Temperatura de compensação em modelos de Ising em camadas (Parte 1)

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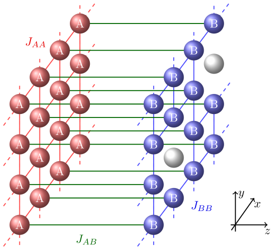
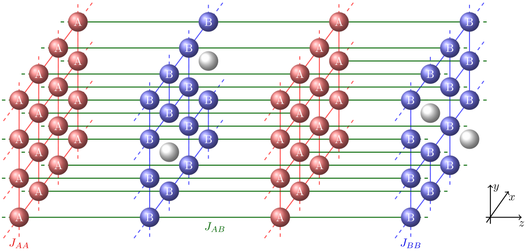
3. Resultados e Discussão

- Materiais magnéticos em camadas têm sido amplamente estudados nas últimas décadas.
- Aplicações tecnológicas
  - Magnetorresistência gigante [Camley e Barnaś 1989].
  - Efeito magnetocalórico [Phan e Yu 2007].

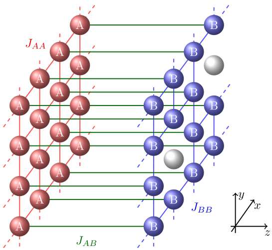
- Camadas monoatômicas de tipos **A** e **B** dispostas alternadamente
- Interação entre átomos **A-A** (J_{AA}): ferromagnética
- Interação entre átomos **B-B** (J_{BB}): ferromagnética
- Interação entre átomos **A-B** (J_{AB}): antiferromagnética
- Apenas camadas do tipo **B** apresentam diluição

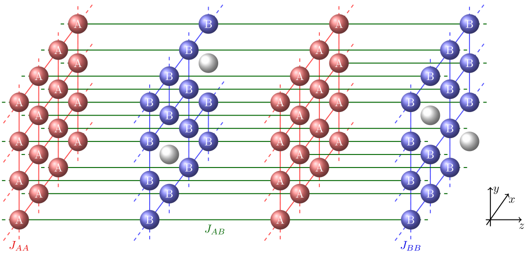




Hamiltoniano (Ising)

$$\mathcal{H} = -\sum_{\langle i\in A, j\in A\rangle} J_{AA} s_i s_j - \sum_{\langle i\in B, j\in B\rangle} J_{BB} s_i s_j \epsilon_i \epsilon_j - \sum_{\langle i\in A, j\in B\rangle} J_{AB} s_i s_j \epsilon_j$$





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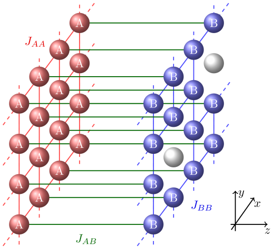


- $s_i = \pm 1$
- $J_{AA}, J_{BB} > 0, \; J_{AB} < 0$
- $\epsilon_i = 1$ (sítio magnético)
- $\epsilon_i = 0$ (vacância)

- Solução analítica $\rightarrow$ não existe
- Métodos aproximados:
  - Matriz de transferência
  - Grupo de renormalização
  - Aproximação de campo médio (CM/MFA)
  - Aproximação de campo efetivo (CE/EFA)
  - Aproximação de pares (AP)
  - Simulações de Monte Carlo (MC)

- Solução analítica $\rightarrow$ não existe
- Métodos aproximados:
  - Matriz de transferência
  - Grupo de renormalização
  - Aproximação de campo médio (CM/MFA) $\rightarrow$ seminário de hoje
  - Aproximação de campo efetivo (CE/EFA) $\rightarrow$ seminário de hoje
  - Aproximação de pares (AP)
  - Simulações de Monte Carlo (MC)

- Solução analítica $\rightarrow$ não existe
- Métodos aproximados:
  - Matriz de transferência
  - Grupo de renormalização
  - Aproximação de campo médio (CM/MFA)
  - Aproximação de campo efetivo (CE/EFA)
  - Aproximação de pares (AP) $\rightarrow$ próximos seminários [Balcerzak e Szałowski 2014, Szałowski e Balcerzak 2014]
  - Simulações de Monte Carlo (MC) $\rightarrow$ próximos seminários [Diaz e Branco 2017][Diaz e Branco 2017]

Hamiltoniano

$$\mathcal{H} = -\sum_{\langle i\in A, j\in A\rangle} J_{AA} s_i s_j - \sum_{\langle i\in B, j\in B\rangle} J_{BB} s_i s_j \epsilon_i \epsilon_j - \sum_{\langle i\in A, j\in B\rangle} J_{AB} s_i s_j \epsilon_j$$

Identidade [Callen 1963, Callen 1985]

$$m_\Lambda = \overline{\langle \tanh\left(\beta_T E_{i\in\Lambda}\right)\rangle}$$

$$\Lambda = A, B;\ \beta_T \equiv \left(k_B T\right)^{-1}$$

$$E_{i\in A} = J_{AA} \sum_{\delta} s_{(i+\delta)\in A} + J_{AB} \sum_{\delta'} s_{(i+\delta')\in B} \epsilon_{(i+\delta')}$$

$$E_{i\in B} = J_{BB} \sum_{\delta} s_{(i+\delta)\in B} \epsilon_{(i+\delta)} + J_{AB} \sum_{\delta'} s_{(i+\delta')\in A}$$

Hamiltoniano

$$\mathcal{H} = -\sum_{\langle i\in A, j\in A\rangle} J_{AA} s_i s_j - \sum_{\langle i\in B, j\in B\rangle} J_{BB} s_i s_j \epsilon_i \epsilon_j - \sum_{\langle i\in A, j\in B\rangle} J_{AB} s_i s_j \epsilon_j$$

Identidade [Callen 1963, Callen 1985]

$$m_\Lambda = \overline{\langle \tanh\left(\beta_T E_{i\in\Lambda}\right)\rangle} \approx \tanh \overline{\langle \beta_T E_{i\in\Lambda}\rangle} \leftarrow \text{campo médio}$$

$$\Lambda = A, B;\ \beta_T \equiv \left(k_B T\right)^{-1}$$

$$E_{i\in A} = J_{AA} \sum_{\delta} s_{(i+\delta)\in A} + J_{AB} \sum_{\delta'} s_{(i+\delta')\in B}\, \epsilon_{(i+\delta')}$$

$$E_{i\in B} = J_{BB} \sum_{\delta} s_{(i+\delta)\in B}\, \epsilon_{(i+\delta)} + J_{AB} \sum_{\delta'} s_{(i+\delta')\in A}$$

- Sistema bicamada

$$m_A = \tanh\left\{\beta_T(4J_{AA}m_A + pJ_{AB}m_B)\right\}$$
$$m_B = \tanh\left\{\beta_T(4pJ_{BB}m_B + J_{AB}m_A)\right\}$$

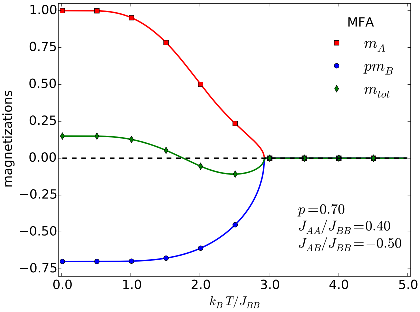
- Sistema multicamadas

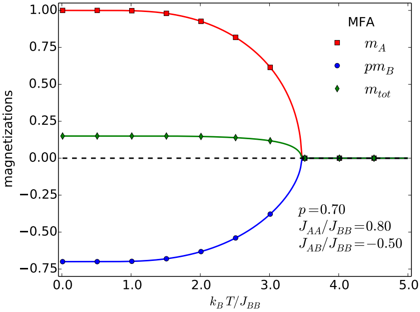
$$m_A = \tanh\left\{\beta_T(4J_{AA}m_A + 2pJ_{AB}m_B)\right\}$$
$$m_B = \tanh\left\{\beta_T(4pJ_{BB}m_B + 2J_{AB}m_A)\right\}$$

- Magnetização total

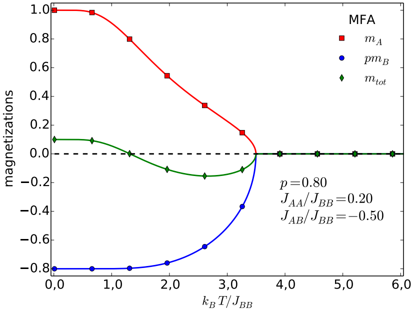
$$m_{\text{tot}} = \frac{1}{2}(m_A + pm_B)$$

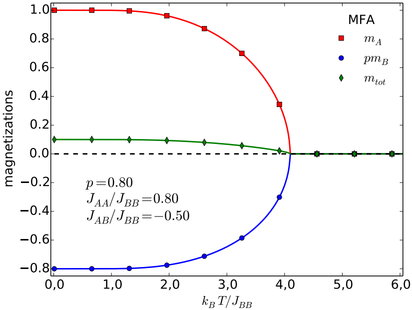
Sistema bicamada: campo médio





Sistema multicamadas: campo médio





Na aproximação de **campo efetivo**
[Honmura e Kaneyoshi 1979, Aguiar, Moreira e Engelsberg 1986], usamos o operador diferencial

$$e^{\lambda D} f(x) = f(x+\lambda), \qquad D \equiv \frac{\partial}{\partial x},$$

para reescrever a identidade de Callen como:

Identidade

$$m_\Lambda = \overline{\langle \exp\left(\beta_T E_{i\in\Lambda} D\right)\rangle} \tanh x \Big|_{x=0}$$

$$\Lambda = A, B;\ \beta_T \equiv (k_B T)^{-1}$$

$$E_{i\in A} = J_{AA} \sum_{\delta} s_{(i+\delta)\in A} + J_{AB} \sum_{\delta'} s_{(i+\delta')\in B} \epsilon_{(i+\delta')}$$

$$E_{i\in B} = J_{BB} \sum_{\delta} s_{(i+\delta)\in B} \epsilon_{(i+\delta)} + J_{AB} \sum_{\delta'} s_{(i+\delta')\in A}$$

Identidade

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Identidade

$$m_\Lambda = \overline{\langle \exp\left(\beta_T E_{i\in\Lambda} D\right)\rangle} \tanh x \Big|_{x=0}$$

$$\begin{aligned}
\exp\left(\beta_T E_{i\in A} D\right) = & \left\{\Pi_\delta \exp\left(\beta_T J_{AA} s_{(i+\delta)\in A} D\right)\right\} \\
& \times \left\{\Pi_{\delta'} \exp\left(\beta_T J_{AB} s_{(i+\delta')\in B} \epsilon_{(i+\delta')} D\right)\right\} \\
\exp\left(\beta_T E_{i\in B} D\right) = & \left\{\Pi_\delta \exp\left(\beta_T J_{BB} s_{(i+\delta)\in B} \epsilon_{(i+\delta)} D\right)\right\} \\
& \times \left\{\Pi_{\delta'} \exp\left(\beta_T J_{AB} s_{(i+\delta')\in A} D\right)\right\}
\end{aligned}$$

Identidade

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$$\begin{aligned}
\exp\left(\beta_T E_{i\in A} D\right) =& \left\{\Pi_\delta \exp\left(\beta_T J_{AA} s_{(i+\delta)\in A} D\right)\right\} \\
& \times \left\{\Pi_{\delta'} \exp\left(\beta_T J_{AB} s_{(i+\delta')\in B} \epsilon_{(i+\delta')} D\right)\right\} \\
\exp\left(\beta_T E_{i\in B} D\right) =& \left\{\Pi_\delta \exp\left(\beta_T J_{BB} s_{(i+\delta)\in B} \epsilon_{(i+\delta)} D\right)\right\} \\
& \times \left\{\Pi_{\delta'} \exp\left(\beta_T J_{AB} s_{(i+\delta')\in A} D\right)\right\}
\end{aligned}$$

- Identidades (válidas pois $s_i = \pm 1$ e $\epsilon_i = 0$ ou 1):
  - $e^{x s_i} = \cosh\left(x\right) + s_i \sinh\left(x\right)$
  - $e^{x s_i \epsilon_i} = 1 + \epsilon_i \left[\cosh\left(x s_i\right) + s_i \sinh\left(x s_i\right) - 1\right]$

Identidade

$$m_\Lambda = \overline{\langle \exp\left(\beta_T E_{i\in\Lambda} D\right)\rangle} \tanh x \Big|_{x=0}$$

$$\begin{aligned}
\exp\left(\beta E_{i\in A} D\right) &= \Pi_\delta \Big\{ \cosh\left(\beta_T J_{AA} D\right) + s_{(i+\delta)\in A} \sinh\left(\beta_T J_{AA} D\right) \Big\} \\
&\quad \times \Pi_{\delta'} \Big\{ 1 + \epsilon_{i+\delta'} \left[\cosh\left(\beta_T J_{AB} D\right) + s_{(i+\delta')\in B} \sinh\left(\beta_T J_{AB} D\right) - 1 \right] \Big\} \\
\exp\left(\beta E_{i\in B} D\right) &= \Pi_\delta \Big\{ 1 + \epsilon_{i+\delta} \left[\cosh\left(\beta_T J_{BB} D\right) + s_{(i+\delta)\in B} \sinh\left(\beta_T J_{BB} D\right) - 1 \right] \Big\} \\
&\quad \times \Pi_{\delta'} \Big\{ \cosh\left(\beta_T J_{AB} D\right) + s_{(i+\delta')\in A} \sinh\left(\beta_T J_{AB} D\right) \Big\}
\end{aligned}$$

Identidade

$$m_\Lambda = \overline{\langle \exp\left(\beta_T E_{i\in\Lambda} D\right)\rangle} \tanh x \Big|_{x=0}$$

$$\exp\left(\beta E_{i\in A} D\right) = \Pi_\delta \Big\{ \cosh\left(\beta_T J_{AA} D\right) + s_{(i+\delta)\in A} \sinh\left(\beta_T J_{AA} D\right) \Big\}$$
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$$\times \Pi_{\delta'} \Big\{ \cosh\left(\beta_T J_{AB} D\right) + s_{(i+\delta')\in A} \sinh\left(\beta_T J_{AB} D\right) \Big\}$$

- Identidades: $\overline{\epsilon_i} = p$; $\overline{\{\Pi_{i=1}^{n} \epsilon_i\}} = p^n$; $\overline{\langle s_{i\in\Lambda}\rangle} = m_\Lambda$
- Aproximação: $\langle s_i s_j \cdots s_k \rangle = \langle s_i \rangle \langle s_j \rangle \cdots \langle s_k \rangle$

Identidade

$$m_\Lambda = \overline{\langle \exp\left(\beta_T E_{i\in\Lambda} D\right)\rangle} \tanh x \Big|_{x=0}$$

$$\begin{aligned}
\overline{\langle \exp\left(\beta E_{i\in A} D\right)\rangle} &= \Pi_\delta \Big\{ \cosh\left(\beta_T J_{AA} D\right) + m_A \sinh\left(\beta_T J_{AA} D\right) \Big\} \\
&\times \Pi_{\delta'} \Big\{ 1 + p \big[\cosh\left(\beta_T J_{AB} D\right) + m_B \sinh\left(\beta_T J_{AB} D\right) - 1 \big] \Big\} \\
\overline{\langle \exp\left(\beta E_{i\in B} D\right)\rangle} &= \Pi_\delta \Big\{ 1 + p \big[\cosh\left(\beta_T J_{BB} D\right) + m_B \sinh\left(\beta_T J_{BB} D\right) - 1 \big] \Big\} \\
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&\times \Pi_{\delta'} \Big\{ \cosh\left(\beta_T J_{AB} D\right) + m_A \sinh\left(\beta_T J_{AB} D\right) \Big\}
\end{aligned}$$

- Identidade: $\cosh a + x \sinh a = \frac{1}{2}\Big[(1+x)e^{a} + (1-x)e^{-a} \Big]$

Sistema bicamada:

$$
\begin{aligned}
m_A =&\frac{1}{2^5}\left\{(1+m_A)e^{\beta_T J_{AA} D}+(1-m_A)e^{-\beta_T J_{AA} D}\right\}^4 \\
&\times\left\{2(1-p)+p\left[(1+m_B)e^{\beta_T J_{AB} D}+(1-m_B)e^{-\beta_T J_{AB} D}\right]\right\}\tanh x\Big|_{x=0} \\
m_B =&\frac{1}{2^5}\left\{2(1-p)+p\left[(1+m_B)e^{\beta_T J_{BB} D}+(1-m_B)e^{-\beta_T J_{BB} D}\right]\right\}^4 \\
&\times\left\{(1+m_A)e^{\beta_T J_{AB} D}+(1-m_A)e^{-\beta_T J_{AB} D}\right\}\tanh x\Big|_{x=0}
\end{aligned}
$$

Magnetização total:

$$m_{\text{tot}} = \frac{1}{2}(m_A + p m_B)$$

Sistema multicamadas:

$$
\begin{aligned}
m_A =& \frac{1}{2^6}\left\{(1+m_A)e^{\beta_T J_{AA} D} + (1-m_A)e^{-\beta_T J_{AA} D}\right\}^4 \\
& \times \left\{2(1-p) + p\left[(1+m_B)e^{\beta_T J_{AB} D} + (1-m_B)e^{-\beta_T J_{AB} D}\right]\right\}^2 \tanh x \Big|_{x=0} \\
m_B =& \frac{1}{2^6}\left\{2(1-p) + p\left[(1+m_B)e^{\beta_T J_{BB} D} + (1-m_B)e^{-\beta_T J_{BB} D}\right]\right\}^4 \\
& \times \left\{(1+m_A)e^{\beta_T J_{AB} D} + (1-m_A)e^{-\beta_T J_{AB} D}\right\}^2 \tanh x \Big|_{x=0}
\end{aligned}
$$

Magnetização total:

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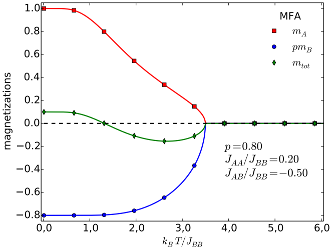
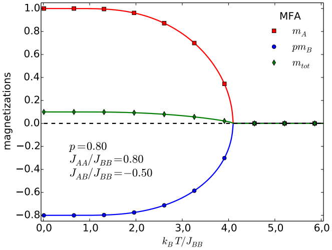
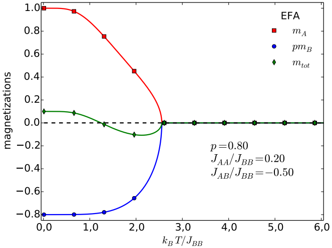
m_{\text{tot}} = \frac{1}{2}(m_A + p m_B)
$$

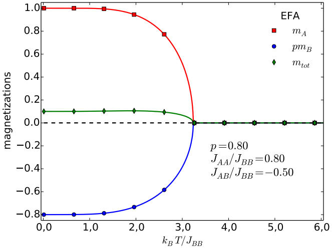
Sistema multicamadas: campo médio



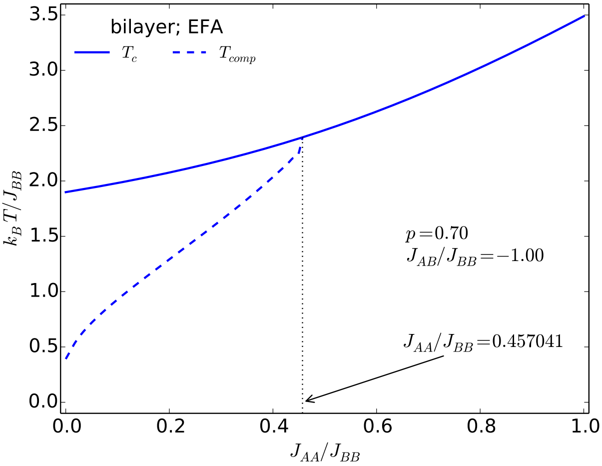


Sistema multicamadas: campo efetivo

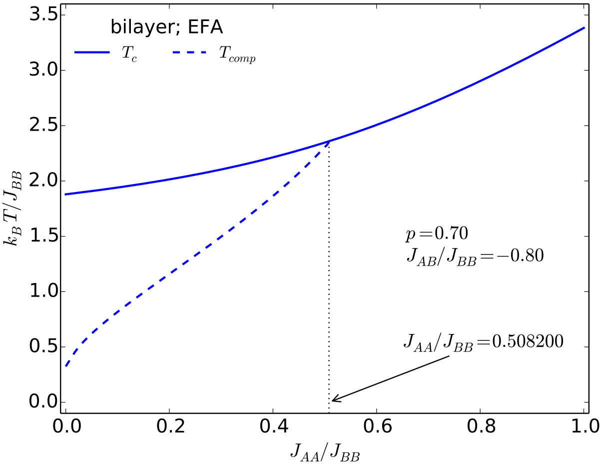




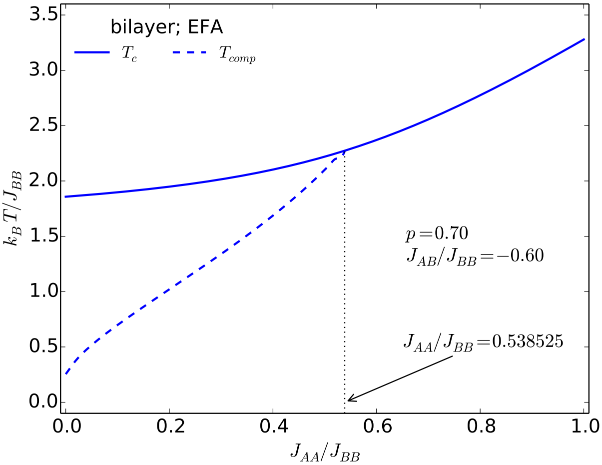
Sistema bicamada: $p = 0.7$; campo efetivo



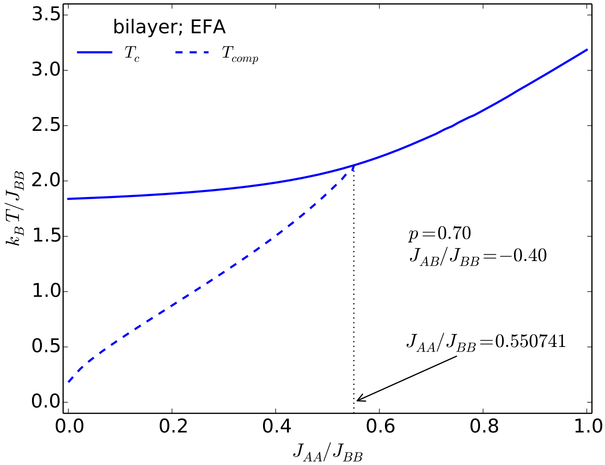
Sistema bicamada: $p = 0.7$; campo efetivo



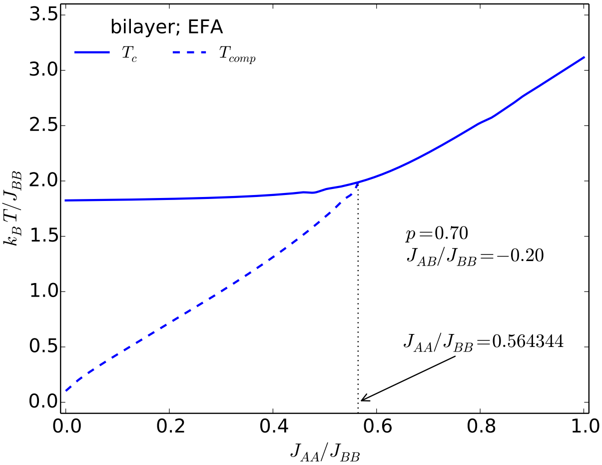
Sistema bicamada: $p = 0.7$; campo efetivo



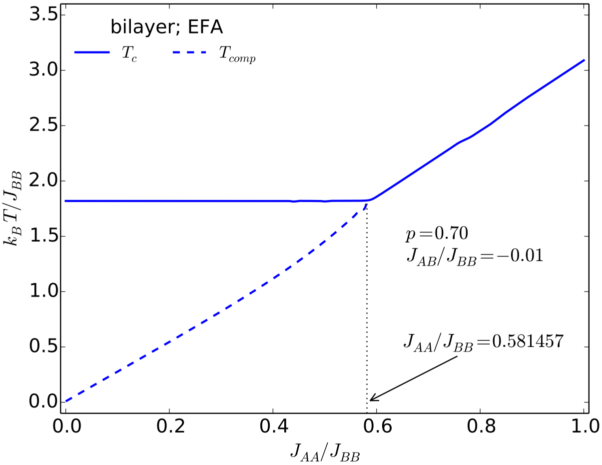
Sistema bicamada: $p = 0.7$; campo efetivo



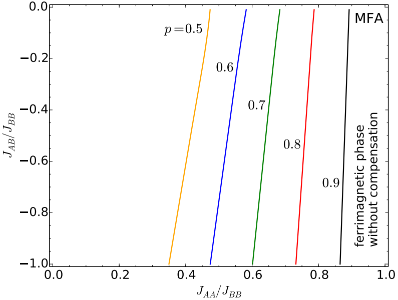
Sistema bicamada: $p = 0.7$; campo efetivo

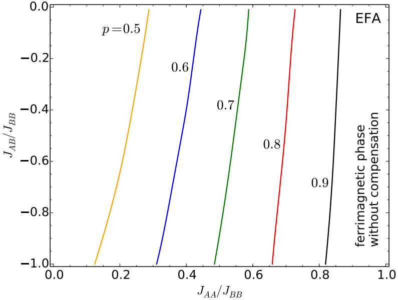


Sistema bicamada: $p = 0.7$; campo efetivo

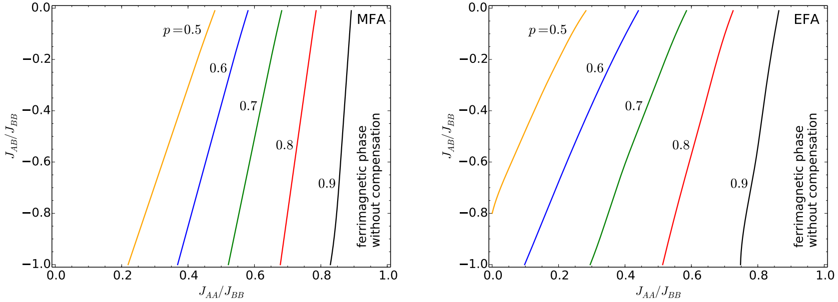


Sistema bicamada: campo médio/campo efetivo





Sistema multicamadas: campo médio/campo efetivo



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