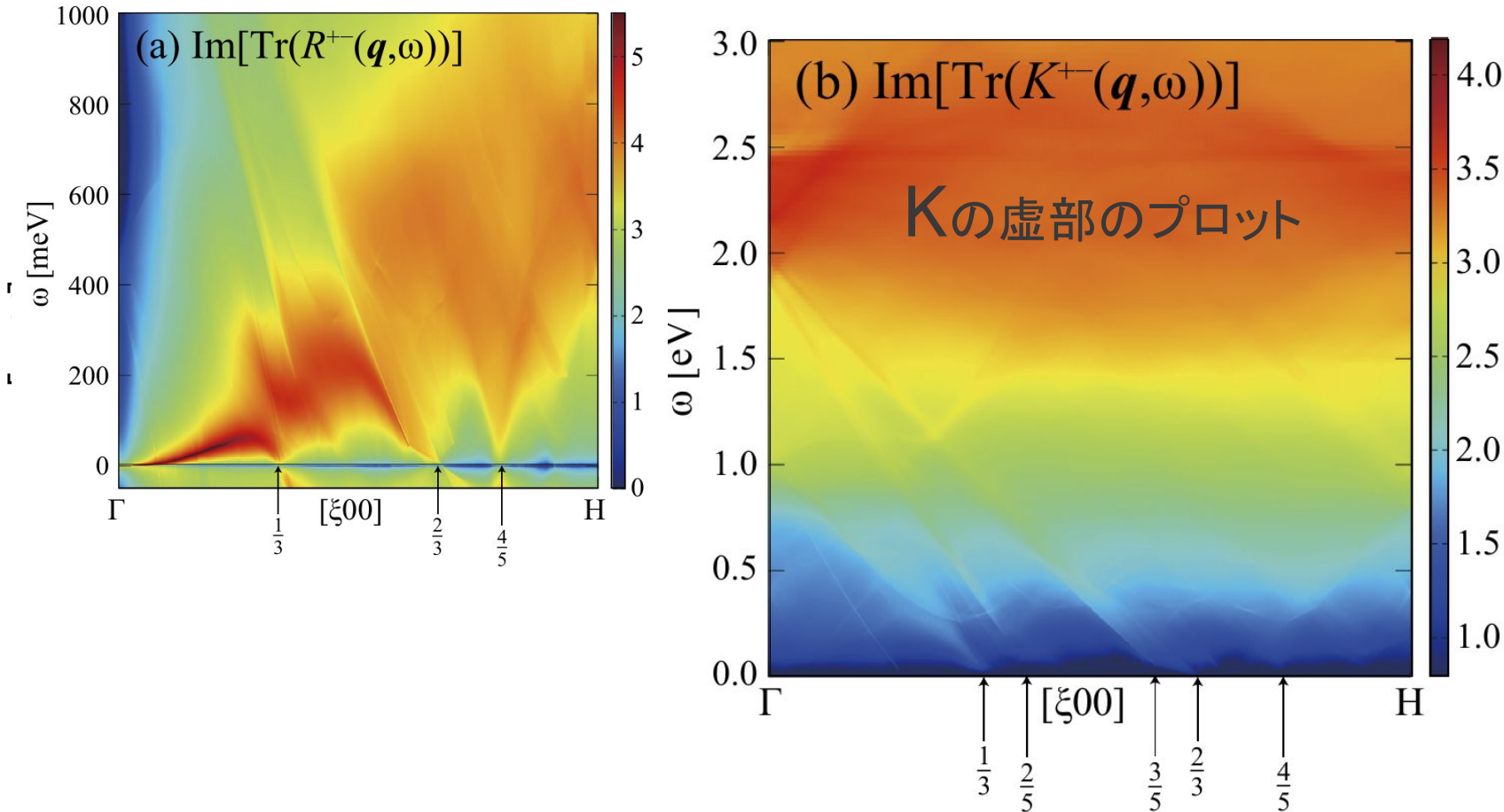


過去計算; C.Friedrich M.C Muller, S.Blugel (2018)



- Gilbert damping、
Kamberskyメカニズムはこれとは別の減衰メカニズム
- Stoner excitation boundary

$$R_{\mathbf{R}m\mathbf{R}'m'}^{+-}(t-t') = K(1-WK)^{-1}$$



Kにおいて、たとえ $q=0$ でも0エネルギーから有限の値 (一様電子ガスとの違い)
磁氣的フェルミ面交差 : upフェルミ面とdnフェルミ面の交差が避けられない



普通のハイゼンベルグモデル

$$\hbar \dot{\mathbf{S}}_{\mathbf{R}}(t) = \mathbf{S}_{\mathbf{R}}(t) \times \sum_{\mathbf{R}'} (J_{\mathbf{R}\mathbf{R}'} \mathbf{S}_{\mathbf{R}'}(t) - g \delta_{\mathbf{R}\mathbf{R}'} \mu_{\text{B}} \mathbf{B}_{\mathbf{R}'}(t)).$$

Lichtenstein公式(線形応答)で J を求める

拡張したハイゼンベルグモデルを考える

$$\hbar \dot{\mathbf{S}}_{\mathbf{R}m}(t) = \mathbf{S}_{\mathbf{R}m}(t) \times \left(\sum_{\mathbf{R}'m'} \int_{-\infty}^{\infty} dt' (J_{\mathbf{R}m\mathbf{R}'m'}(t-t') \mathbf{S}_{\mathbf{R}'m'}(t') - g \mu_{\text{B}} \mathbf{B}_{\mathbf{R}'m'}(t') \delta(t-t')) \right)$$

注: 最近見つけた。Valiulin, V.E., Chtchelkatchev, N.M., Mikheyenkov, A.V. *et al.*

'Time-dependent exchange creates the time-frustrated state of matter' *Sci Rep* 12, 16177 (2022).



$$\hbar \dot{\mathbf{S}}_{\mathbf{R}m}(t) = \mathbf{S}_{\mathbf{R}m}(t) \times \left(\sum_{\mathbf{R}'m'} \int_{-\infty}^{\infty} dt' (J_{\mathbf{R}m\mathbf{R}'m'}(t-t') \mathbf{S}_{\mathbf{R}'m'}(t') - g\mu_B \mathbf{B}_{\mathbf{R}'m'}(t') \delta(t-t')) \right)$$

拡張ハイゼンベルグ方程式を線形化して解いて得たスピンゆらぎ = 線形応答で得られるスピンゆらぎ $R_{\mathbf{R}m\mathbf{R}'m'}^{+-}(t-t')$

とおいて求めれば良い。

$$J_{\mathbf{R}m\mathbf{R}'m'}(\omega) = -\mu_B g (K^{-1} - W)_{\mathbf{R}m\mathbf{R}'m'}(\omega) \quad \text{for } \mathbf{R}m \neq \mathbf{R}'m',$$

$$J_{\mathbf{R}m\mathbf{R}m}(\omega) = \frac{-\hbar\omega}{S_{\mathbf{R}mz}} + \mu_B g (K^{-1} - W)_{\mathbf{R}m\mathbf{R}m}(\omega) + \frac{1}{S_{\mathbf{R}mz}} \sum_{\mathbf{R}'m' \neq \mathbf{R}m} \mu_B g (K^{-1} - W)_{\mathbf{R}m\mathbf{R}'m'}(0) S_{\mathbf{R}'m'z}.$$

Z component for ground state

時間依存を無視すればLichtenstein公式に帰着する

$$\hbar \dot{\mathbf{S}}_{\mathbf{R}}(t) = \mathbf{S}_{\mathbf{R}}(t) \times \sum_{\mathbf{R}'} (J_{\mathbf{R}\mathbf{R}'} \mathbf{S}_{\mathbf{R}'}(t) - g \delta_{\mathbf{R}\mathbf{R}'} \mu_{\text{B}} \mathbf{B}_{\mathbf{R}'}(t)).$$

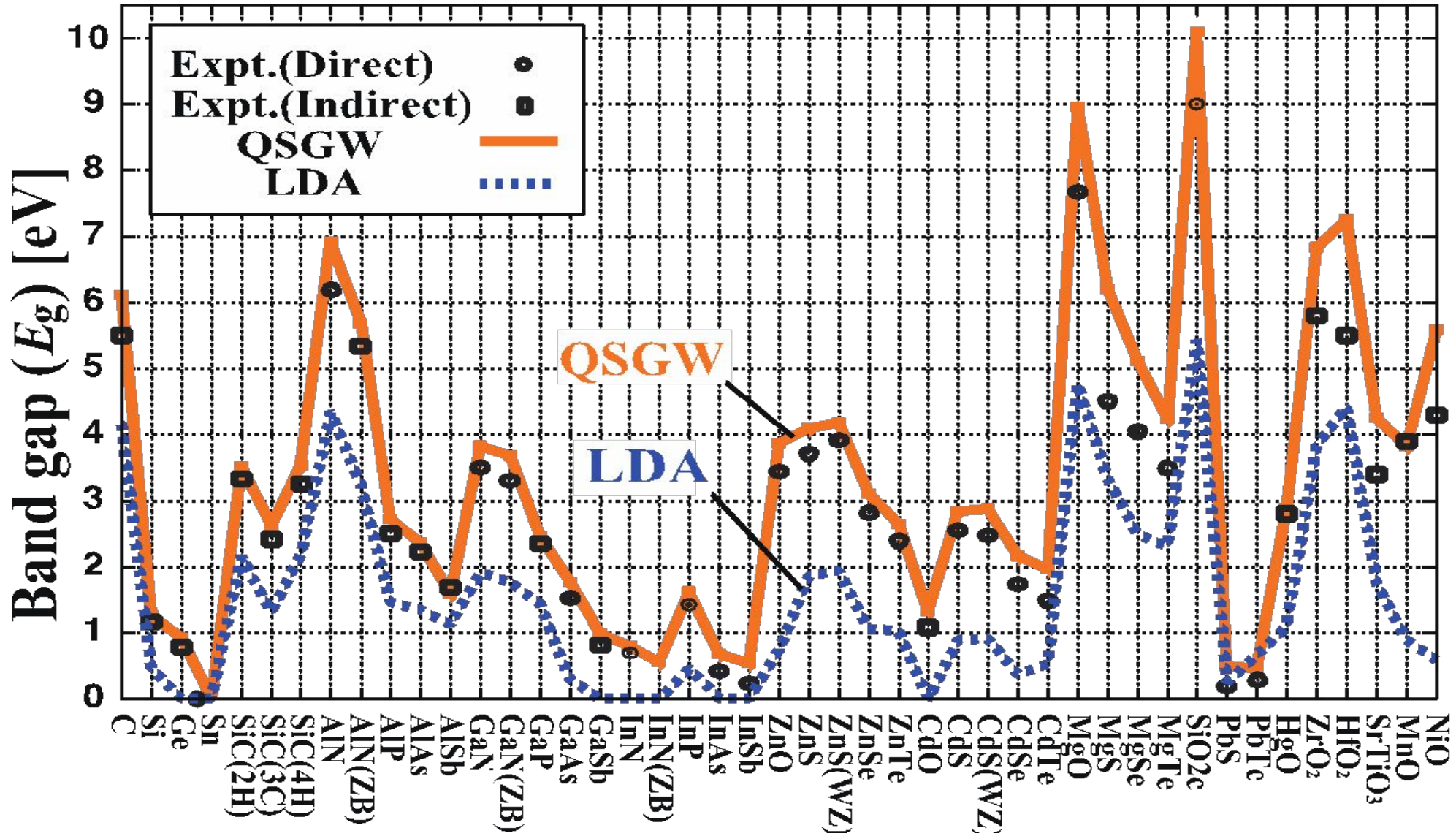
$$\hbar \dot{\mathbf{S}}_{\mathbf{R}m}(t) = \mathbf{S}_{\mathbf{R}m}(t) \times \left(\sum_{\mathbf{R}'m'} \int_{-\infty}^{\infty} dt' (J_{\mathbf{R}m\mathbf{R}'m'}(t-t') \mathbf{S}_{\mathbf{R}'m'}(t') - g \mu_{\text{B}} \mathbf{B}_{\mathbf{R}'m'}(t') \delta(t-t')) \right)$$

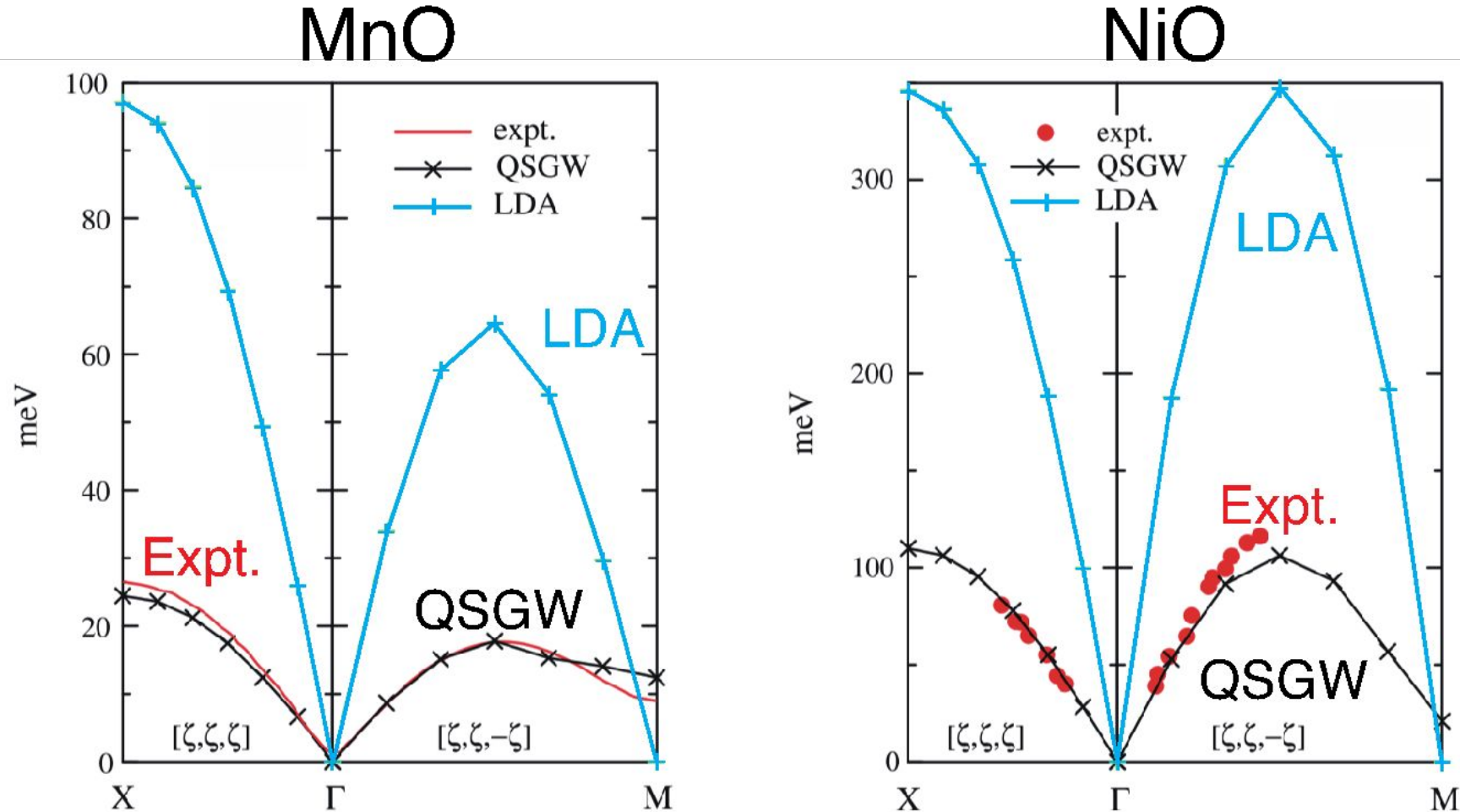
1. Retarded effects
2. Orbital dependence

For example, we can use Tc by the method .Baker and G.Bauer(PRB.100.140401)
(Classical simulation but mimicking quantum noise)

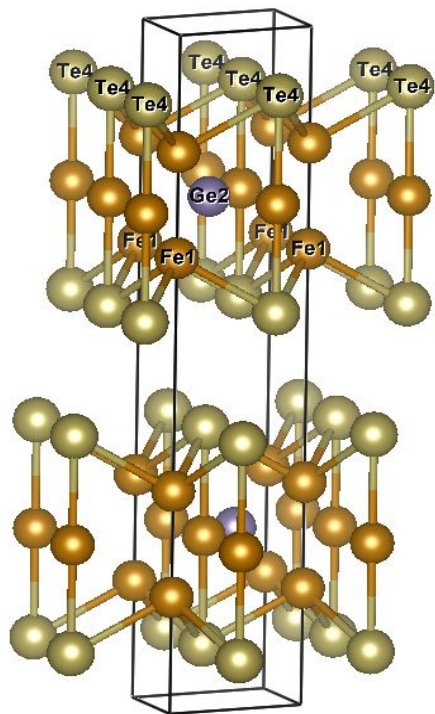
⇒ **Spin dynamics (extended LLG equation)**

D. Deguchi, K. Sato, H. Kino, and T. Kotani, *Jpn. J. Appl. Phys.* **55**, (2016).





QSGWはMnOとNiOのバンドギャップエネルギーを再現でき、スピン波のエネルギーも実験値に一致する。



$a=3.99\text{\AA}$

$c=16.33\text{\AA}$

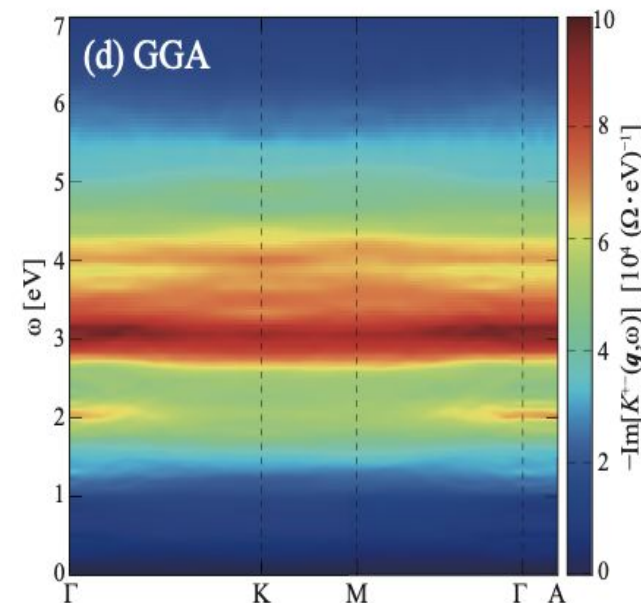
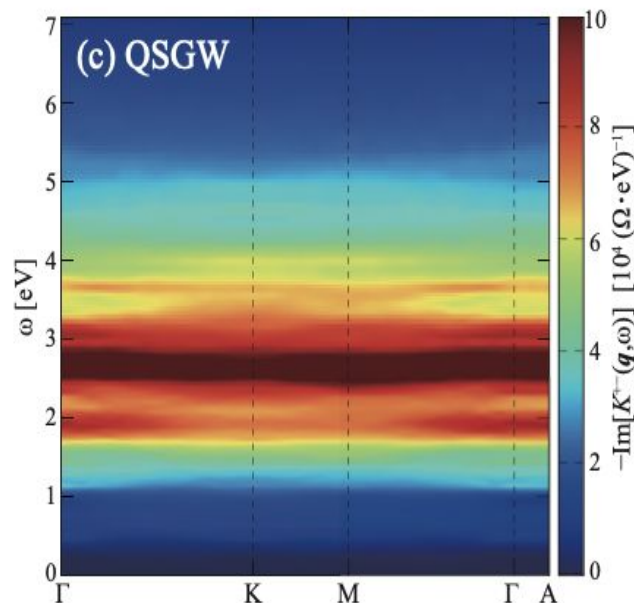
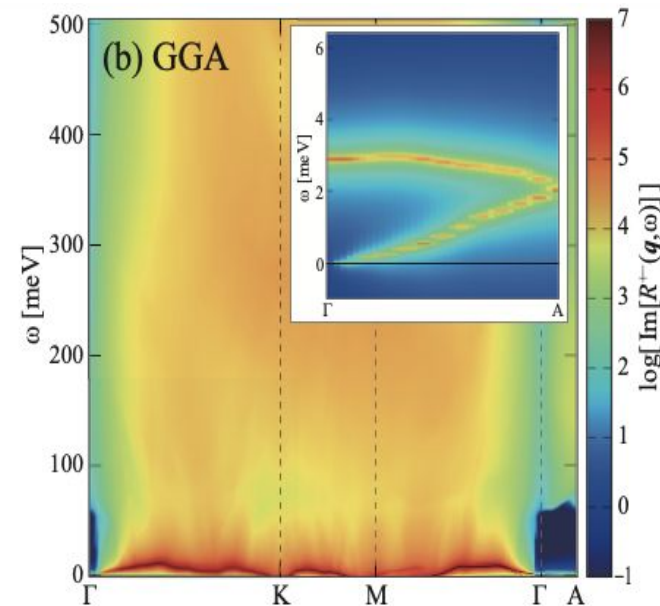
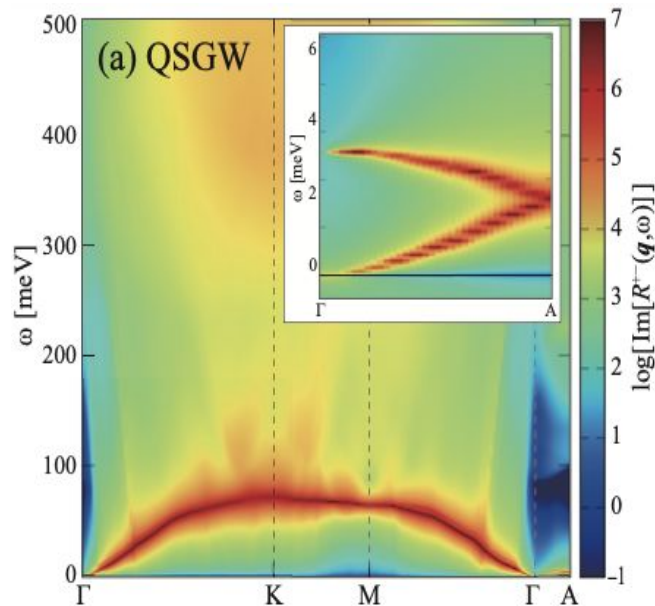
Wannier functions:

Fe spd (6 atoms)

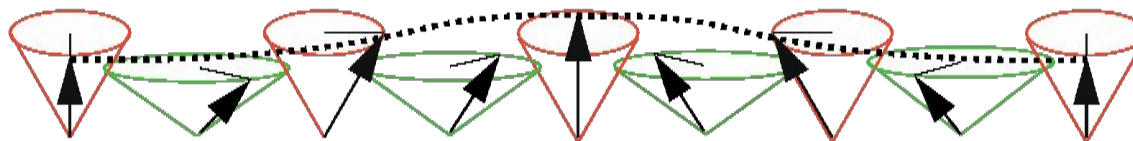
Ge sp (2 atoms)

Te sp (4 atoms)

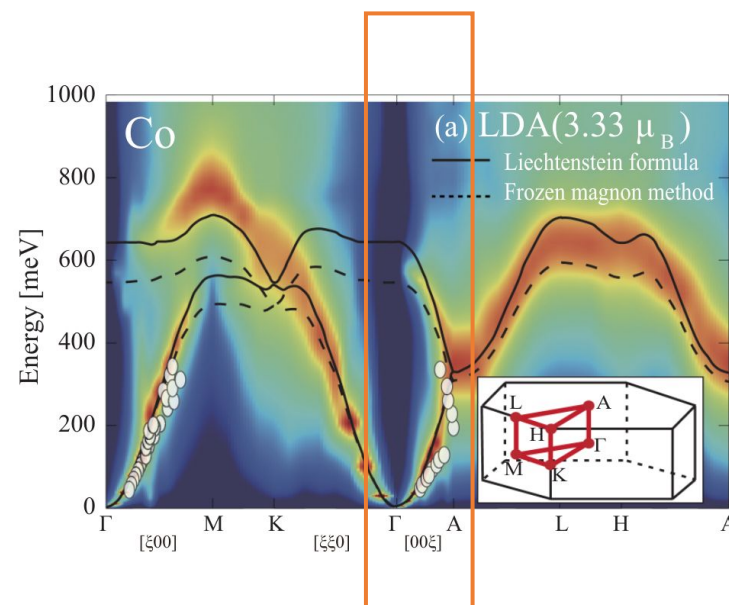
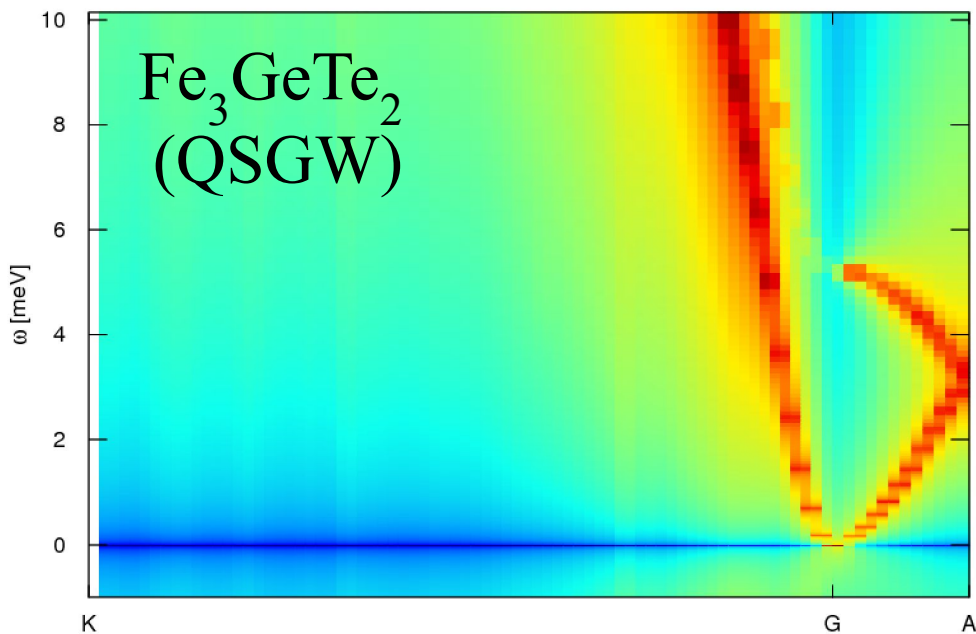
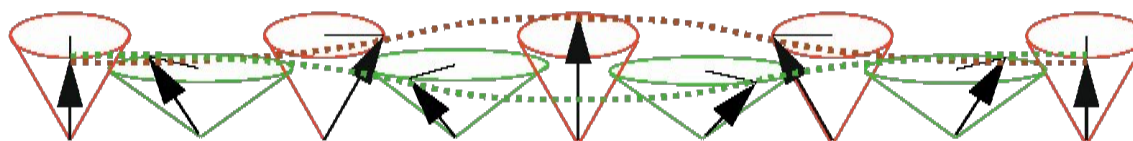
total number of Wannier functions (nwf) = 78



Spin-wave (acoustic mode)



Spin-wave (optical mode)



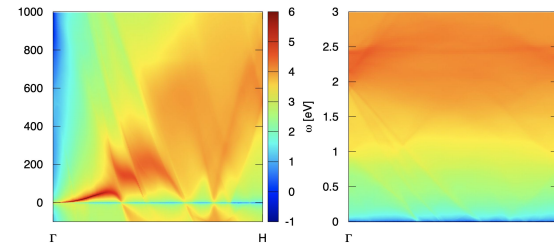
H. Okumura, K. Sato, and T. Kotani, Phys. Rev. B 100, 54419 (2019).

荒い計算

1. We introduced extended Heisenberg model. $J(t-t')$

$$\hbar\dot{\mathbf{S}}_{\mathbf{R}m}(t) = \mathbf{S}_{\mathbf{R}m}(t) \times \left(\sum_{\mathbf{R}'m'} \int_{-\infty}^{\infty} dt' (J_{\mathbf{R}m\mathbf{R}'m'}(t-t')\mathbf{S}_{\mathbf{R}'m'}(t') - g\mu_B\mathbf{B}_{\mathbf{R}'m'}(t')\delta(t-t')) \right)$$

2. High resolution calculation of spin fluctuation



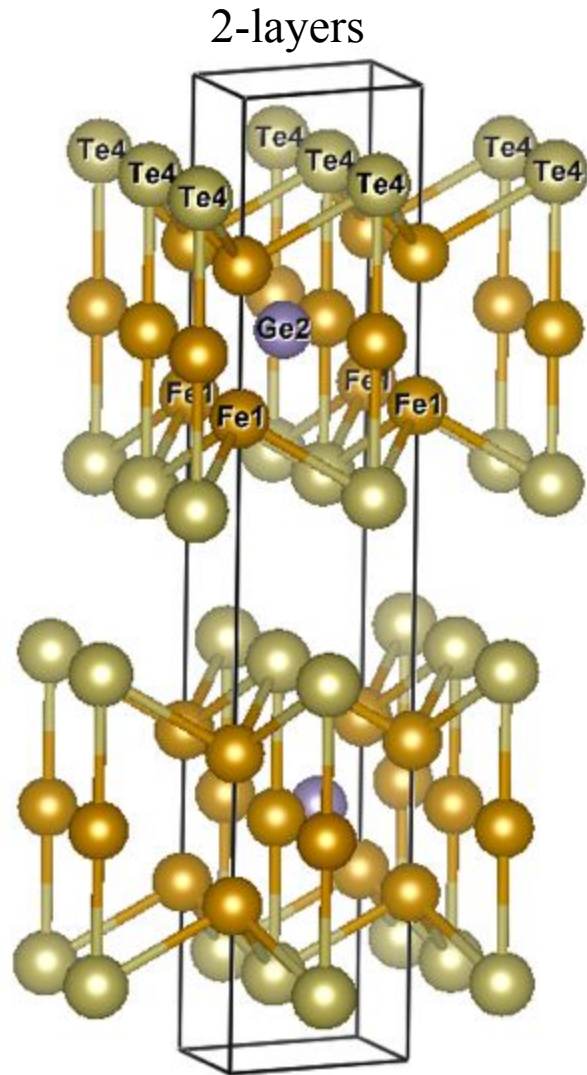
3. For Fe₃GeTe₂, we need to be on top of QSGW.

Future

- LLG方程式としてダイナミクスを解く。T_c
- SOC included.



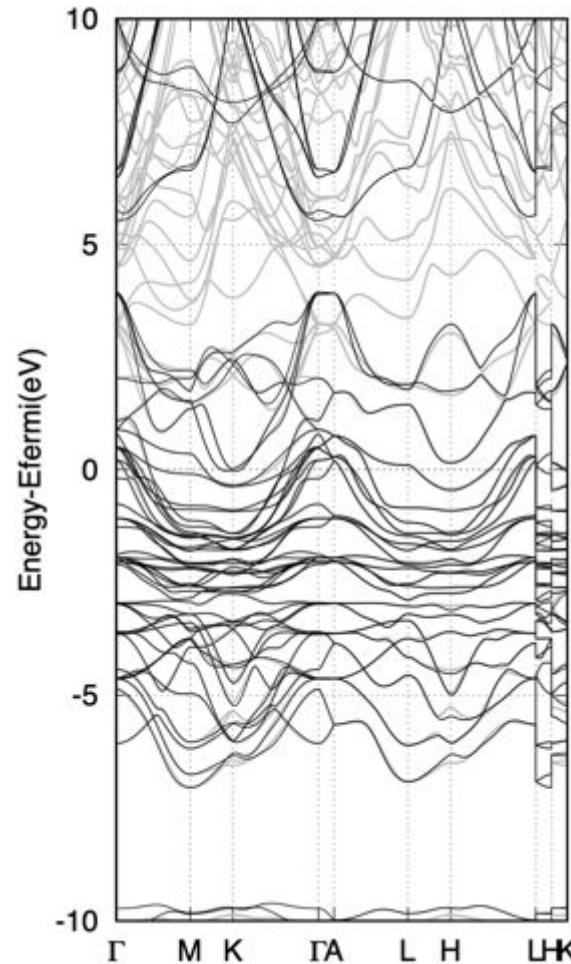
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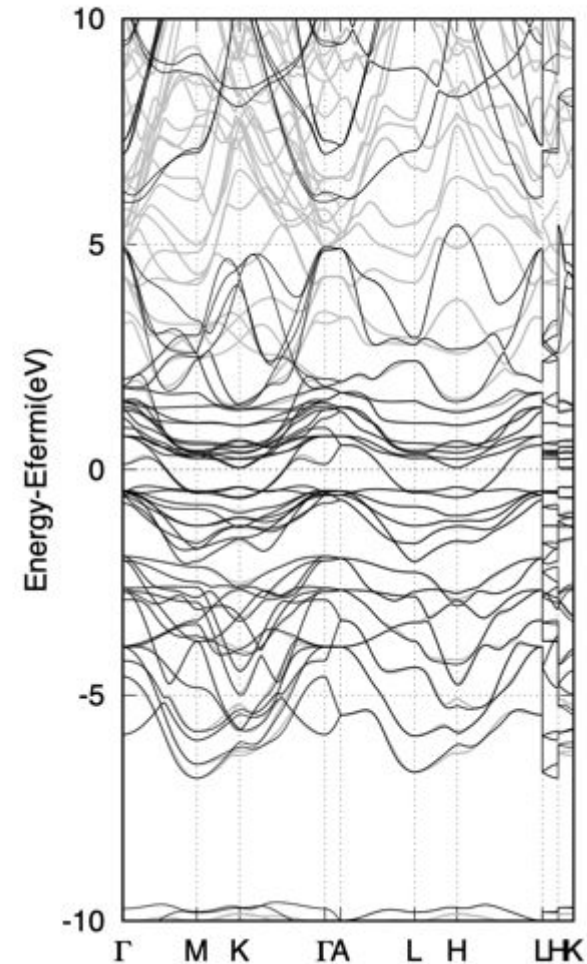
$a=3.99\text{\AA}$

$c=16.33\text{\AA}$

FGT (minority)



FGT (minority)



Wannier functions:

Fe spd (6 atoms)

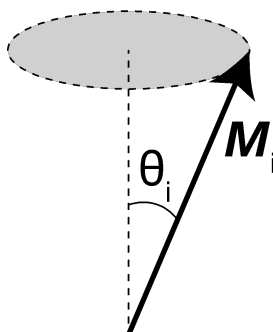
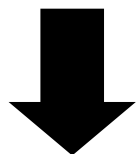
Ge sp (2 atoms)

Te sp (4 atoms)

total number of Wannier functions (nwf) = 78

Ground state ($T=0K$)

First-principle calculations
(Density functional theory (DFT))



Frozen-magnon

- Adiabatic approach
- Infinitesimal θ_i
- Not including Stoner excitation

Linear response

- Dynamical susceptibility: $R^{\mathbb{Z}}(\omega, \mathbf{q})$
- Including Stoner excitation

I. Galanakis and E. Şaşıoğlu, *J. Mater. Sci.* **47**, 7678 (2012).

