#7 Feroelektrici i feromagneti

I Feroelektrici

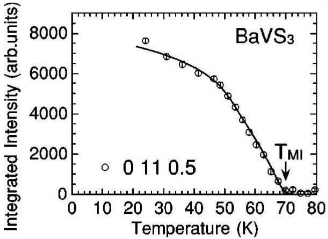
II Feromagneti

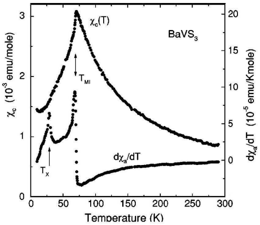
predavanja 20**

Motivacija I i II

što je to parametar uređenja u teoriji faznih prijelaza?

- primjer: valovi gustoće naboja u $BaVS_3$ [Inami *et al.*, 2002], [Mihaly *et al.*, 2000]
- u feroelektricima (FE) i feromagnetima (FM)?
- u antiferoelektricima (AFE) i antiferomagnetima (AFM)?
- u sustavima s valovima gustoće spina (SDW)?
- u supravodičima (SC)?





Gibbsov potencijal u feroelektricima

na koji način možemo istovremeno studirati stabilizaciju FE faze i odrediti pripadne odzivne funkcije

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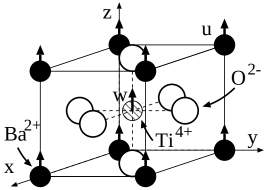
- Gibbsov potencijal na temperaturama $T > T_c$ i $T < T_c$

$$\widetilde{F}(T, \mathbf{P}, \mathbf{E}) = F(T, \mathbf{P}) - \sum_{\mathbf{k}'} \left[\mathbf{P}(\mathbf{k}') \cdot \mathbf{E}(-\mathbf{k}') + (1/8\pi) \left| \mathbf{E}(\mathbf{k}') \right|^2 \right]$$

$$F(T, \mathbf{P}) = \sum_{\mathbf{k}'} \left[\left| \mathbf{P}(\mathbf{k}') \right|^2 / (2\chi_0(\mathbf{k}')) + \dots \right]$$

- FE uređenje (u $BaTiO_3$, na primjer) je povezano uz pojavu permanentne polarizacije

$$\mathbf{P}(\mathbf{k}') \to \mathbf{P}^0(\mathbf{k}' = 0) = f(\mathbf{w}, \mathbf{u})$$



Landauova teorija feroelektrika (druge vrste)

konstrukcija termodinamičkog potencijala za $\mathbf{E} = 0$

- termodinamički potencijal ($A = a(T - T_c)$ te $B \approx B(T_c) > 0$)

$$\Phi(P_z) = \Phi_0 + AP_z^2 + BP_z^4$$

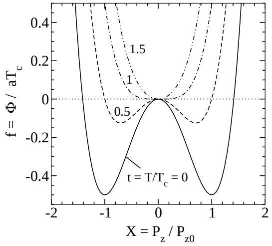
- minimizacija termodinamičkog potencijala

$$\partial\Phi/\partial P_z = 2P_z(A + 2BP_z^2) = 0, \quad \partial^2\Phi/\partial P_z^2 = 2A + 12BP_z^2$$

- rješenja za $T > T_c$ i za $T < T_c$ (kritični eksponent $1/2$)

$$P_{z0}^{(1)} = 0, \quad P_{z0}^{(2)} = \sqrt{-(A/2B)} \propto (T_c - T)^{1/2}$$

$$\Delta\Phi(P_z) = (1/2)AP_{z0}^2$$



Odzivne funkcije u feroelektricima

kako odrediti dielektričnu susceptibilnost χ za $T > T_c$ i za $T < T_c$

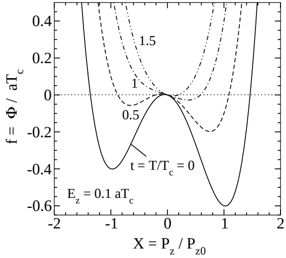
- termodinamički potencijal za $\mathbf{E} \neq 0$

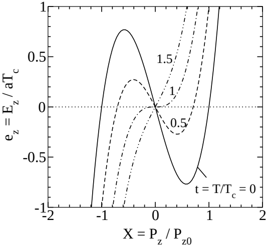
$$\widetilde{\Phi}(\mathbf{P}, \mathbf{E}) = \Phi(\mathbf{P}, 0) - \mathbf{P} \cdot \mathbf{E} - (1/8\pi)\mathbf{E}^2$$

- minimizacija termodinamičkog potencijala

$$\partial\Phi/\partial P_z = 2AP_z + 4BP_z{}^3 - E_z = 0, \quad \partial^2\Phi/\partial P_z^2 = 2A + 12BP_z^2$$

- rješenje? $(P_z \approx P_{z0} + \chi E_z \equiv P_{z0} + \delta P_z)$





Odzivne funkcije u feroelektricima

rješenje

- razvoj po malom δP_z

$$2A(P_{z0} + \delta P_z) + 4B(P_{z0}^3 + 3P_{z0}^2 \delta P_z) - E_z = 0$$

- opći zapis susceptibilnosti

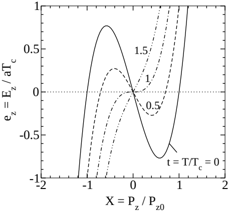
$$\chi = 1/[2A + 12BP_{z0}^2]$$

- eksplicitni oblik inverzne susceptibilnosti

$$\begin{aligned} 1/\chi(T) = 1/\chi^{(1)} &= 2a(T - T_\mathrm{c}), \;\; \text{za} \;\; T > T_\mathrm{c} \\ = 1/\chi^{(2)} &= 4a(T_\mathrm{c} - T), \;\; \text{za} \;\; T < T_\mathrm{c} \end{aligned}$$

- alternativni način računa

$$\chi^{(i)} = \partial P_z / \partial E_z = \left[\partial E_z / \partial P_z\right]^{-1}$$



Mikroskopski modeli: red-nered feroelektrici

kakva je mikroskopska struktura koeficijenata $A(T)$ i $B(T)$?

- slobodna energija red-nered feroelektrika u akroksimaciji srednjeg polja, $\mathcal{F} = \mathcal{U} - T\mathcal{S}$

$$\mathcal{U} = -\frac{1}{2} J \sum_{i,\delta} \langle \sigma_i^z \rangle \langle \sigma_{i+\delta}^z \rangle, \qquad \mathcal{S} = k_{\mathrm{B}} \ln \frac{N!}{N_+! N_-!}$$

- aproksimativni rezultat ($\langle \sigma_i^z \rangle \to X = (N_\uparrow - N_\downarrow)/N$)

$$\mathcal{F} \approx -\frac{N}{2} J z X^2 + \frac{N}{2} k_{\mathrm{B}} T \left[(1+X) \ln \frac{1+X}{2} + (1-X) \ln \frac{1-X}{2} \right]$$

- Landauov razvoj

$$\Delta\mathcal{F} \approx \frac{N}{2} k_{\mathrm{B}} (T - T_c) X^2 + \frac{N}{12} k_{\mathrm{B}} T X^4 \equiv a(T - T_c) X^2 + B(T) X^4$$

Landauova teorija feromagnetizma

račun magnetske susceptibilnosti χ

- termodinamički potencijal

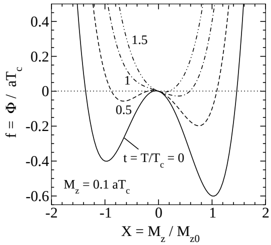
$$\Delta\widetilde{\Phi}(M_z, H_z) = AM_z^2 + BM_z^4 - M_z H_z - (1/8\pi)H_z^2$$

- ukupni termodinamički potencijal

$$\Delta\widetilde{\Phi}(M_z, H_z) = (1/2)AM_{z0}^2 - M_{z0}H_z - (1/2)\delta M_z H_z - (1/8\pi)H_z^2$$

- Curie-Weissov zakon $[T > T_\mathrm{C}]$

$$\chi(T) = C/[T - T_\mathrm{C}]^{-1}$$



Jednadžbe magnetostatike za $\mathbf{M}^0 \neq 0$

rješavanje jednadžbi magnetostatike za $\mathbf{J} = 0$

- jednadžbe

$$\nabla \cdot \mathbf{B}^{(i)} = 0, \qquad (\mathbf{B}^{(2)} - \mathbf{B}^{(1)}) \cdot \mathbf{n}_{21} = 0$$
$$\nabla \times \mathbf{H}^{(i)} = 0, \qquad \mathbf{n}_{21} \times (\mathbf{H}^{(2)} - \mathbf{H}^{(1)}) = 0$$

- skalarni magnetski potencijal $[\nabla \times \mathbf{H}^{(i)} = 0]$

$$\mathbf{H}^{(i)}(\mathbf{x}) = -\nabla \Phi_M^{(i)}(\mathbf{x})$$

- struktura Maxwellove jednadžbe II

$$\nabla \cdot \mathbf{B}^{(i)} = \nabla \cdot (\mathbf{H}^{(i)} + 4\pi \mathbf{M}^{(i)}) = -\nabla^2 \Phi_M^{(i)} + 4\pi \nabla \cdot \mathbf{M}^{(i)} = 0$$

- treba riješiti Poissonovu jednadžbu $[\rho_M^{(i)}(\mathbf{x}) = -\nabla \cdot \mathbf{M}^{(i)}(\mathbf{x})]$

$$\nabla^2 \Phi_M^{(i)}(\mathbf{x}) = -4\pi \rho_M^{(i)}(\mathbf{x}) \rightarrow \Phi_M^{(i)}(\mathbf{x}) = -\int \mathrm{d}^3 x' \frac{\nabla' \cdot \mathbf{M}^{(i)}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

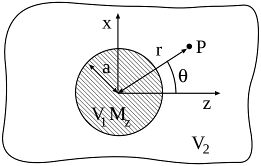
Primjer: feromagnetska kugla

- homogena feromagnetska kugla $[\mathbf{n}' \cdot \mathbf{M} \equiv \sigma_M(\mathbf{x})]$

$$\Phi_M^{(i)}(\mathbf{x}) = -\int \mathrm{d}^3x' \frac{\nabla' \cdot \mathbf{M}^{(i)}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} = \int \mathrm{d}a' \frac{\mathbf{n}' \cdot \mathbf{M}^{(i)}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

- rješenje integrala

$$\Phi_M(r,\theta) = M_{z0}a^2 \int \mathrm{d}\Omega' \frac{\cos\theta'}{|\mathbf{x}-\mathbf{x}'|} = \frac{4\pi}{3} M_{z0}a^2 \frac{r_<}{r_>^2} \cos\theta$$



Primjer: feromagnetska kugla

- skalarni magnetski potencijal $[\mathbf{m} = (4\pi a^3/3)\mathbf{M}]$

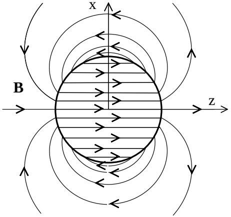
$$\Phi_M^{(1)}(r,\theta) = (4\pi/3)M_{z0}\, r\cos\theta = (4\pi/3)M_{z0}\, z, \quad \Phi_M^{(2)}(r,\theta) = \mathbf{m}\cdot\mathbf{x}/r^3$$

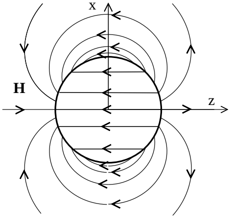
- magnetska polja unutar

$$\mathbf{H}^{(1)} = -(4\pi/3)\mathbf{M}, \quad \mathbf{B}^{(1)} = (8\pi/3)\mathbf{M}$$

- i izvan kugle

$$\mathbf{H}^{(2)}(\mathbf{x}) = \mathbf{B}^{(2)}(\mathbf{x}) = -\nabla\left(\mathbf{m}\cdot\mathbf{x}/r^3\right)$$





FM nestabilnost itinerantnih elektrona

postoji li mogućnost da se realizira FM stanje u sustavu delokaliziranih elektrona?
koji je kritični parametar za ovakvu vrstu FM faznih prijelaza?

- termodinamički potencijal [$U \leq U_c$ i $T = 0$]

$$\Delta\widetilde{\Phi}(\mathbf{M},\mathbf{H}) \;=\; \frac{1}{4\mu^2}\big(U_c - U\big)M_z^2 - \mathbf{M}\cdot\mathbf{H} - \frac{1}{8\pi}\mathbf{H}^2$$

- parametri 3D slobodnog elektronskog plina

$$U_c = (4\varepsilon_{\rm F}/3N), \;\; n(\varepsilon_{\rm F}) = (3N/2\varepsilon_{\rm F})$$

- paramagnetska susceptibilnost [$M_z = \mu(N_\uparrow - N_\downarrow)$]

$$\chi(U) = \frac{n(\varepsilon_{\rm F})\mu^2}{1 - (1/2)n(\varepsilon_{\rm F})U}$$

- što se događa za $U \to U_c$? [Stonerov kriterij]