Theory

Superconductivity in MoS_2 surface

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博士 1 年　中村康晴

Dispersion

$$
\begin{aligned}
\varepsilon_{\mathrm{Mo}}(\boldsymbol{k}) = 2t_1 &\left(\cos k_{\mathrm{y}}a + 2\cos\frac{\sqrt{3}}{2}k_{\mathrm{x}}a\cos\frac{1}{2}k_{\mathrm{y}}a\right) \\
+\, 2t_2 &\left(\cos\sqrt{3}k_{\mathrm{x}}a + 2\cos\frac{\sqrt{3}}{2}k_{\mathrm{x}}a\cos\frac{3}{2}k_{\mathrm{y}}a\right) \\
+\, 2t_3 &\left(\cos 2k_{\mathrm{y}}a + 2\cos\sqrt{3}k_{\mathrm{x}}a\cos k_{\mathrm{y}}a\right) - \mu
\end{aligned}
$$

Band calculation

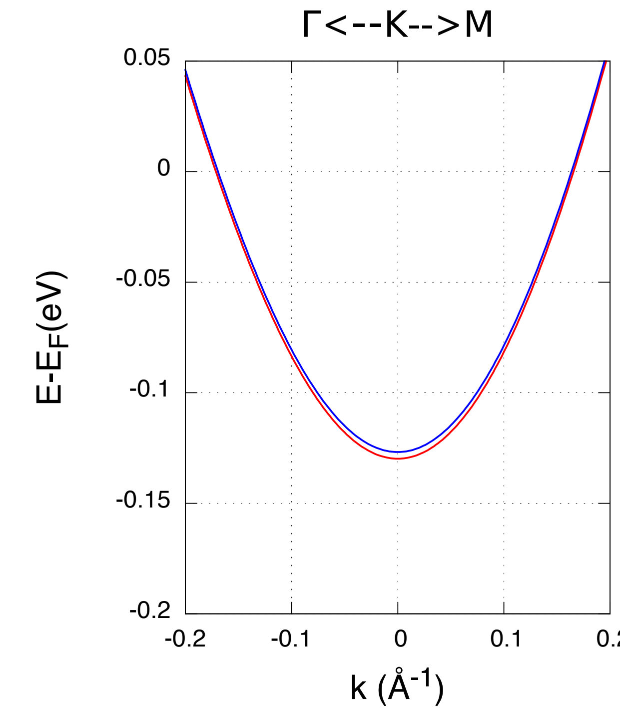
at mono-layer

G.B Lin et.al:PRB

$$t_2/t_1 = -0.40$$

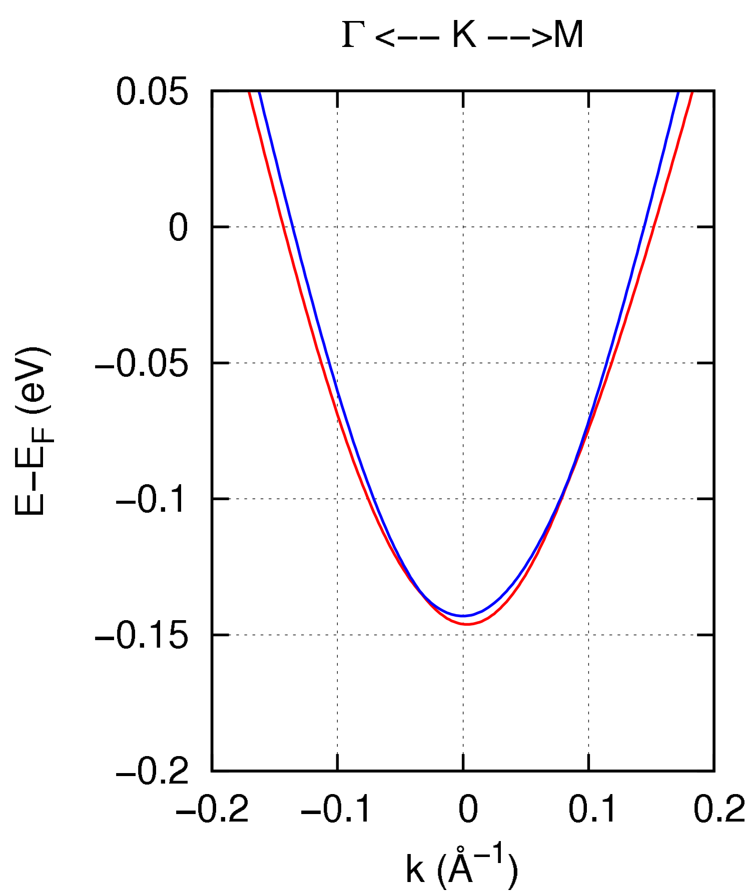
$$t_3/t_1 = 0.25$$

$$t_1 = 146\ meV$$



Band calculation

$$N \sim 8.9 \times 10^{13} cm^{-2}$$



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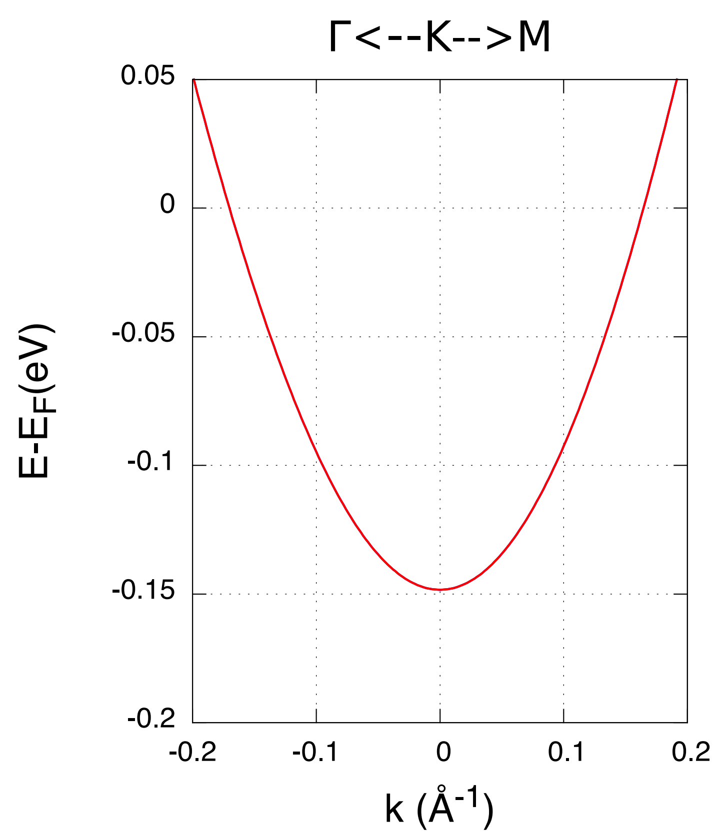
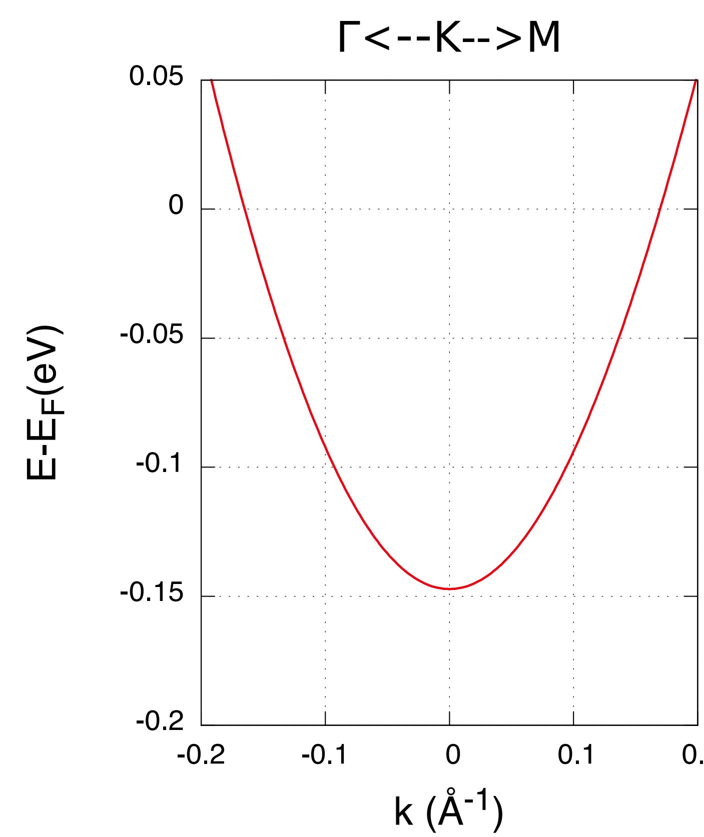


$$t_3/t_1 = 0.05$$



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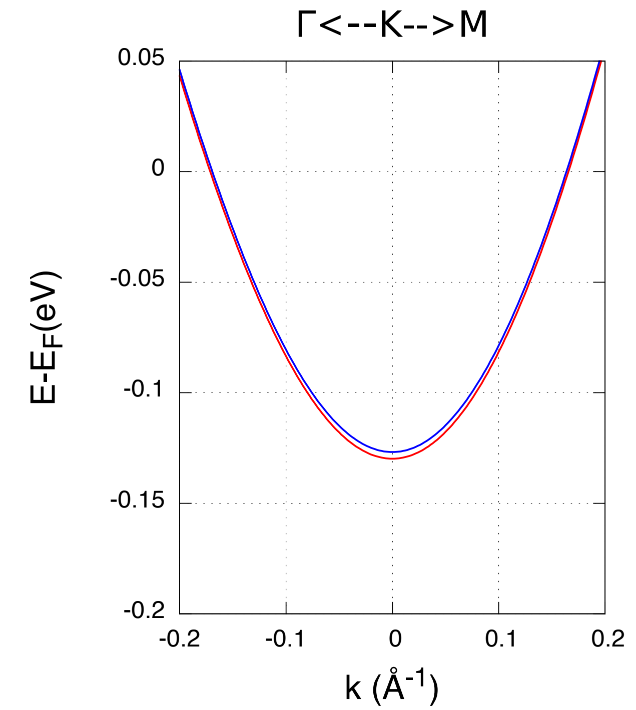

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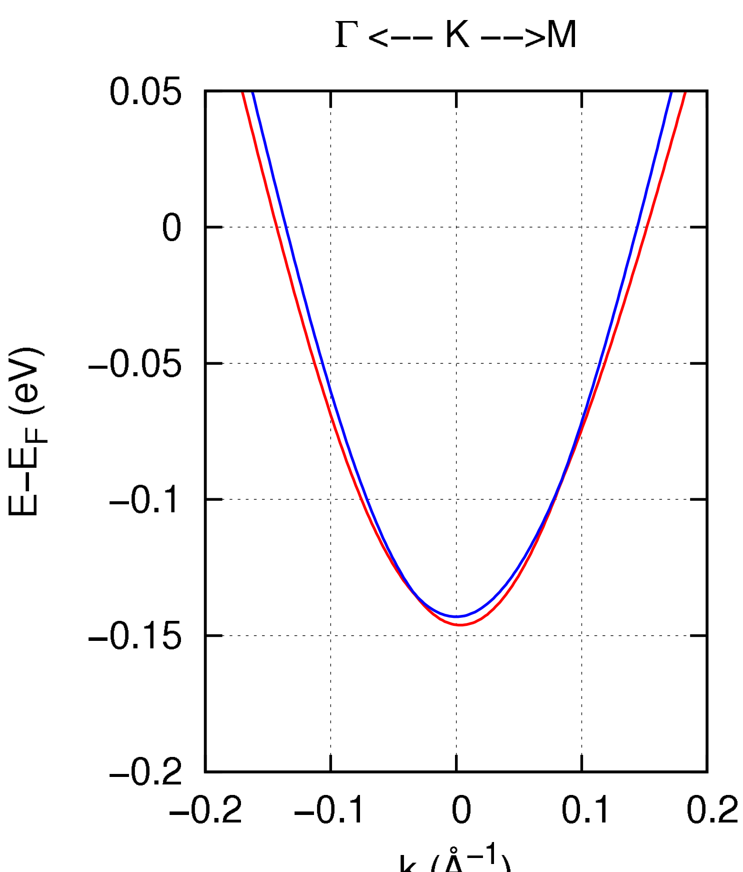
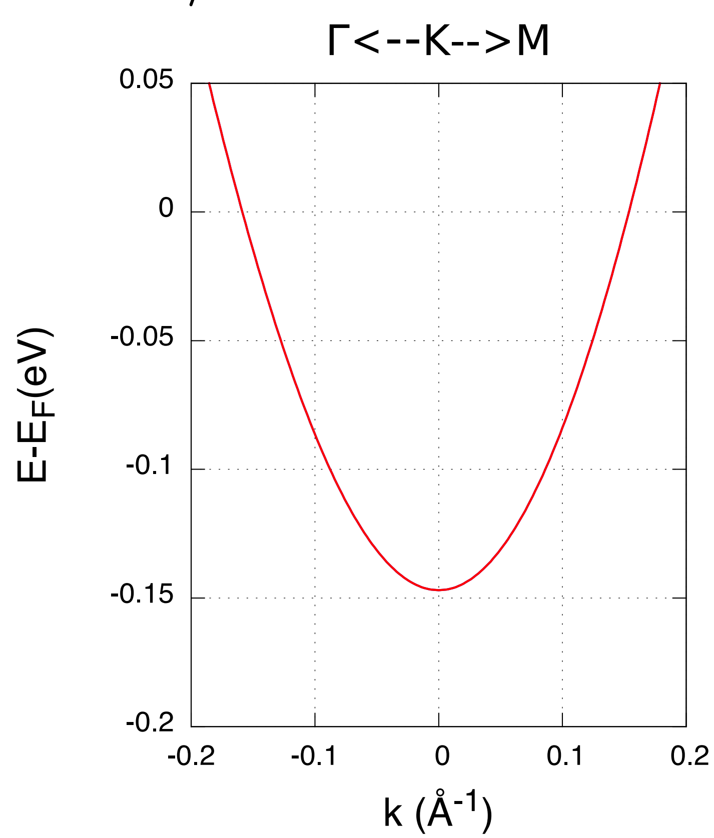


$$N \sim 7.7 \times 10^{13} cm^{-2}$$

$$t_3/t_1 = 0.25$$



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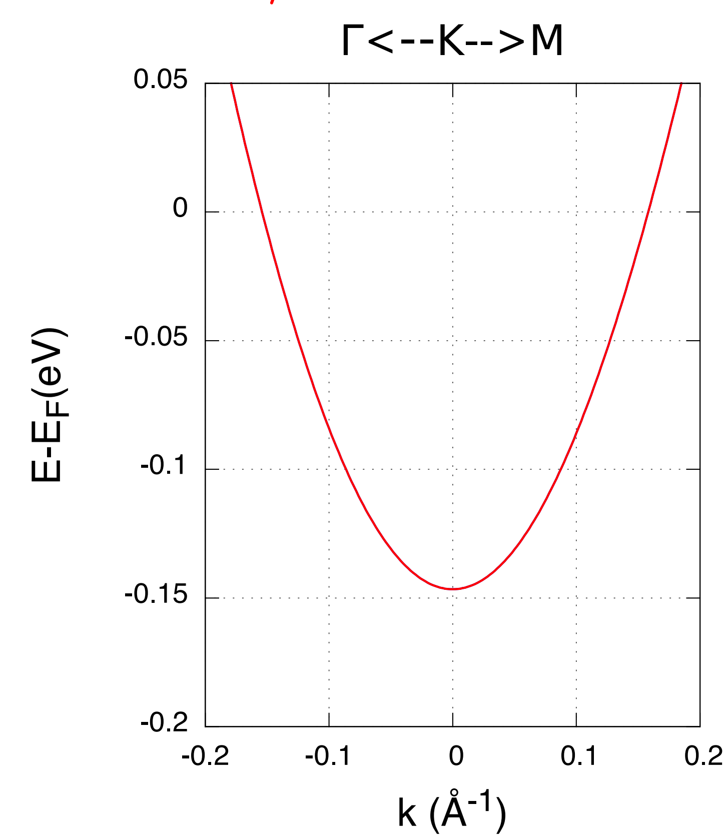
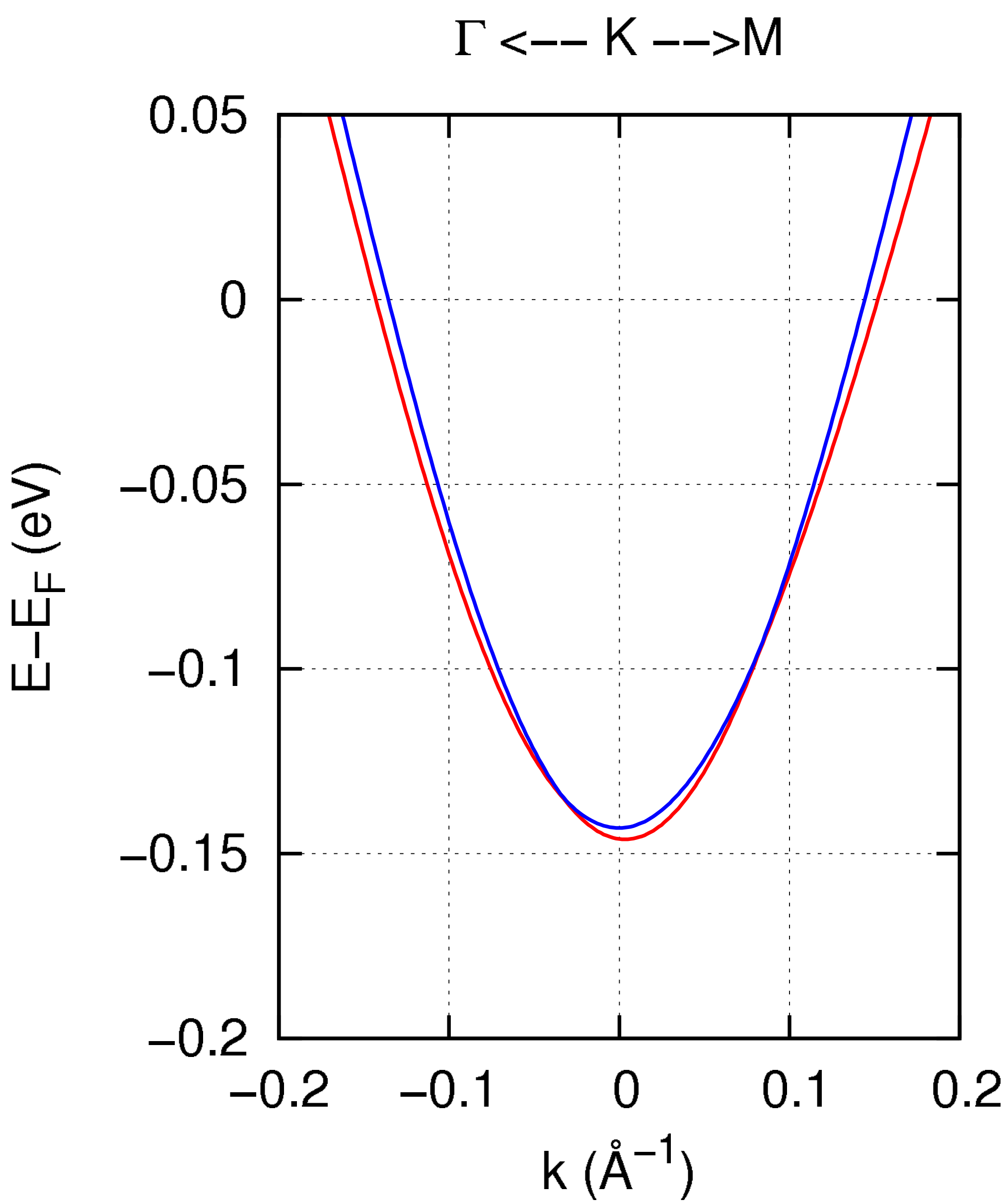
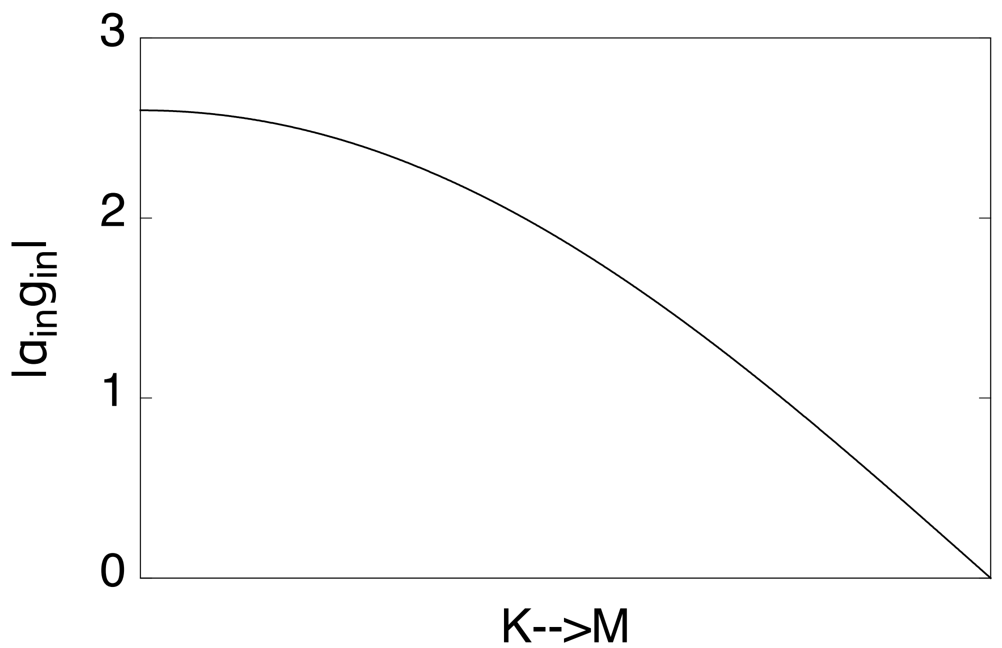


Spin split

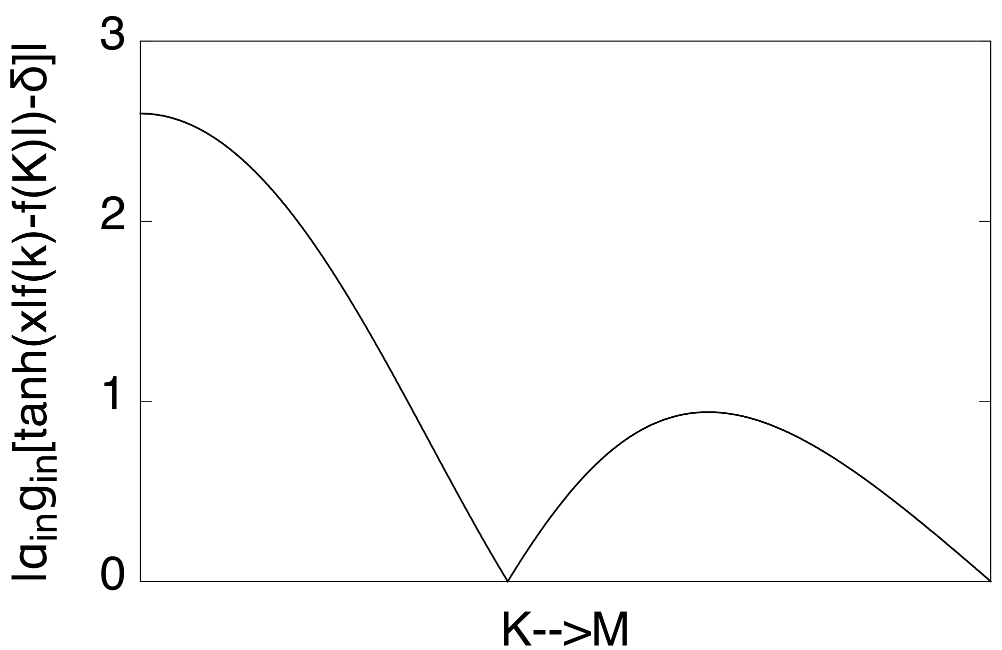
Band calculation



$$\sum_{\mathbf{k},s,s'} \alpha_{\rm in} \boldsymbol{g}_{\rm in}(\mathbf{k}) \cdot \boldsymbol{\sigma}_{s,s'} \hat{c}^\dagger_{\mathbf{k},s} \hat{c}_{\mathbf{k},s'}$$



$$\sum_{\mathbf{k},s,s'} \alpha_{\rm in} \boldsymbol{g}_{\rm in}(\mathbf{k}) \cdot \boldsymbol{\sigma}_{s,s'} [\tanh(x|f(\mathbf{k}) - f(K)|) - \delta] \hat{c}^\dagger_{\mathbf{k},s} \hat{c}_{\mathbf{k},s'}$$



Spin split

$$\hat{H}_{\mathrm{in}} = \sum_{\mathbf{k},s,s'} \alpha_{\mathrm{in}} \boldsymbol{g}_{\mathrm{in}}(\mathbf{k}) \cdot \boldsymbol{\sigma}_{s,s'} \left[\tanh\left(x|f(\mathbf{k}) - f(K)|\right) - \delta\right] \hat{c}^{\dagger}_{\mathbf{k},s} \hat{c}_{\mathbf{k},s'}$$

$$\boldsymbol{g}_{\mathrm{in}}(\mathbf{k}) = \left(0, 0, \sin k_{\mathrm{y}} - 2\cos\frac{\sqrt{3}}{2}k_{\mathrm{x}} \sin\frac{1}{2}k_{\mathrm{y}}\right)$$

$$\hat{H}_{\mathrm{ra}} = \sum_{\mathbf{k},s,s'} \alpha_{\mathrm{ra}} \boldsymbol{g}_{\mathrm{ra}}(\mathbf{k}) \cdot \boldsymbol{\sigma}_{s,s'} \hat{c}^{\dagger}_{\mathbf{k},s} \hat{c}_{\mathbf{k},s'}$$

$$\boldsymbol{g}_{\mathrm{ra}}(\mathbf{k}) = \left(-\sin k_{\mathrm{y}} - \cos\frac{\sqrt{3}}{2}k_{\mathrm{x}} \sin\frac{1}{2}k_{\mathrm{y}}, \sqrt{3}\sin\frac{\sqrt{3}}{2}k_{\mathrm{x}} \cos\frac{1}{2}k_{\mathrm{y}}, 0\right)$$

Spin splitを決める変数は４つ

Parameter　$(\alpha_{\mathrm{in}}, \alpha_{\mathrm{ra}}, x, \delta)$

パラメーターの決定

束縛条件

$$\frac{|\alpha_{\rm ra} g_{\rm ra}(k_{\rm F})|}{\left|\alpha_{\rm in} g_{\rm in}(k_{\rm F}) \tilde{f}^{(x,\delta)}(k_{\rm F})\right|} = 0.02$$

$$2\sqrt{[\alpha_{\rm ra} g_{\rm ra}(k_{\rm F})]^2 + \left[\alpha_{\rm in} g_{\rm in}(k_{\rm F}) \tilde{f}^{(x,\delta)}(k_{\rm F})\right]^2} = 13 \quad (meV)$$

$$2\sqrt{[\alpha_{\rm ra} g_{\rm ra}(K)]^2 + \left[\alpha_{\rm in} g_{\rm in}(K) \tilde{f}^{(x,\delta)}(K)\right]^2} = 3 \quad (meV)$$

$$\tilde{f}^{(x,\delta)}(\mathbf{k}) = \tanh\left(x|f(\mathbf{k}) - f(K)|\right) - \delta$$

Definition of $k_{\rm F}$:

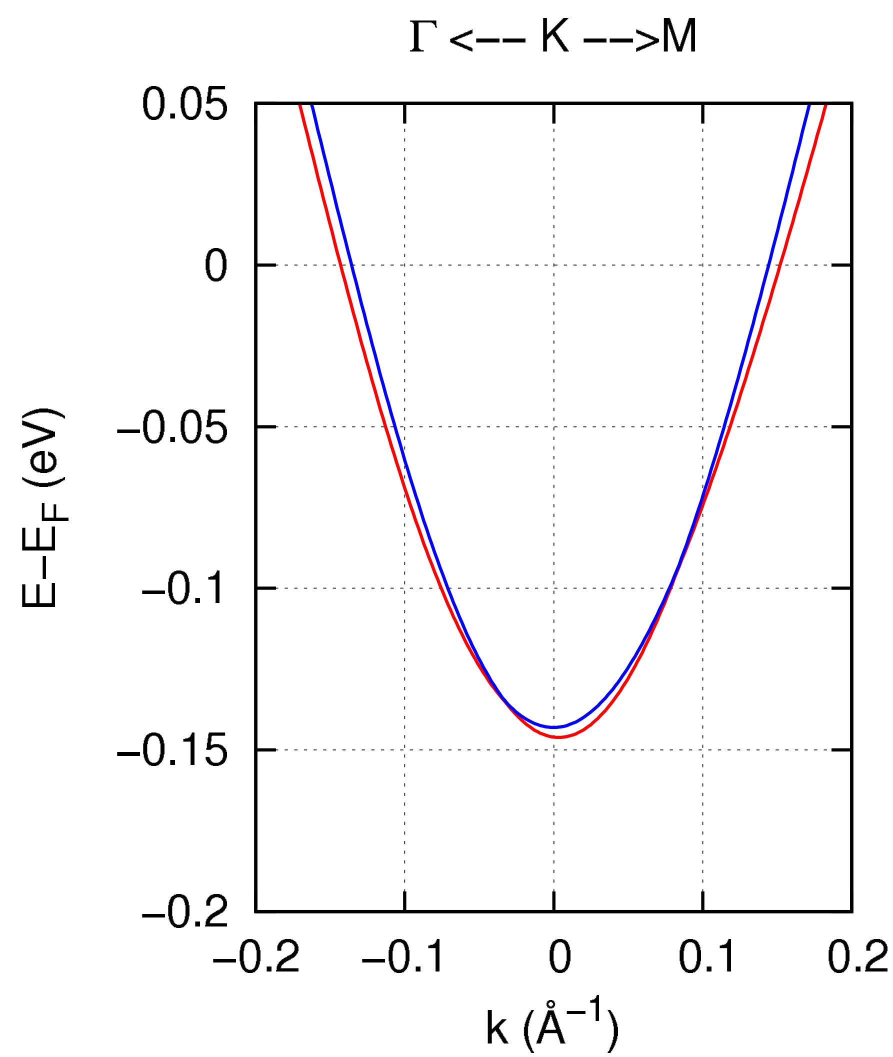
$$\frac{E_+(k_{\rm F}) + E_-(k_{\rm F})}{2} = 0$$

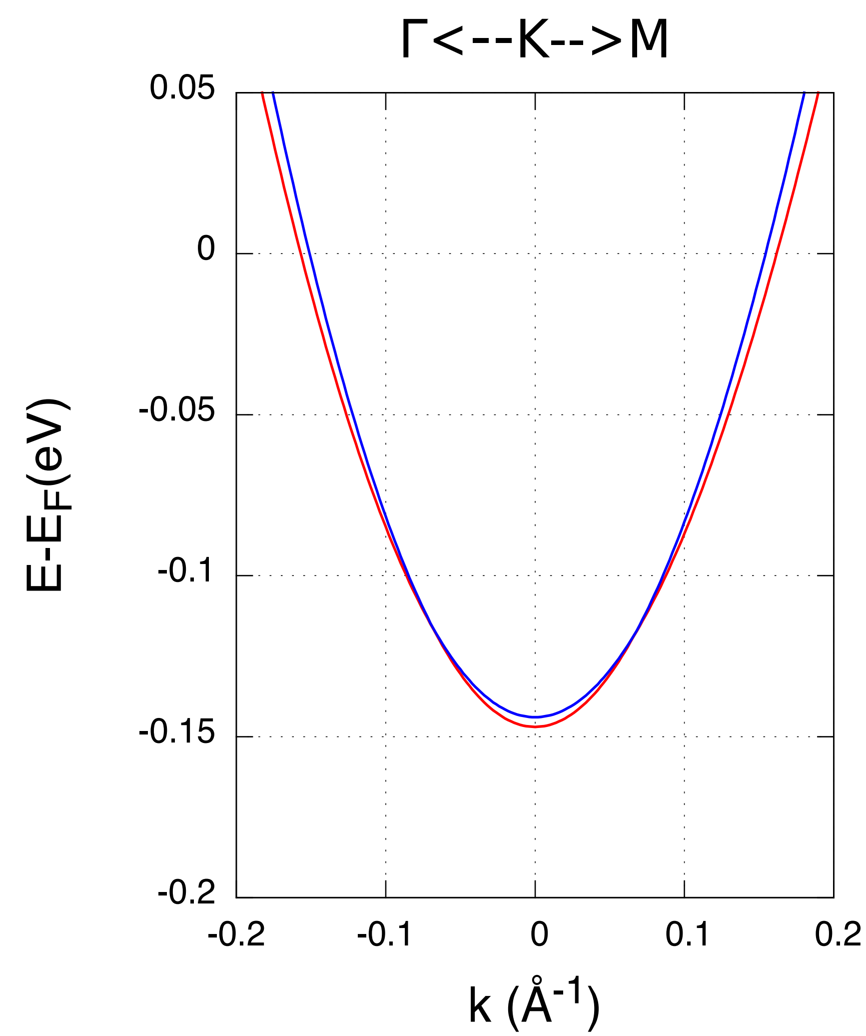
変数４つに対して束縛条件が３つ

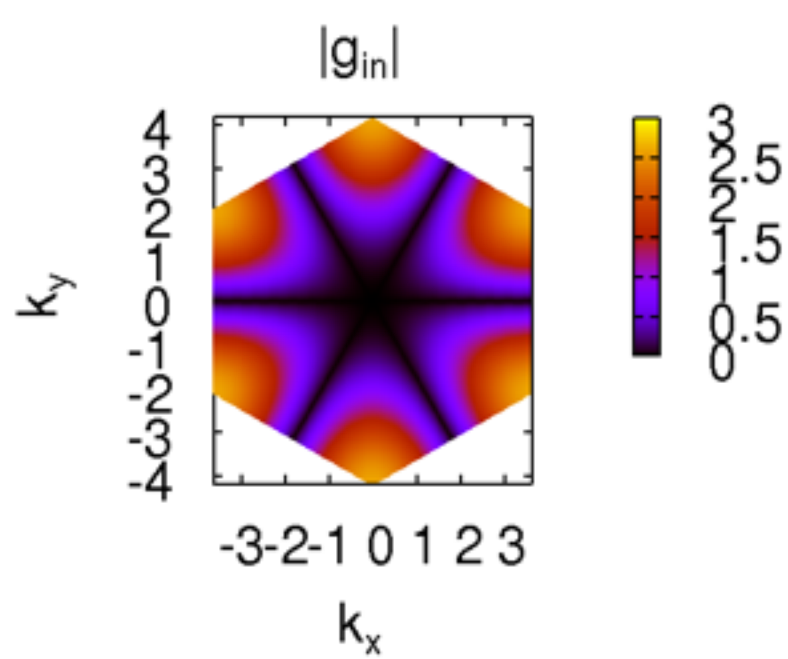
↓

変数を一つを決めれば他がユニークに決まる

Band calculation



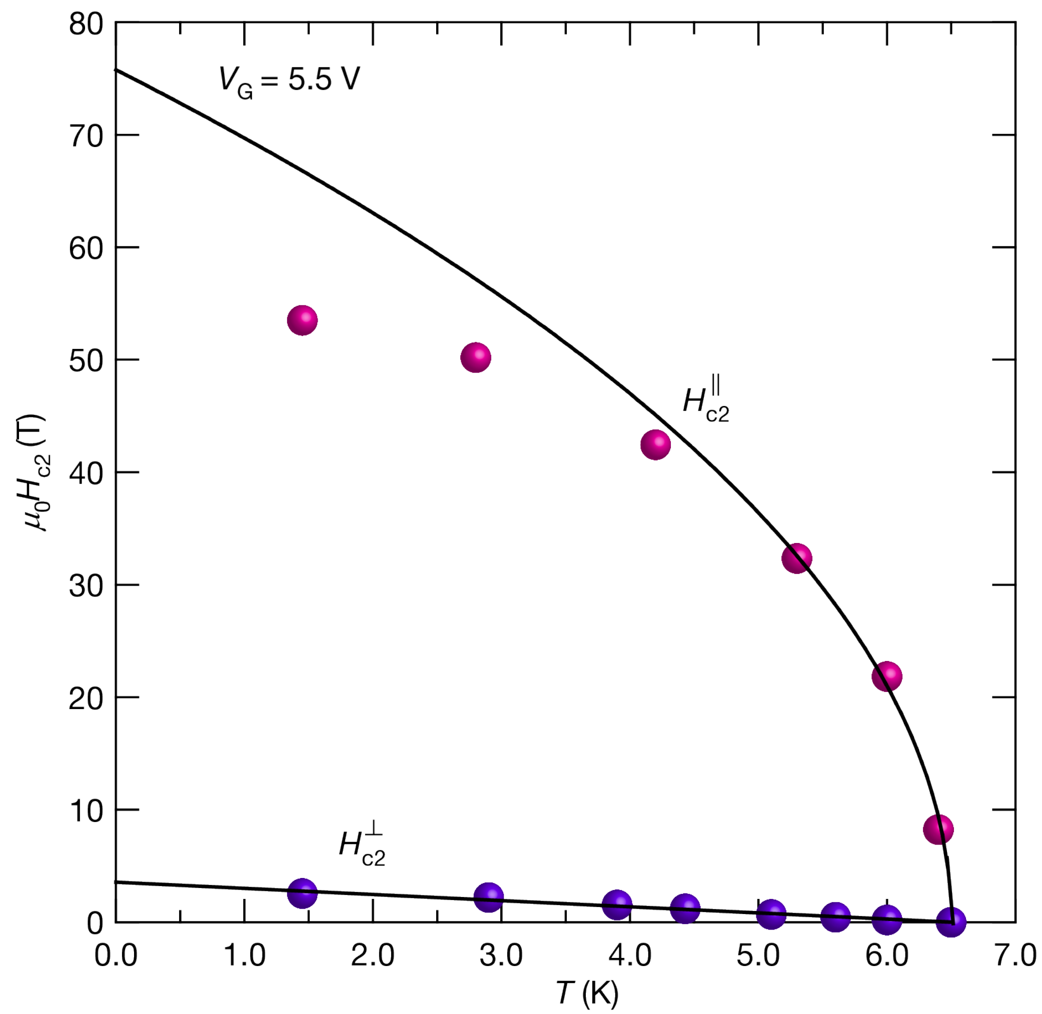




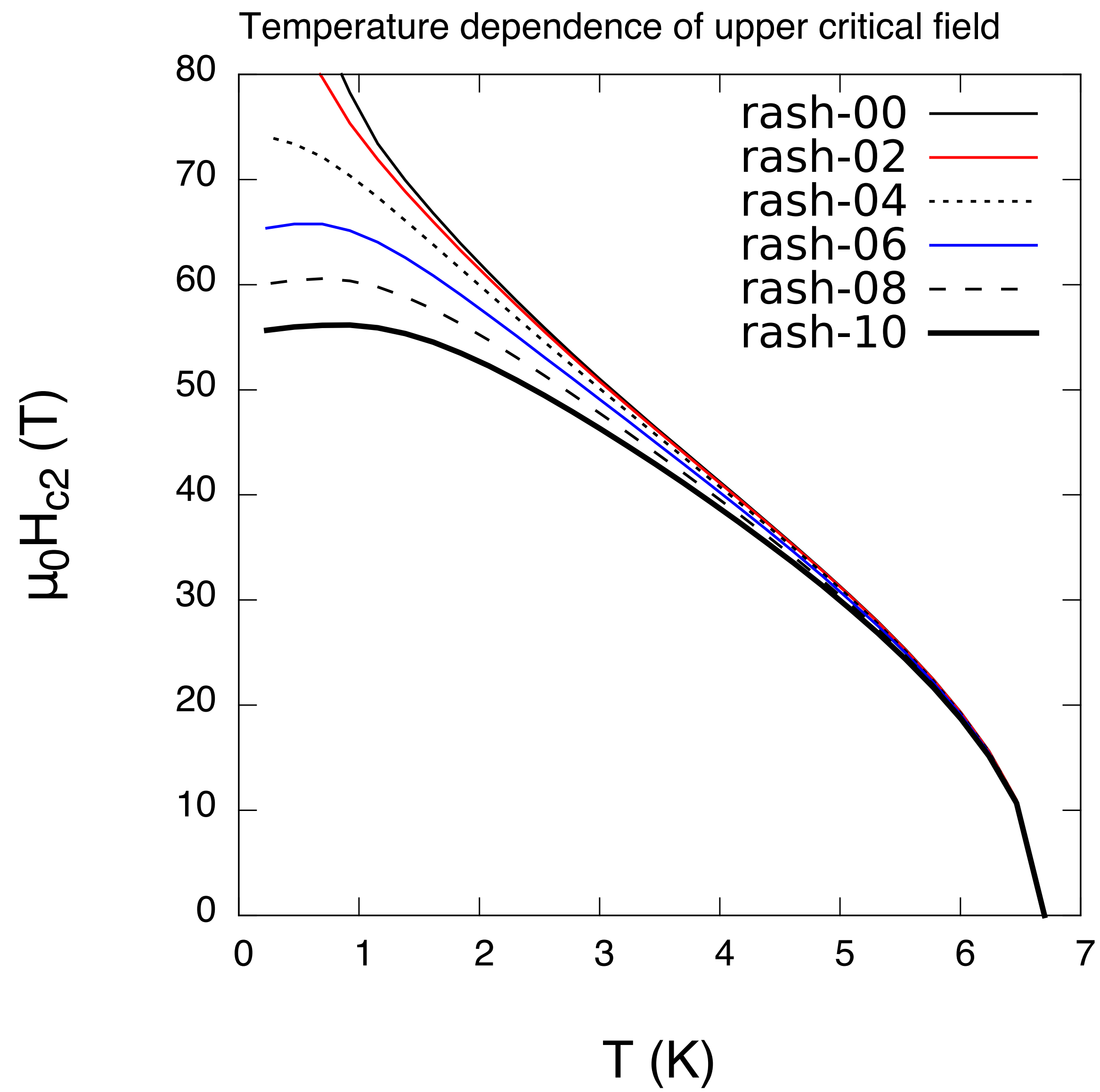
$$
\begin{aligned}
f(\mathbf{k}) &= \left| \sin k_{\mathrm{y}} - 2\cos\frac{\sqrt{3}}{2}k_{\mathrm{x}} \sin\frac{1}{2}k_{\mathrm{y}} \right| \\
&= |\boldsymbol{g}_{\mathrm{in}}(\mathbf{k})|
\end{aligned}
$$

実験との比較

実験

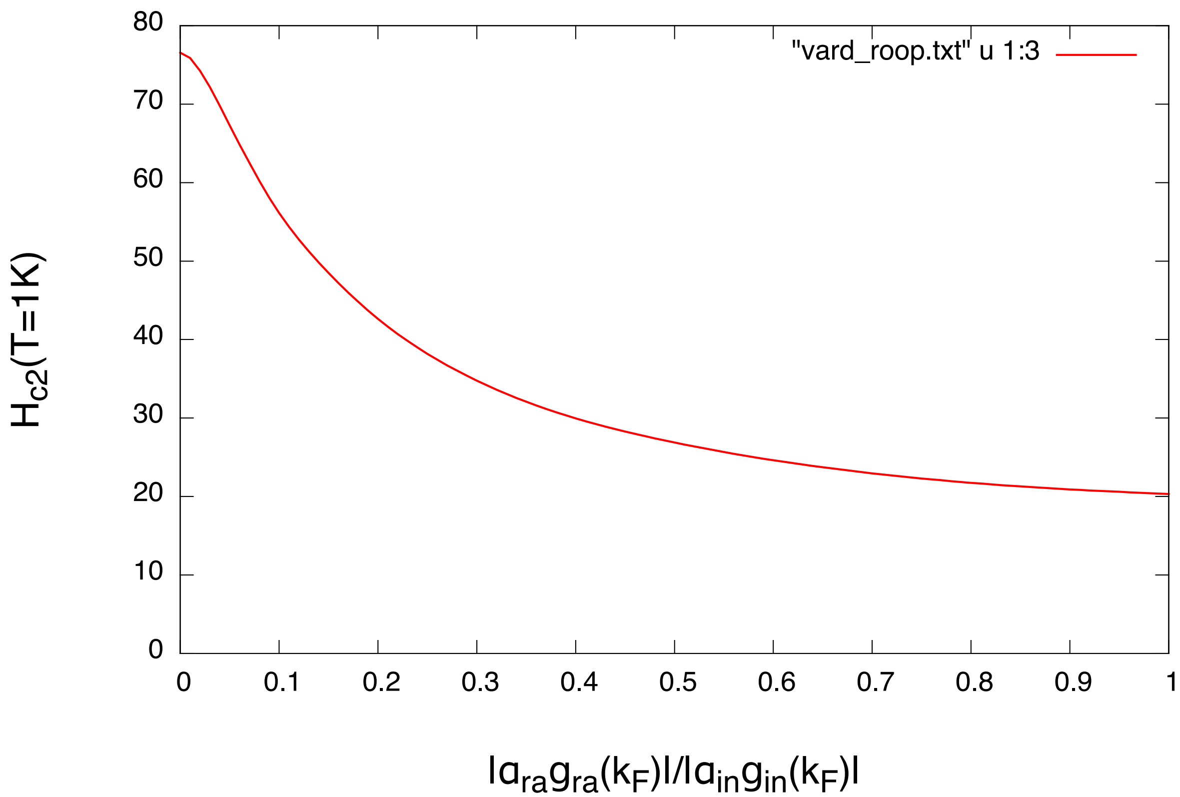


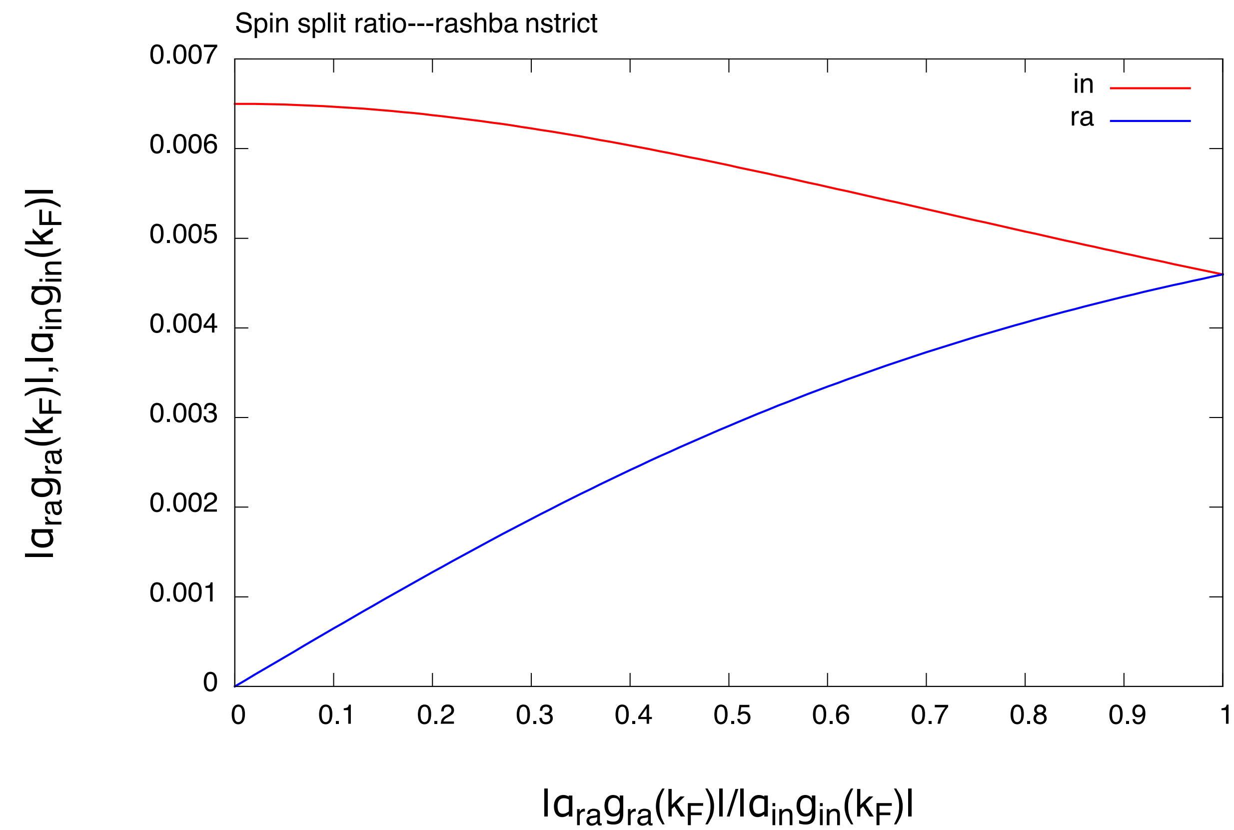
理論　$H \parallel [1,0,0]$



- Rashba型ASOCがInstinctASOCの１０％程度で実験とほぼ一致
- Rashba型ASOCがInstinctASOCの６％程度から低温高磁場領域でH_{c2}が温度に対してフラットになる

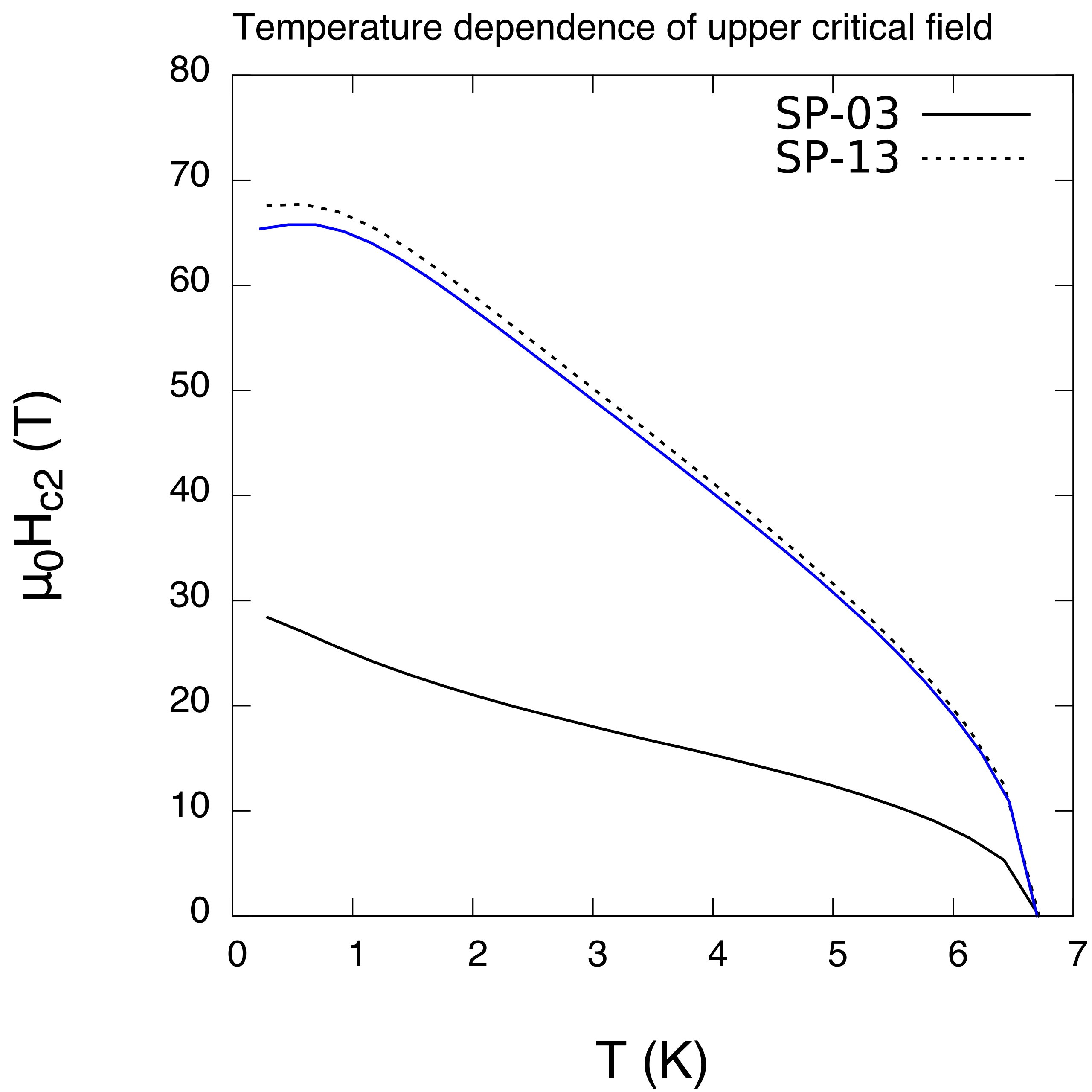
ASOCの比とH_{c2}

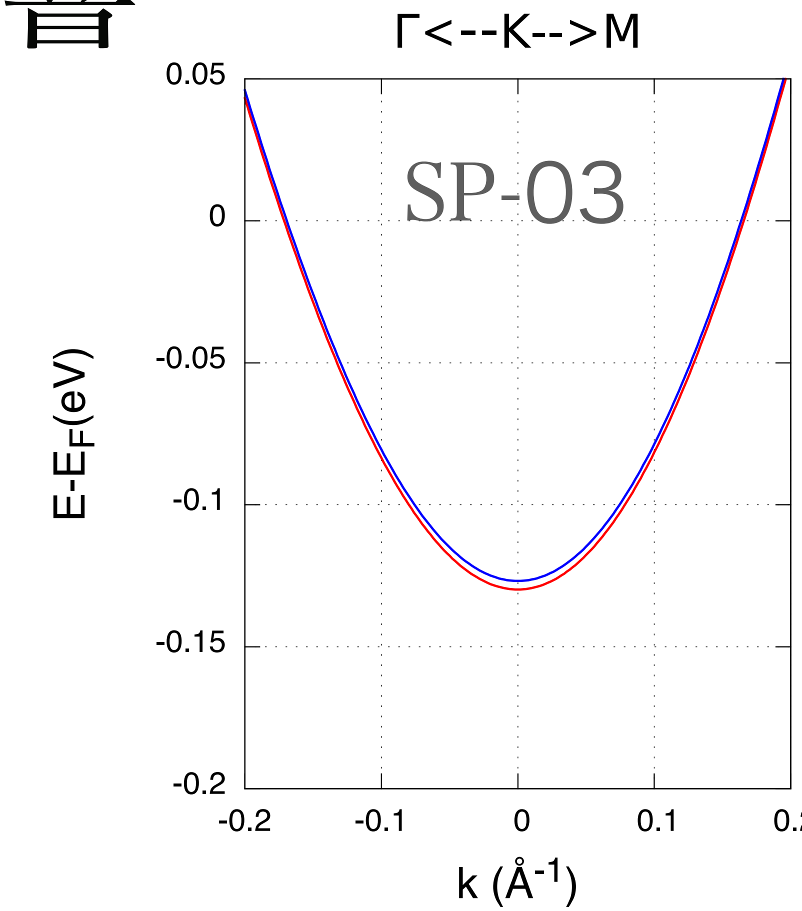


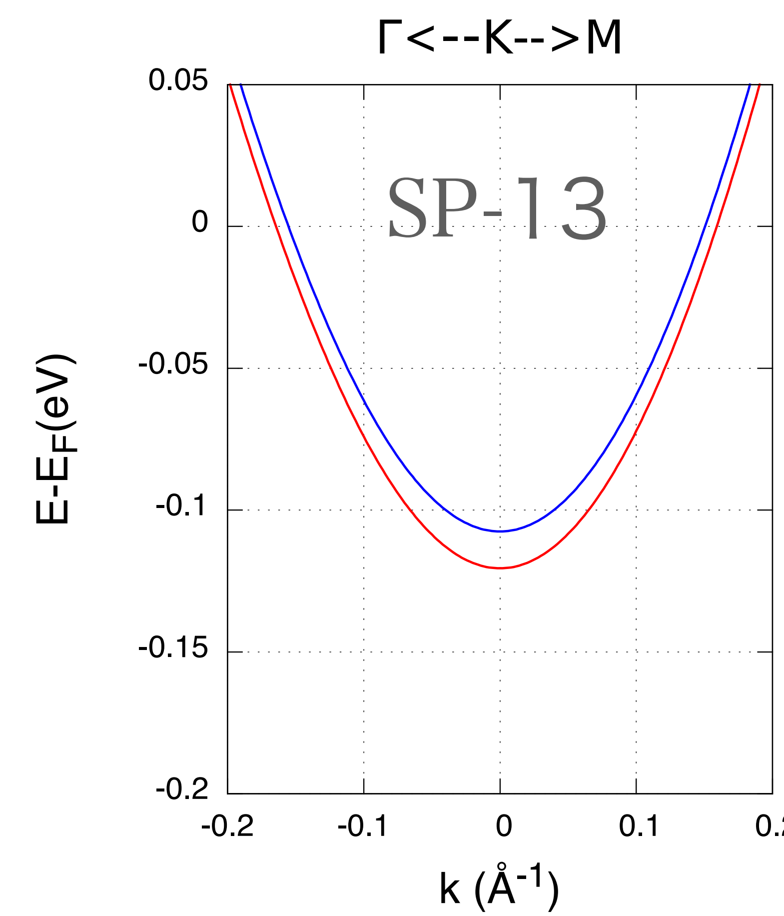


Rashba型ASOCによるSpin splitの割合が小さくてもH_{c2}は大きく減少する

バンドが変化する影響



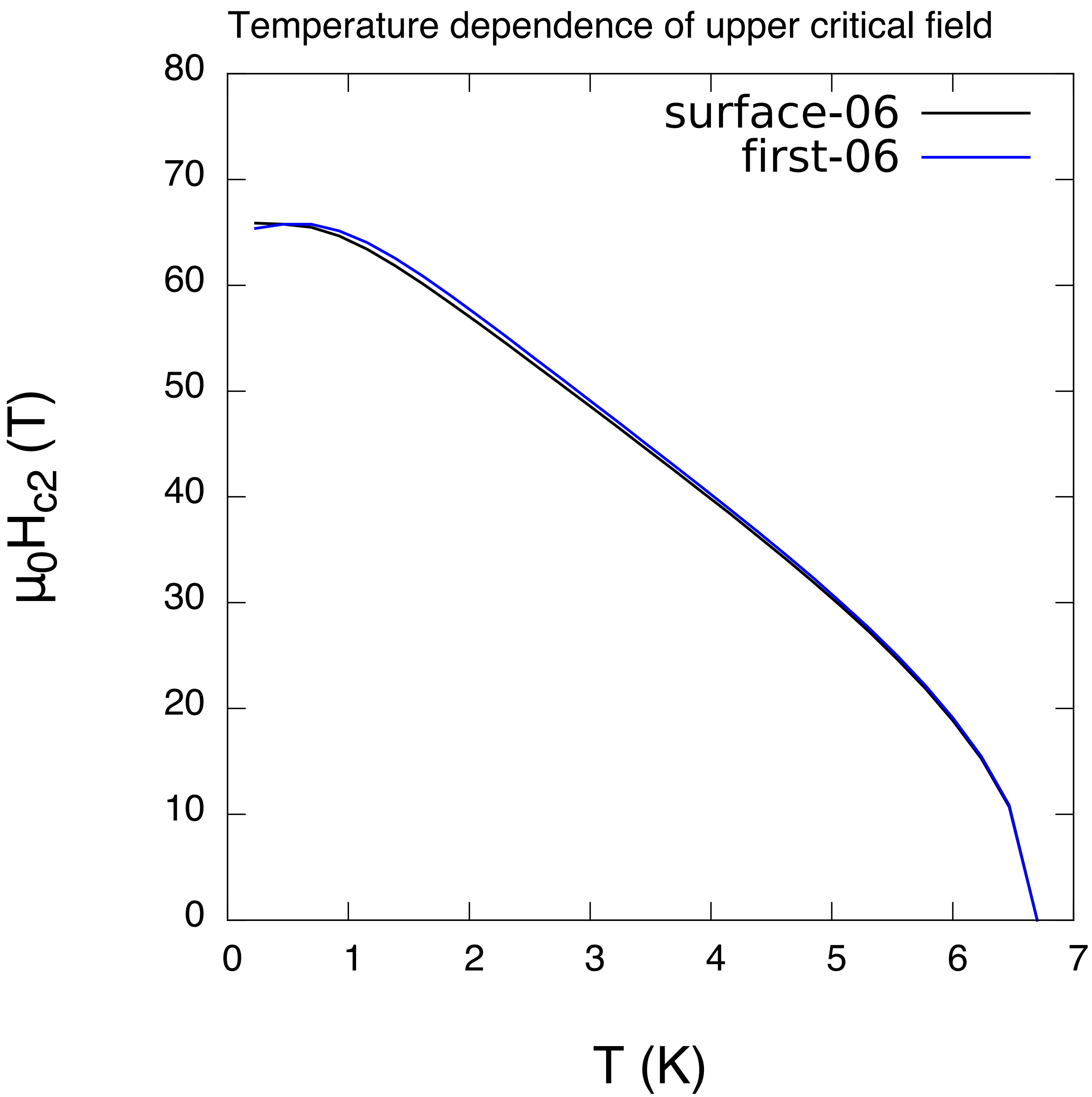




- 通常のmono-layerの場合と異なり
  Fermi levelでのspin splitが13meVあることが重要

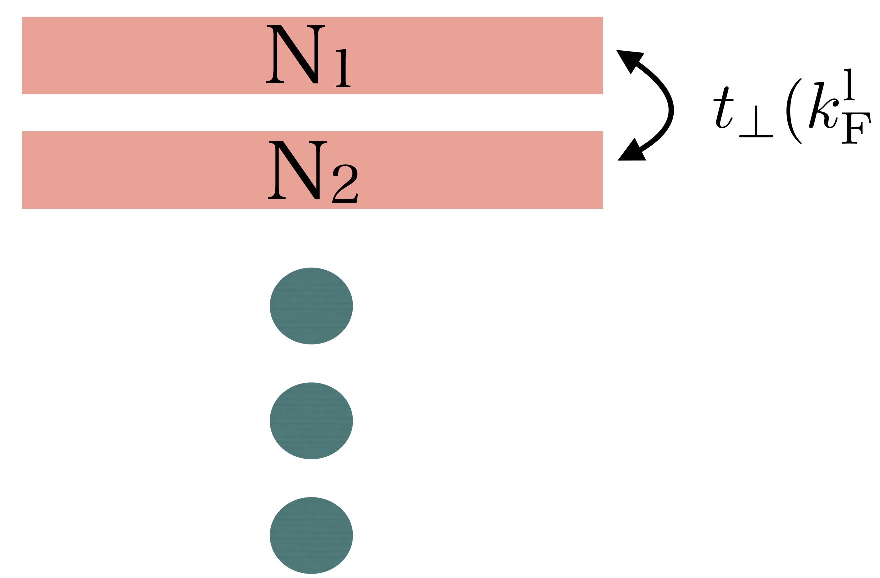
2 層目の影響

$$\frac{|\alpha_{\rm ra} g_{\rm ra}(k_{\rm F})|}{\left|\alpha_{\rm in} g_{\rm in}(k_{\rm F}) \tilde{f}^{(x,\delta)}(k_{\rm F})\right|} = 0.06$$



Surface

$N_1 \sim 7.7 \times 10^{13} cm^{-2}$
$N_2 \sim 1.2 \times 10^{13} cm^{-2}$

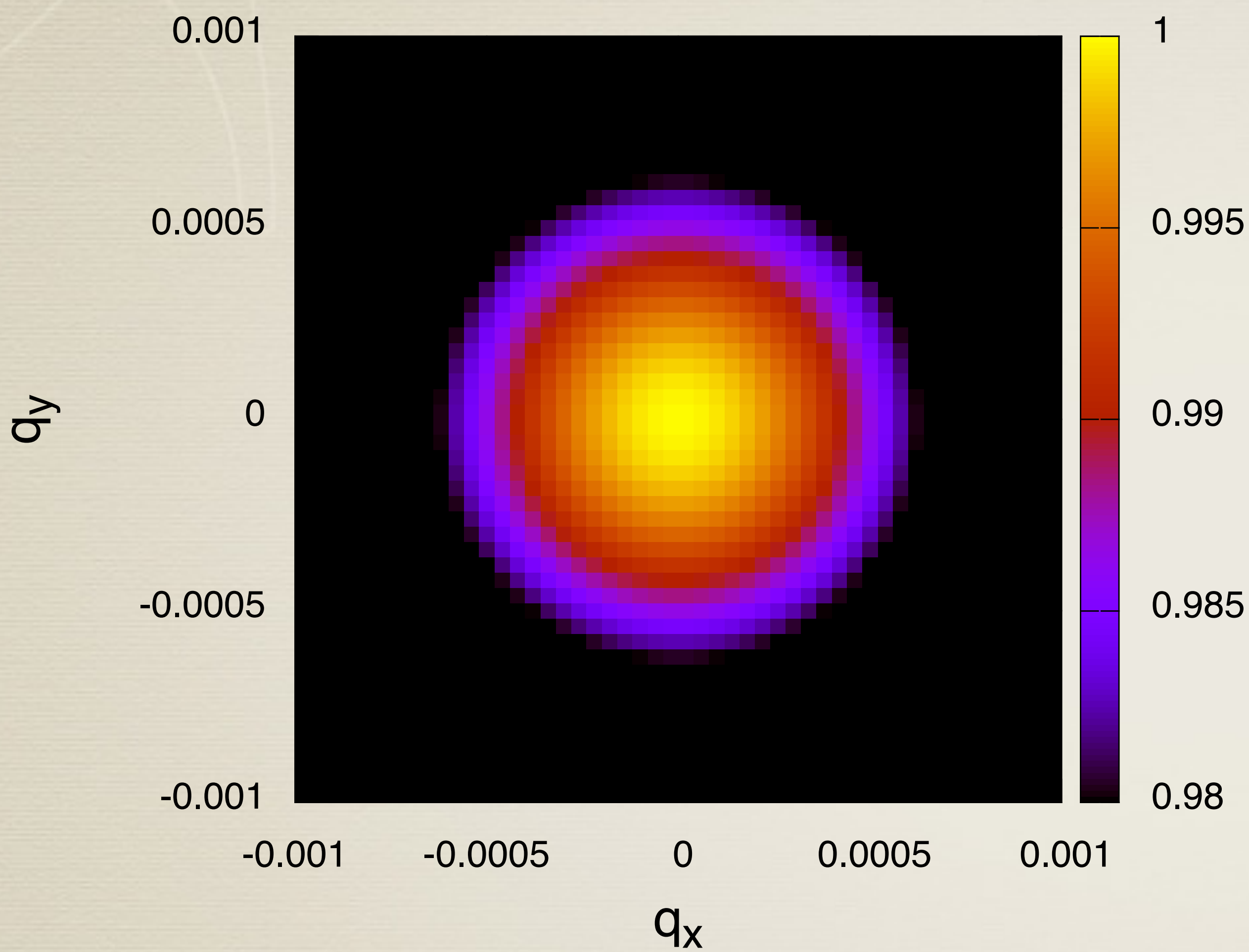


$t_{\perp}(k_{\rm F}^{\rm l}) \sim 6.5\ meV$

理論的にも 1 層目までの計算で十分であると考えられる

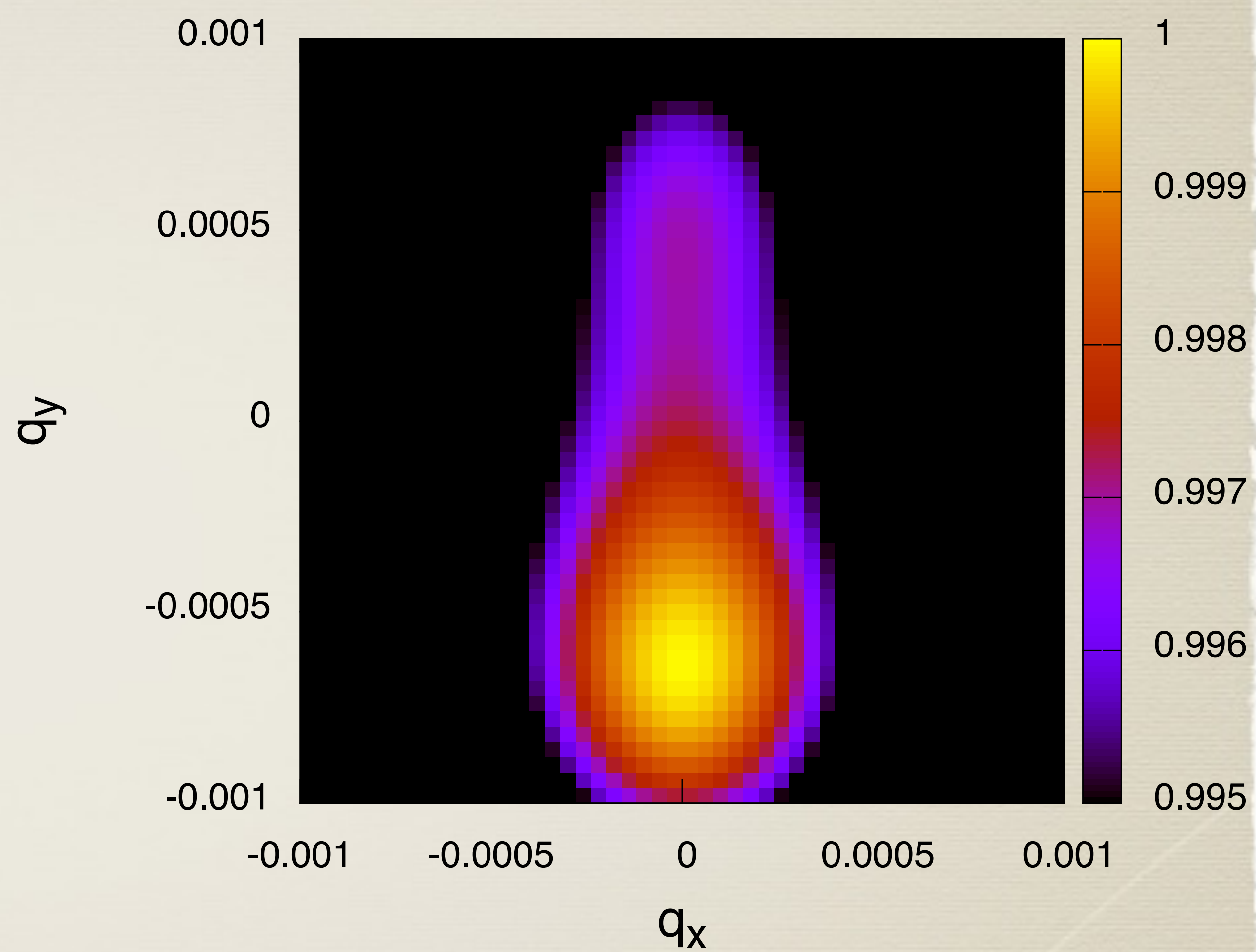
Helical 超伝導　　$T \sim 1K$

$$\frac{|\alpha_{\rm ra} g_{\rm ra}(k_{\rm F})|}{\left|\alpha_{\rm in} g_{\rm in}(k_{\rm F}) \tilde{f}^{(x,\delta)}(k_{\rm F})\right|} = 0.00$$



BCS超伝導

$$\frac{|\alpha_{\rm ra} g_{\rm ra}(k_{\rm F})|}{\left|\alpha_{\rm in} g_{\rm in}(k_{\rm F}) \tilde{f}^{(x,\delta)}(k_{\rm F})\right|} = 0.06$$



Helical超伝導