Effect of asymmetry on the bias dependence of perpendicular spin torque in magnetic tunnel junction (MTJ)

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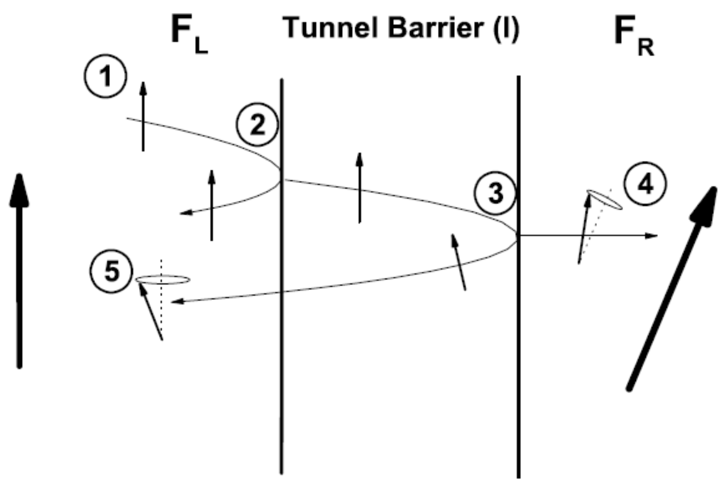
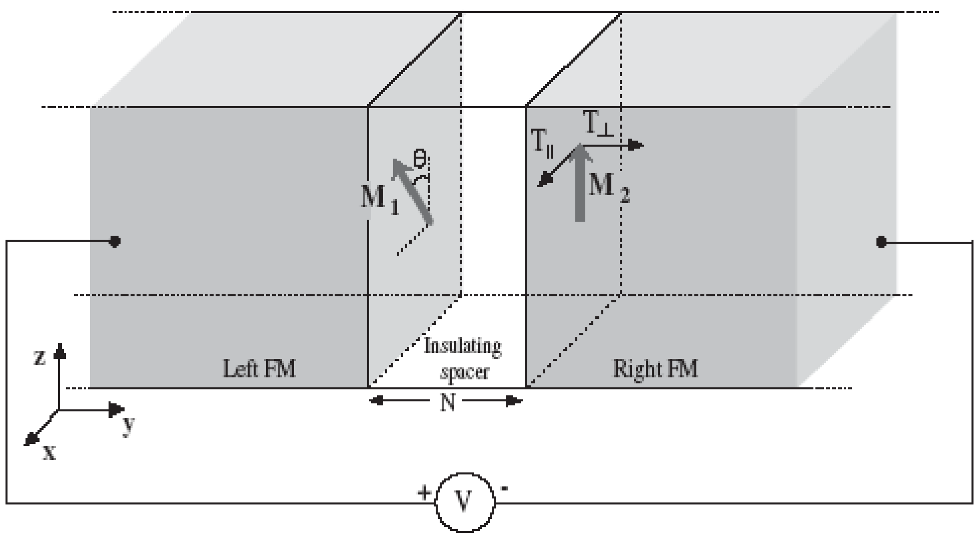


Non-collinear MTJ

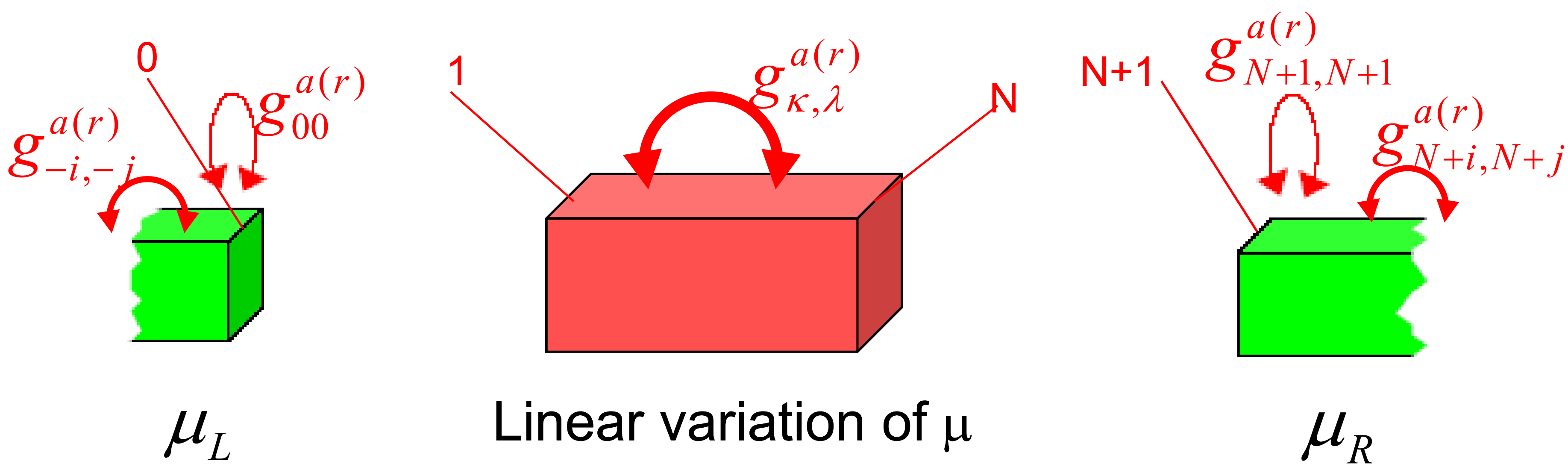


At CSUN, Dec19, 2008

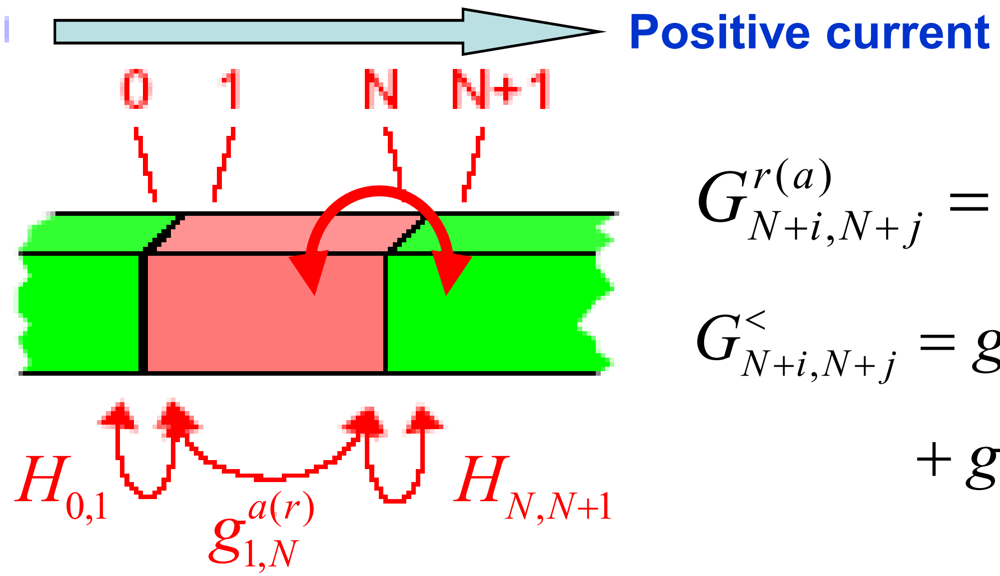
Calculation method

The tight-binding calculation method with the non-equilibrium Keldysh formalism is used to calculate spin torque in MTJ.

(1) Calculate surface and bulk Green's function for the **isolated semi-infinite** left and right electrods and the **isolated** barrier.



(2) Using Dyson equations to calculate coupled Green's functions, $G^{r(a)}_{N+i,N+j}$ and non-equilibrium Keldysh Green's function $G^{<}_{N+i,N+j}$.



$$G^{r(a)}_{N+i,N+j} = g^{r(a)}_{N+i,N+1} H_{N+1,N} G^{r(a)}_{N,N+j}$$

$$G^{<}_{N+i,N+j} = g^{<}_{N+i,N+j} + g^{r}_{N+i,N+1} H_{N+1,N} G^{<}_{N,N+j} + g^{<}_{N+i,N+1} H_{N+1,N} G^{a}_{N,N+j}$$

(3) **Average spin torque in the right FM electrode** can be calculated by

Integrate over all occupied states

$$T_{\perp} = \frac{H_{N,N+1}}{16\pi^3} \int \mathrm{Im}\{ G^{<\,\uparrow\downarrow}_{N+1,N} - G^{<\,\downarrow\uparrow}_{N+1,N} - G^{<\,\uparrow\downarrow}_{N,N+1} + G^{<\,\downarrow\uparrow}_{N,N+1} \}] dE dk_{\parallel}$$

Importance of integration of 2d BZ

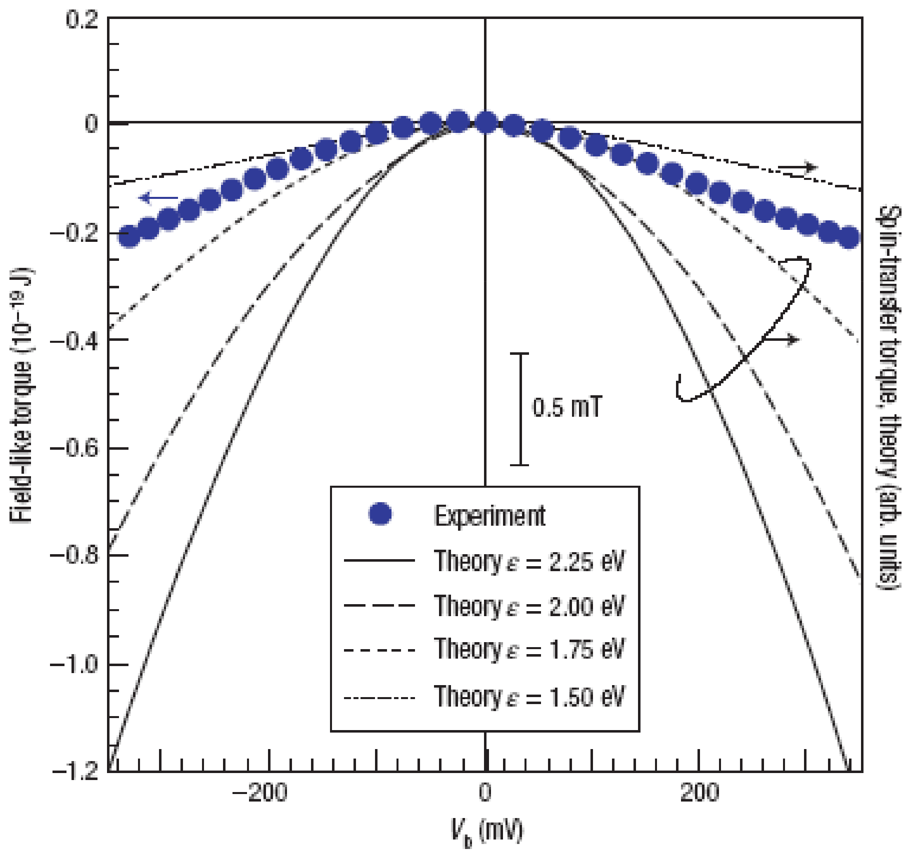
Bias dependence of perpendicular spin torque

One outstanding question which remains unresolved and controversial is the **" bias dependence of $T_\perp$ "**

- **Theoretically**, the bias dependence of $T_\perp$ is purely quadratic for symmetric and perfect MTJ.
- **Experimentally**, the inconsistence still exists.

Kubota et al. [1] used a layer structure $3Co_{60}Fe_{20}B_{20}$ /1MgO/ $2Co_{60}Fe_{20}B_{20}$.

$T_\perp$ has a **quadratic** bias dependence with **negative curvature**, which agrees with previous theoretical results by Theodonis et al. [2].

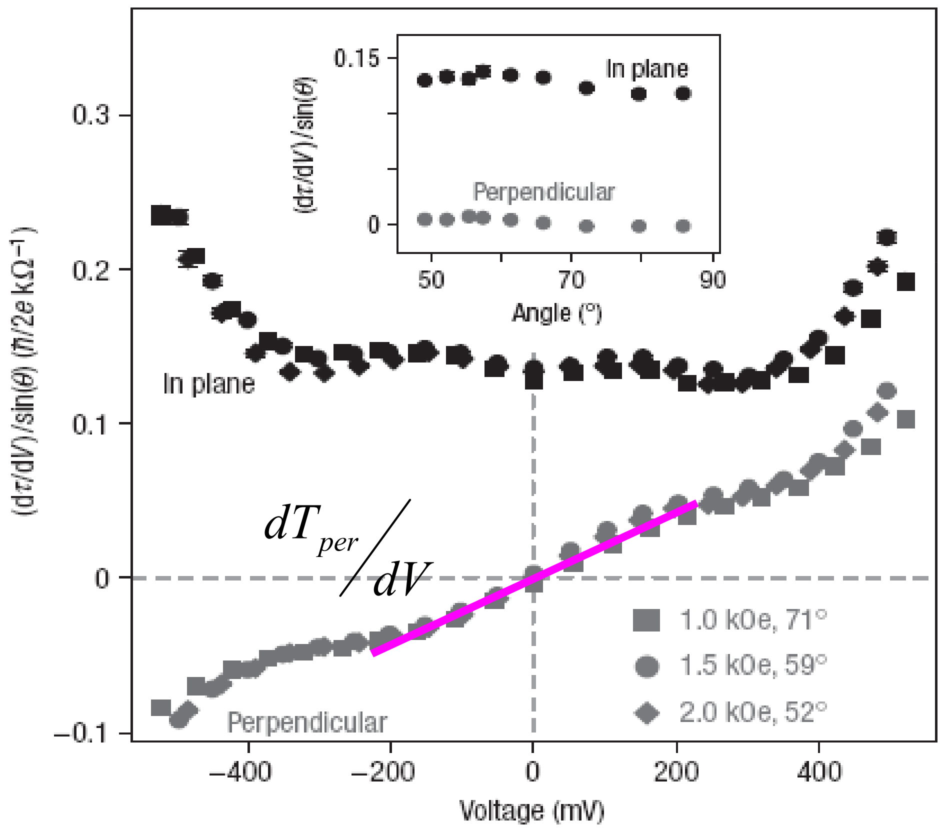


[1] Kubota et al., Nature Physics **4**, 37 (2008).
[2] Theodonis et al. Phys. Rev. Lett **97**, 237205 (2006)

Sankey et al. [3] used a layer structure $3Co_{60}Fe_{20}B_{20}$ /1.5MgO/ $2.5Co_{60}Fe_{20}B_{20}$.

dT_{per}/dV has a nearly linear bias dependence with positive slope for small bias.

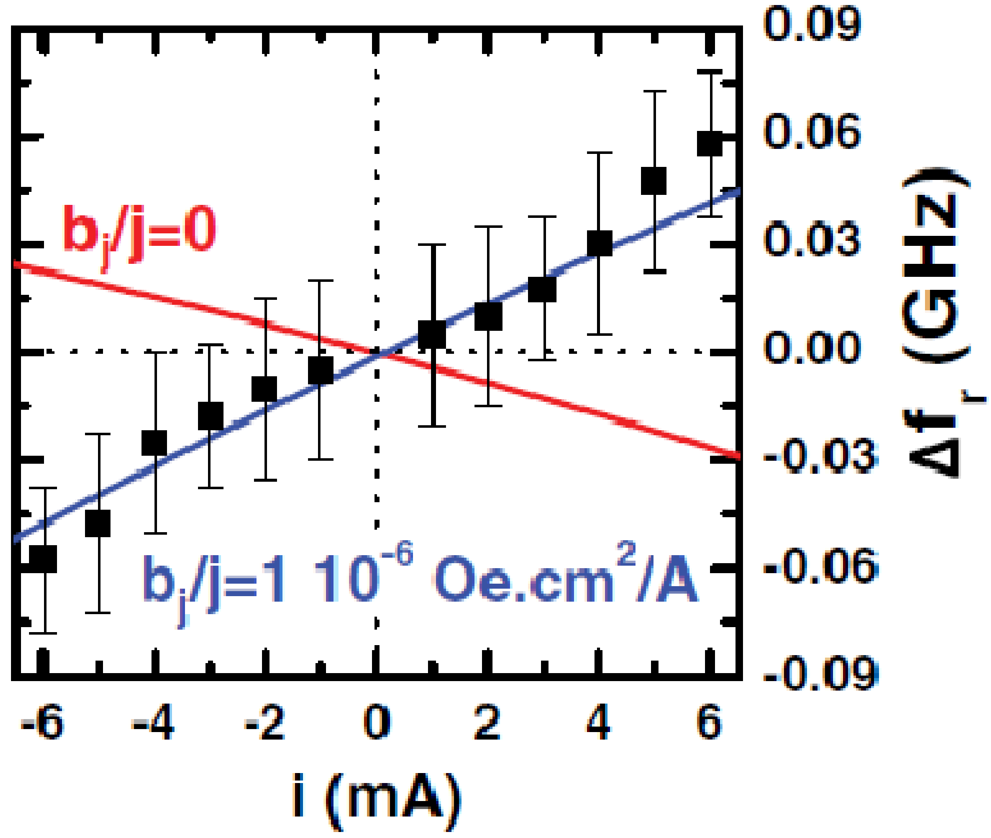
$T_{\perp}$ has **quadratic** bias dependence with **positive curvature** for small bias.



[3] Sankey et al., Nature Physics **4**, 67 (2008).

Petit et al. [4] used a layer structure $CoFe_{(2.5)} / Al_2O_{3(0.7)} / CoFe_{(1)}$.

They suggest that **linear bias dependence** with positive slope of $T_\perp$ has to be taken into account for MTJ.



[4] Petit et al., Phys. Rev. Lett **98**, 077203 (2007).

The discrepancy in these experimental results may be due to :

- Asymmetric left and right electrodes --- Asymmetric MTJ
- Disorder in the barrier or at barrier/FM interface

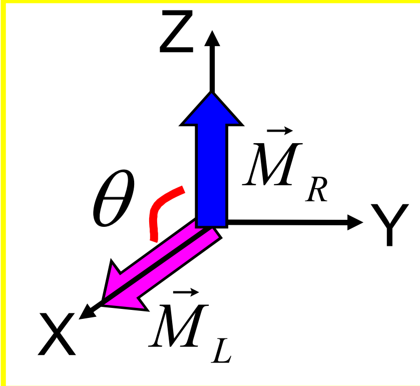
  --- Disordered MTJ (In progress !!)

In this study,

- Find the underlying mechanism responsible for the bias dependence of $T_\perp$ (interlayer exchange coupling, J).
- Explain the discrepancy in previous experimental results.
- Understand how to control the bias dependence of $T_\perp$.

For **non-collinear** MTJ, the exact expression of $T_\perp$ is

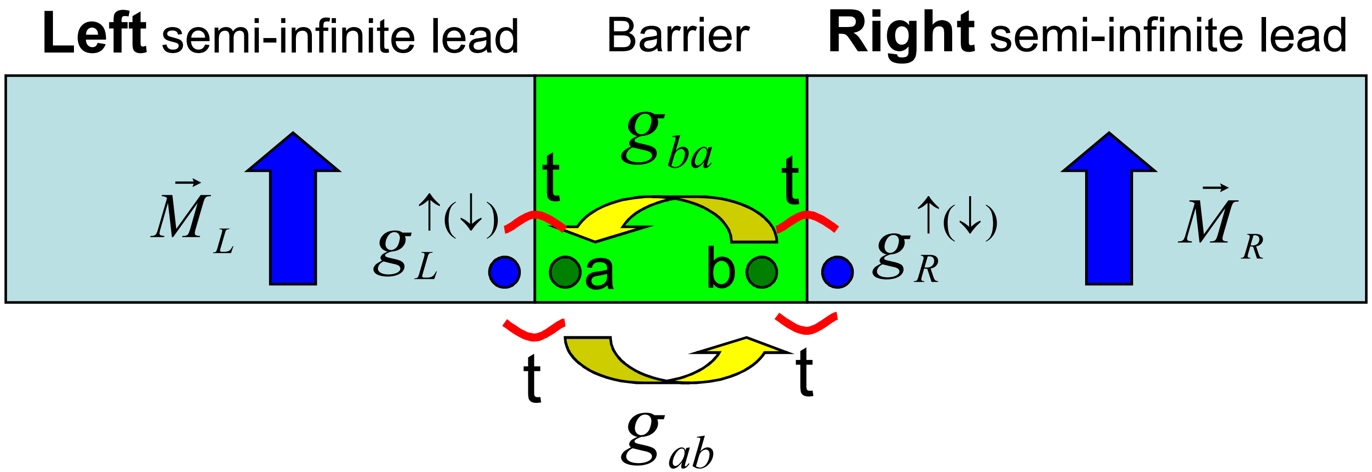
$$T_\perp(\boxed{\theta}) = \frac{t}{16\pi^3}\int \mathrm{Im}\underbrace{\{G_{0,-1}^{<\,\uparrow\downarrow} - G_{0,-1}^{<\,\downarrow\uparrow} - G_{-1,0}^{<\,\uparrow\downarrow} - G_{-1,0}^{<\,\downarrow\uparrow}\}}_{\theta \text{ dependence}} dEdk_{\parallel}$$



$T_\perp$ also can be expressed by

$$= \frac{\boxed{\sin\theta}}{8\pi^3|D|^2}\underbrace{\int t^4 \cdot g_{ba}\cdot g_{ab}\cdot[f_L\cdot \mathrm{Im}\{(g_L^{\uparrow}-g_L^{\downarrow})\cdot(g_R^{\uparrow}-g_R^{\downarrow})\} + (f_R - f_L)\cdot \mathrm{Re}\{(g_L^{\uparrow}-g_L^{\downarrow})\}\cdot \mathrm{Im}\{(g_R^{\uparrow}-g_R^{\downarrow})\}]dEdk_{\parallel}}_{\text{Collinear } (\theta \text{ independent})}$$

Collinear MTJ



$\times \sin\theta$

Perpendicular spin torque : $T_\perp = -\frac{\partial E_{IEC}}{\partial \theta} = -J \boxed{\sin\theta}$

$$T_\perp(\boxed{\theta}) = \frac{\boxed{\sin\theta} \cdot t^4}{8\pi^3 |D|^2} \cdot \int g_{ba} \cdot g_{ab} \cdot [\underline{f_L \cdot \mathrm{Im}\{(g_L^\uparrow - g_L^\downarrow)\cdot(g_R^\uparrow - g_R^\downarrow)}\}$$

$$+ \underline{(f_R - f_L)\cdot \mathrm{Re}\{(g_L^\uparrow - g_L^\downarrow)\}\cdot \mathrm{Im}\{(g_R^\uparrow - g_R^\downarrow)}\}]dEdk_{\|}$$

$$= -\boxed{\sin\theta} \cdot [J_{FM}^{\uparrow\uparrow} - J_{FM}^{\downarrow\uparrow} - J_{FM}^{\uparrow\downarrow} + J_{FM}^{\downarrow\downarrow}]$$

$|D|^2 \sim 1$ for thick barrier

with collinear (FM) configuration

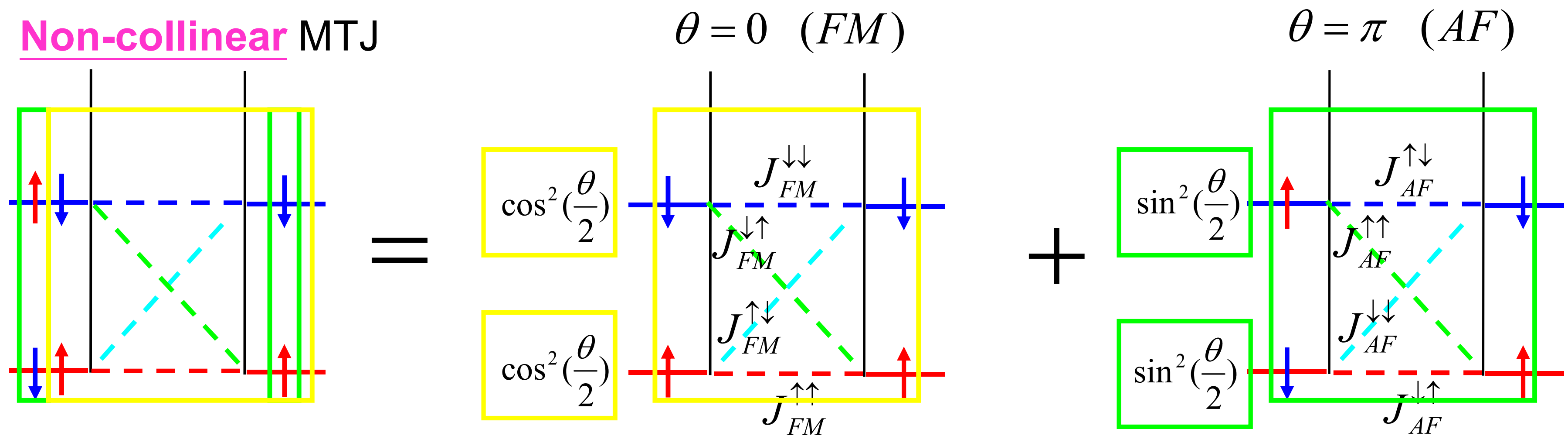
$$-J_{FM}^{\uparrow\uparrow} = \int C(E)\cdot[f_L \cdot \mathrm{Im}\{g_L^\uparrow \cdot g_R^\uparrow\} + (f_R - f_L)\cdot \mathrm{Re}\{g_L^\uparrow\}\cdot \mathrm{Im}\{(g_R^\uparrow\}]dEdk_{\|}$$

$$-J_{FM}^{\downarrow\uparrow} = \int C(E)\cdot[f_L \cdot \mathrm{Im}\{g_L^\downarrow \cdot g_R^\uparrow\} + (f_R - f_L)\cdot \mathrm{Re}\{g_L^\downarrow\}\cdot \mathrm{Im}\{(g_R^\uparrow\}]dEdk_{\|}$$

$$-J_{FM}^{\uparrow\downarrow} = \int C(E)\cdot[f_L \cdot \mathrm{Im}\{g_L^\uparrow \cdot g_R^\downarrow\} + (f_R - f_L)\cdot \mathrm{Re}\{g_L^\uparrow\}\cdot \mathrm{Im}\{(g_R^\downarrow\}]dEdk_{\|}$$

$$-J_{FM}^{\downarrow\downarrow} = \int C(E)\cdot[f_L \cdot \mathrm{Im}\{g_L^\downarrow \cdot g_R^\downarrow\} + (f_R - f_L)\cdot \mathrm{Re}\{g_L^\downarrow\}\cdot \mathrm{Im}\{(g_R^\downarrow\}]dEdk_{\|}$$

Non-zero at V=0



$$|\uparrow\rangle_L = \cos\theta/2\,|\uparrow\rangle_R + \sin\theta/2\,|\downarrow\rangle_R \qquad |\downarrow\rangle_L = -\sin\theta/2\,|\uparrow\rangle_R + \cos\theta/2\,|\downarrow\rangle_R$$

$$\Pr obability : P^{\sigma,\sigma'} = \left|\langle \sigma_L | \sigma'_R \rangle\right|$$

$$\begin{aligned}
E_{xc}(\theta) &= -J(\theta)\cdot\cos(\theta) \\
&= -[\boxed{\cos^2(\tfrac{\theta}{2})\cdot(J_{FM}^{\uparrow\uparrow} - J_{FM}^{\uparrow\downarrow} - J_{FM}^{\downarrow\uparrow} + J_{FM}^{\downarrow\downarrow})} + (\sin^2(\tfrac{\theta}{2})\cdot\boxed{(-J_{AF}^{\downarrow\uparrow} + J_{AF}^{\downarrow\downarrow} - J_{AF}^{\uparrow\downarrow} + J_{AF}^{\uparrow\uparrow})]} \\
&= -[\cos^2(\tfrac{\theta}{2})\cdot(J_{FM}^{\uparrow\uparrow} - J_{FM}^{\uparrow\downarrow} - J_{FM}^{\downarrow\uparrow} + J_{FM}^{\downarrow\downarrow}) + (\sin^2(\tfrac{\theta}{2})\cdot(-J_{FM}^{\uparrow\uparrow} + J_{FM}^{\downarrow\uparrow} - J_{FM}^{\uparrow\downarrow} + J_{AF}^{\uparrow\uparrow})] \\
&= -[\cos^2(\tfrac{\theta}{2}) - \sin^2(\tfrac{\theta}{2})]\cdot[J_{FM}^{\uparrow\uparrow} - J_{FM}^{\uparrow\downarrow} - J_{FM}^{\downarrow\uparrow} + J_{FM}^{\downarrow\downarrow}] \\
&= -[J_{FM}^{\uparrow\uparrow} - J_{FM}^{\uparrow\downarrow} - J_{FM}^{\downarrow\uparrow} + J_{FM}^{\downarrow\downarrow}]\cdot\cos(\theta)
\end{aligned}$$

Non-collinear

$$T_\perp(\theta) = -\frac{\partial E_{xc}(\theta)}{\partial\theta} = -J(\theta)\cdot\sin\theta = -\underbrace{\boxed{[J_{FM}^{\uparrow\uparrow} - J_{AF}^{\uparrow\uparrow} + J_{FM}^{\downarrow\downarrow} - J_{AF}^{\downarrow\downarrow}]}}_{\text{FM configuration}}\cdot\boxed{\sin\theta}$$

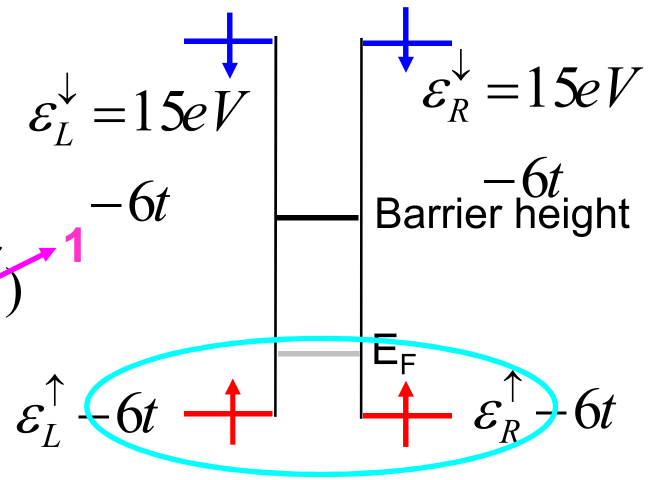
For **one-band symmetric MTJ** with θ=π/2 :

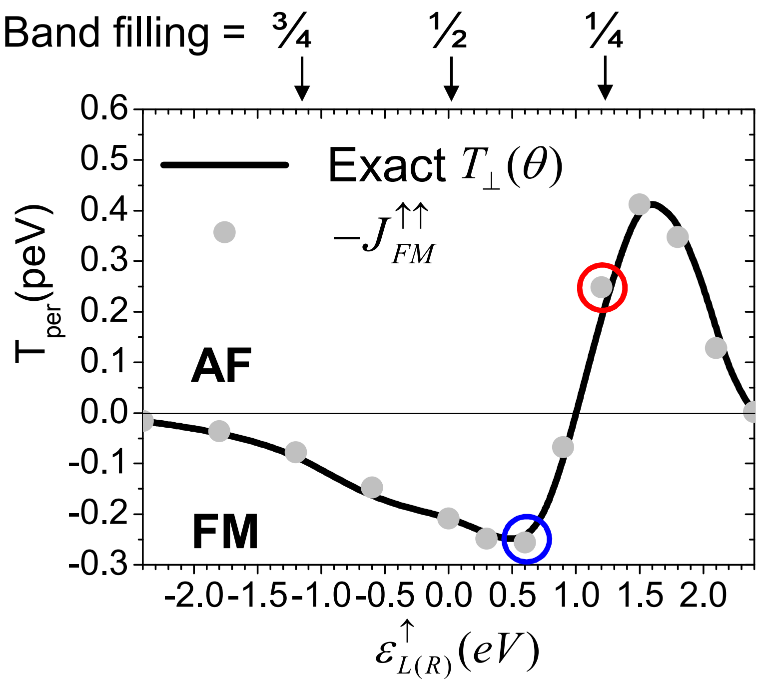
(1) At zero bias

FM configuration

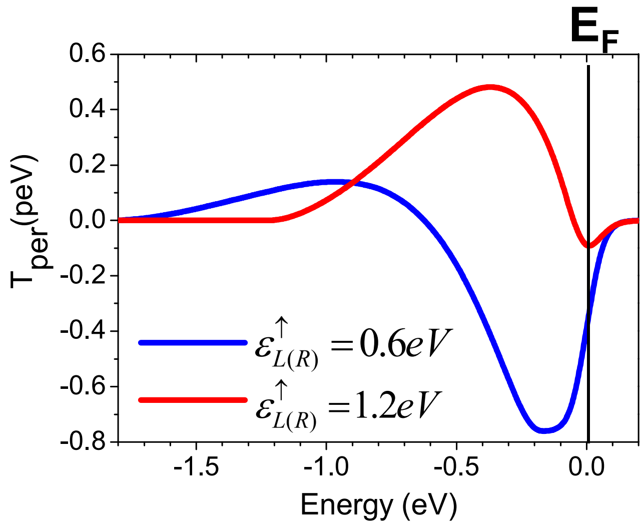
$$T_{\perp}(\pi/2) = \frac{t^4}{8\pi^3}\int g_{ba}\cdot g_{ab}\cdot f_L \,\mathrm{Im}\boxed{\{g_L^{\uparrow}\cdot g_R^{\uparrow}\}}dEdk_{\parallel}\cdot \cancelto{1}{\sin(\pi/2)}$$

$$= -J_{FM}^{\uparrow\uparrow}$$

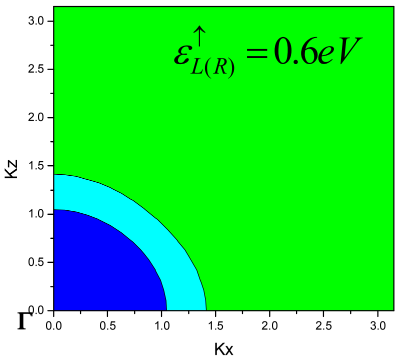


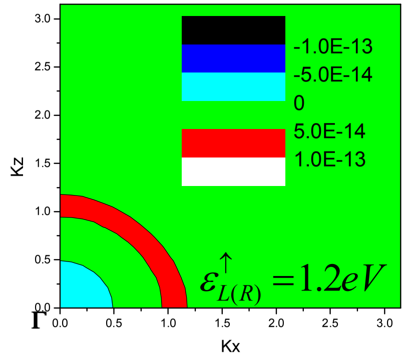


$\int dk_{\parallel}$



$\int_{Occ} dE$



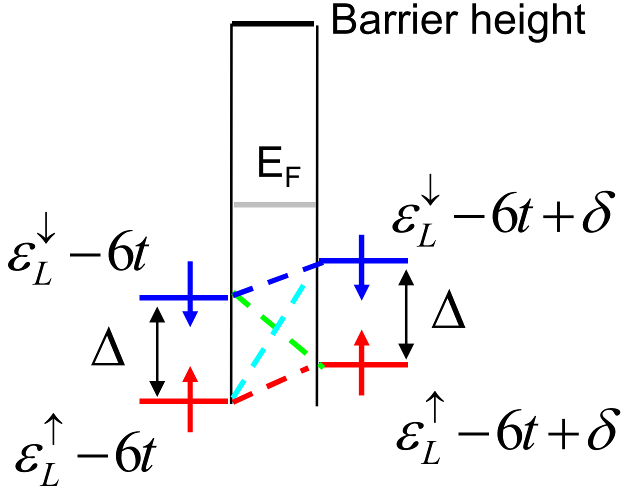


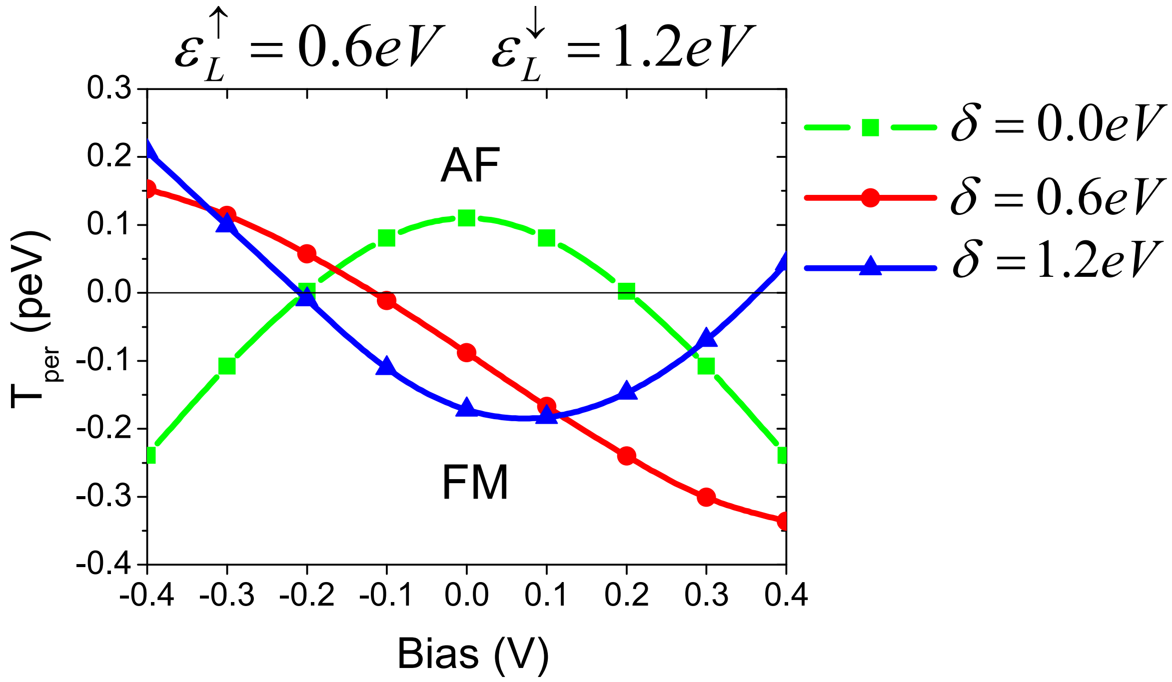
For **two-band MTJ** with θ=π/2 :

$$T_\perp(\pi/2) = \frac{t^4}{8\pi^3}\int g_{ba}\cdot g_{ab}\cdot[f_L\cdot \mathrm{Im}\{(g_L^\uparrow - g_L^\downarrow)\cdot(g_R^\uparrow - g_R^\downarrow)\} \quad \times \cancel{\sin(\pi/2)}\ 1$$

$$+(f_R - f_L)\cdot \mathrm{Re}\{(g_L^\uparrow - g_L^\downarrow)\}\cdot \mathrm{Im}\{(g_R^\uparrow - g_R^\downarrow)\}]dEdk_\parallel$$

$$= -[J_{FM}^{\uparrow\uparrow} - J_{FM}^{\downarrow\uparrow} - J_{FM}^{\uparrow\downarrow} + J_{FM}^{\downarrow\downarrow}]$$

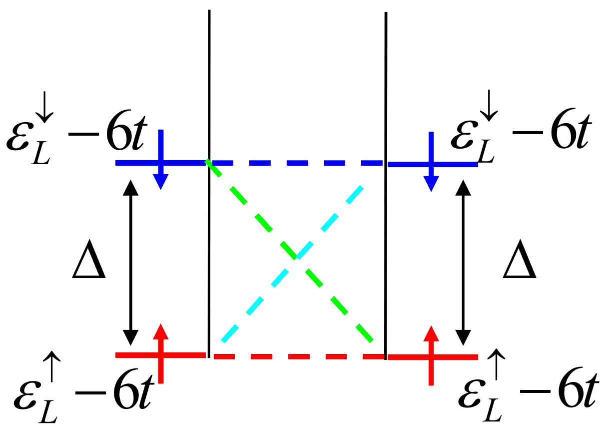




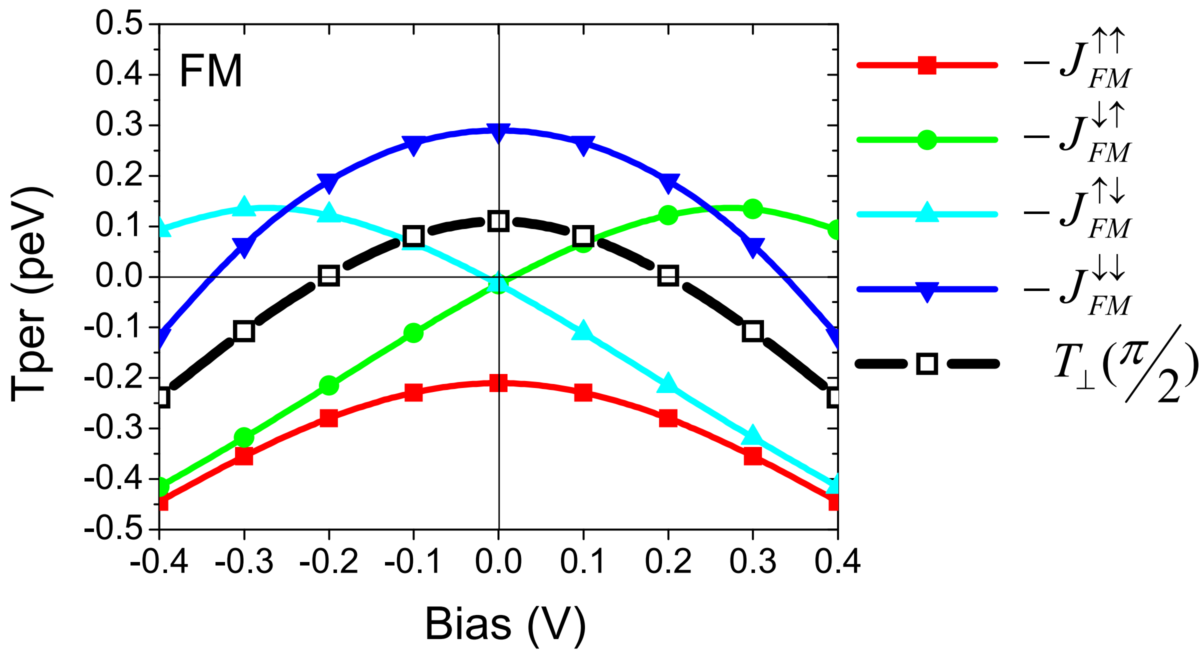
- The bias dependence of $T_\perp$ changes significantly with δ.
- $T_\perp$ can change sign with the bias, which means that one can control the magnetic configuration with bias even in the absent of external magnetic field.

$\varepsilon^{\uparrow}_{L(R)} = 0.6eV \quad \varepsilon^{\downarrow}_{L(R)} = 1.2eV \quad \delta = 0.0eV$ **(Symmetric two-band MTJ)**

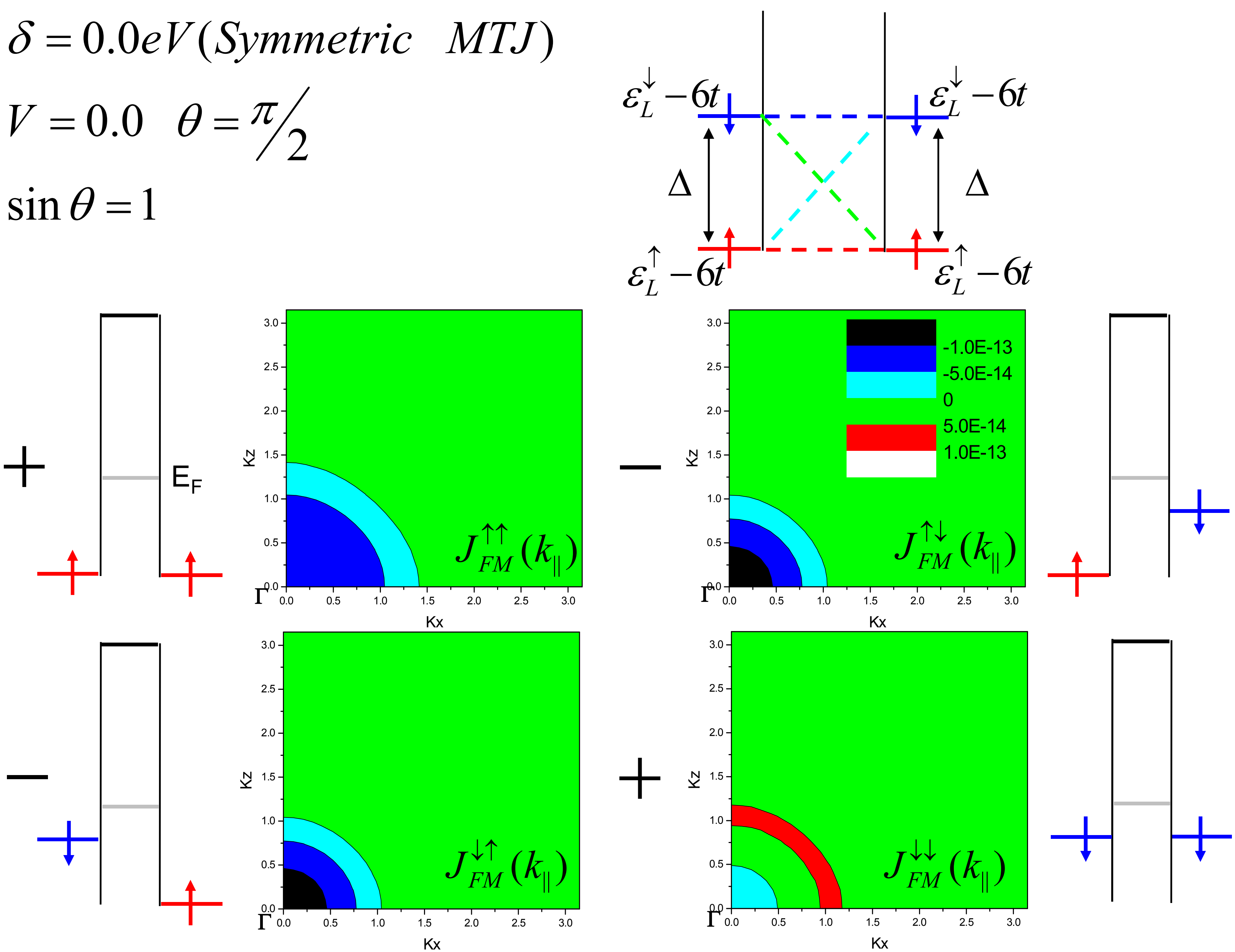
$$T_{\perp}(\pi/2) = \frac{t^4}{8\pi^3}\int g_{ba}\cdot g_{ab}\cdot[f_L\cdot \mathrm{Im}\{(g_L^{\uparrow}-g_L^{\downarrow})\cdot(g_R^{\uparrow}-g_R^{\downarrow})\}$$
$$+(f_R-f_L)\cdot \mathrm{Re}\{(g_L^{\uparrow}-g_L^{\downarrow})\}\cdot \mathrm{Im}\{(g_R^{\uparrow}-g_R^{\downarrow})\}]dEdk_{\|}$$
$$= -[J_{FM}^{\uparrow\uparrow} - J_{FM}^{\downarrow\uparrow} - J_{FM}^{\uparrow\downarrow} + J_{FM}^{\downarrow\downarrow}]$$



Δ **is the exchange splitting.**



$$-J_{FM}^{\downarrow\uparrow}(-V_b) = -J_{FM}^{\uparrow\downarrow}(+V_b)$$



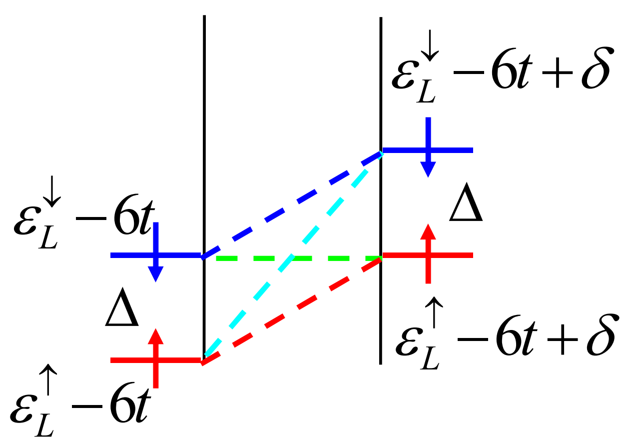
$\delta = 0.0eV\,(Symmetric\ \ MTJ)$
$V = 0.0 \quad \theta = \pi/2$
$\sin\theta = 1$
$\varepsilon_L^{\downarrow} - 6t$
$\varepsilon_L^{\uparrow} - 6t$
Δ
E_F
$J_{FM}^{\uparrow\uparrow}(k_{\|})$
$J_{FM}^{\uparrow\downarrow}(k_{\|})$
$J_{FM}^{\downarrow\uparrow}(k_{\|})$
$J_{FM}^{\downarrow\downarrow}(k_{\|})$
-1.0E-13
-5.0E-14
0
5.0E-14
1.0E-13
Kx
Kz
Γ
+
−

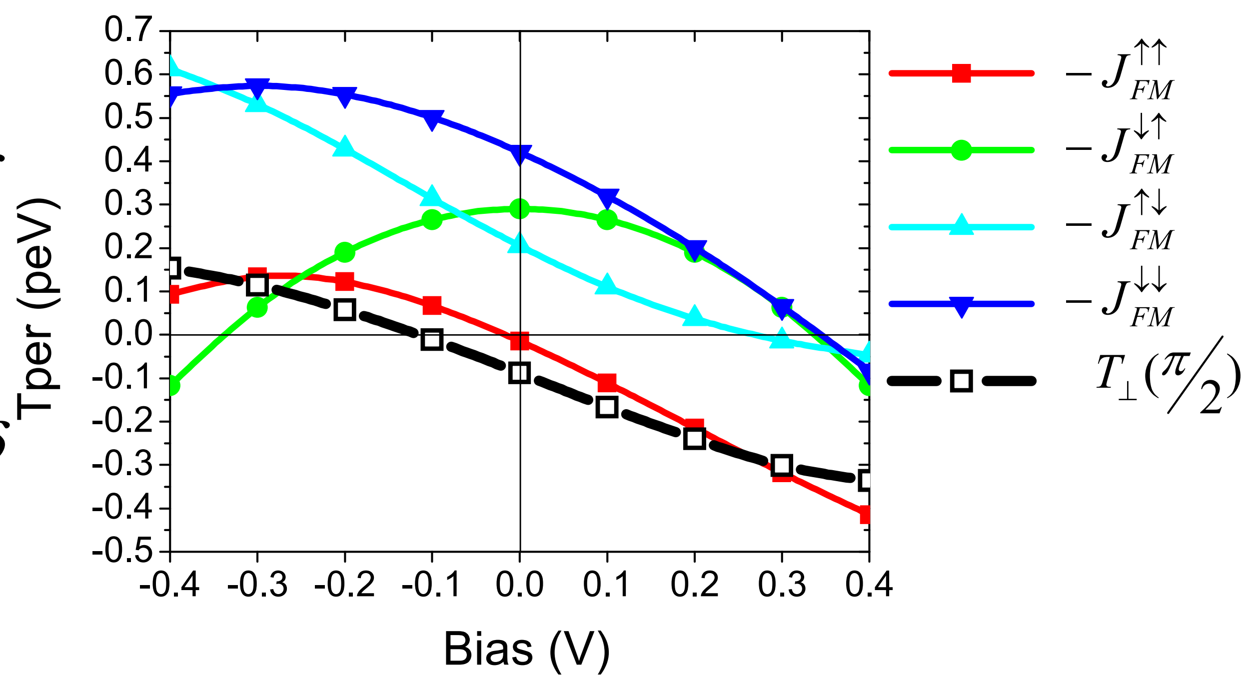
$$\varepsilon_L^{\uparrow} = 0.6eV \quad \varepsilon_L^{\downarrow} = 1.2eV \quad \delta = 0.6eV$$ **(Asymmetric two-band MTJ)**

$$\varepsilon_R^{\uparrow} = 1.2eV \quad \varepsilon_R^{\downarrow} = 1.8eV$$

$$T_{\perp}(\pi/2) = \frac{t^4}{8\pi^3}\int g_{ba}\cdot g_{ab}\cdot[f_L\cdot \mathrm{Im}\{(g_L^{\uparrow}-g_L^{\downarrow})\cdot(g_R^{\uparrow}-g_R^{\downarrow})\} + (f_R - f_L)\cdot \mathrm{Re}\{(g_L^{\uparrow}-g_L^{\downarrow})\}\cdot \mathrm{Im}\{(g_R^{\uparrow}-g_R^{\downarrow})\}]dEdk_{\parallel}$$

$$= -[J_{FM}^{\uparrow\uparrow} - J_{FM}^{\downarrow\uparrow} - J_{FM}^{\uparrow\downarrow} + J_{FM}^{\downarrow\downarrow}]$$



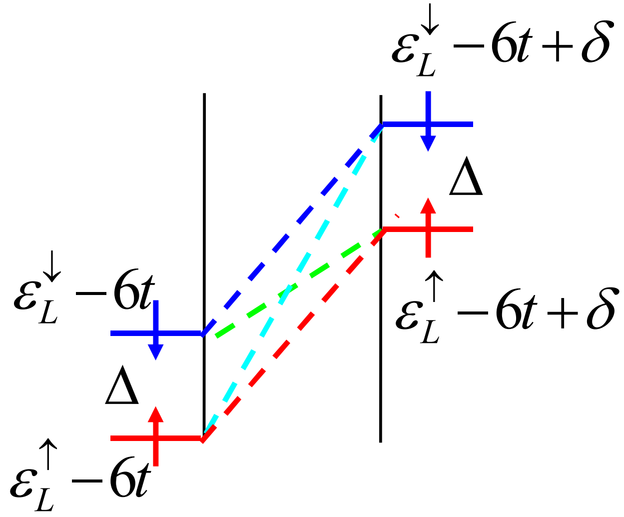


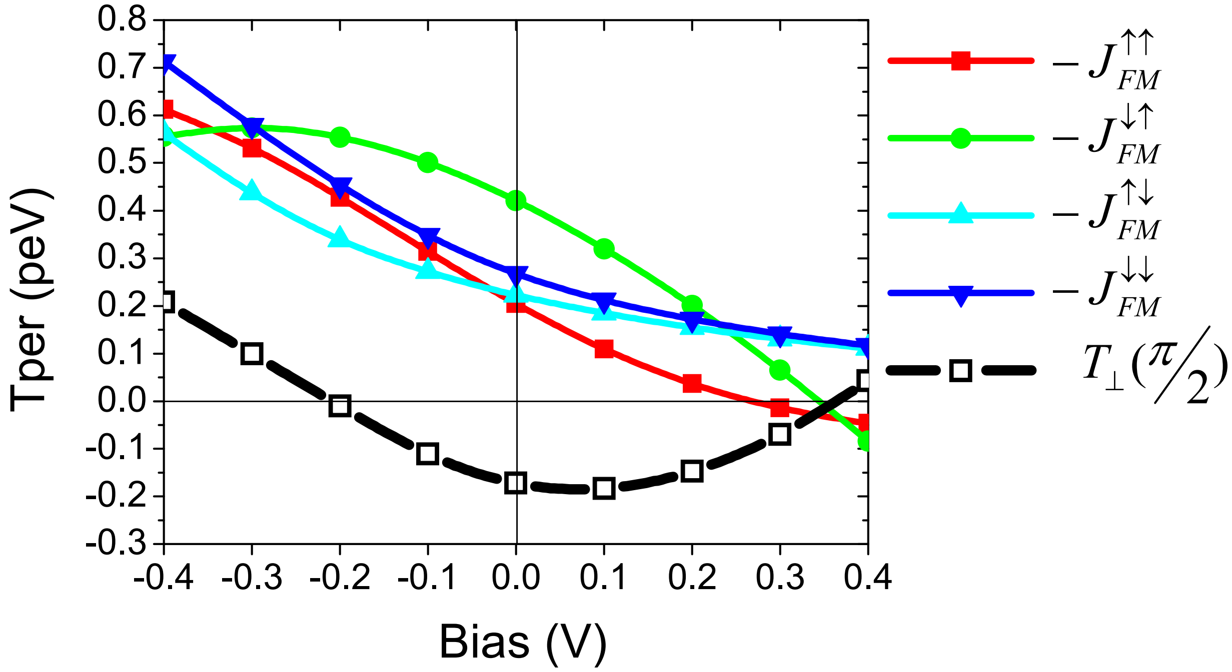
$\varepsilon_L^{\uparrow} = 0.6eV \quad \varepsilon_L^{\downarrow} = 1.2eV \quad \delta = 1.2eV$ **(Asymmetric two-band MTJ)**

$\varepsilon_R^{\uparrow} = 1.8eV \quad \varepsilon_R^{\downarrow} = 2.4eV$

$$T_{\perp}(\pi/2) = \frac{t^4}{8\pi^3}\int g_{ba}\cdot g_{ab}\cdot[f_L\cdot \mathrm{Im}\{(g_L^{\uparrow}-g_L^{\downarrow})\cdot(g_R^{\uparrow}-g_R^{\downarrow})\} + (f_R - f_L)\cdot \mathrm{Re}\{(g_L^{\uparrow}-g_L^{\downarrow})\}\cdot \mathrm{Im}\{(g_R^{\uparrow}-g_R^{\downarrow})\}]dEdk_{\parallel}$$

$$= -[J_{FM}^{\uparrow\uparrow} - J_{FM}^{\downarrow\uparrow} - J_{FM}^{\uparrow\downarrow} + J_{FM}^{\downarrow\downarrow}]$$



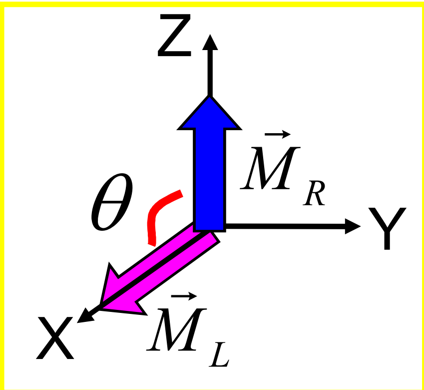


Conclusion

1. For non-collinear MTJ, $T_\perp(\theta)$ can be related to the interlayer exchange coupling of four independent channels in FM configurations.

$$T_\perp(\theta) = \frac{\sin\theta \cdot t^4}{8\pi^3} \cdot \int g_{ba} \cdot g_{ab} \cdot [f_L \cdot \mathrm{Im}\{(g_L^\uparrow - g_L^\downarrow)\cdot(g_R^\uparrow - g_R^\downarrow)\}$$
$$+ (f_R - f_L)\cdot \mathrm{Re}\{(g_L^\uparrow - g_L^\downarrow)\}\cdot \mathrm{Im}\{(g_R^\uparrow - g_R^\downarrow)\}]dEdk_\parallel$$
$$= -\sin\theta \cdot [J_{FM}^{\uparrow\uparrow} - J_{FM}^{\downarrow\uparrow} - J_{FM}^{\uparrow\downarrow} + J_{FM}^{\downarrow\downarrow}]$$

Non-collinear MTJ = **FM configuration** $\times \sin\theta$



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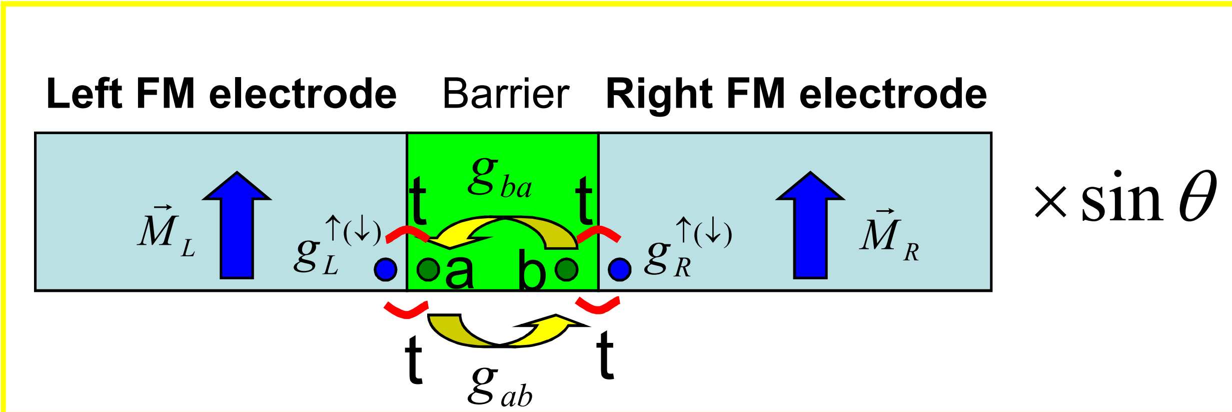
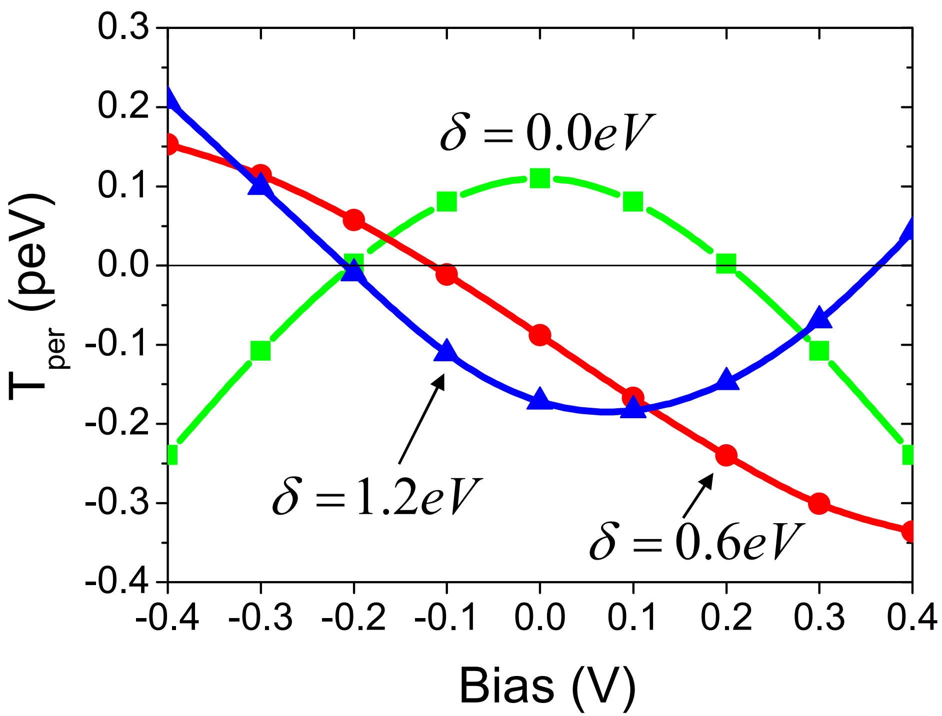


$\times \sin\theta$

2. The bias dependence of $T_\perp$ can be significantly altered by the asymmetry, δ, between left and right electrodes, which can explain the inconsistence of previous experimental findings.



3. Since $T_\perp$ is controlled by four independent FM interlayer exchange couplings, $J_{FM}^{\sigma\sigma'}$, one can systematically create any kind of bias dependence of $T_\perp$ through different combinations of majority- and minority-spin band fillings in both left and right electrodes.

4. The Remaining problem is to understand the physical meanings of $J_{FM}^{\sigma\sigma'}(\mathrm{Im})$ and $J_{FM}^{\sigma\sigma'}(\mathrm{Re}^*\mathrm{Im})$.

$$-J_{FM}^{\uparrow\uparrow}(\mathrm{Im}+\mathrm{Re}^*\mathrm{Im}) = \frac{t^4}{8\pi^3}\int g_{ba}\cdot g_{ab}\cdot[f_L\cdot \mathrm{Im}\{g_L^\uparrow\cdot g_R^\uparrow\} + (f_R - f_L)\cdot \mathrm{Re}\{g_L^\uparrow\}\cdot \mathrm{Im}\{g_R^\uparrow\}]dEdk_\parallel$$

$$= \frac{t^4}{8\pi^3}\int g_{ba}\cdot g_{ab}\cdot[\boxed{f_L\cdot \mathrm{Im}\{g_L^\uparrow\}}\cdot \mathrm{Re}\{g_R^\uparrow\} + \boxed{f_R}\cdot \mathrm{Re}\{g_L^\uparrow\}\cdot \boxed{\mathrm{Im}\{g_R^\uparrow\}}]dEdk_\parallel$$

Occupied LDOS in isolated left electrode

Occupied LDOS in isolated right electrode

Similar to the current ??

What's the relation between $T_\perp$ and other physical quantities, such as LDOS, spin-current, charge-current, …, and so on **????**

Happy Holidays!

Happy Holidays!

Thank you for your attention !!!

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