

Ferron transport from excitonic insulator model of electronic ferroelectricity

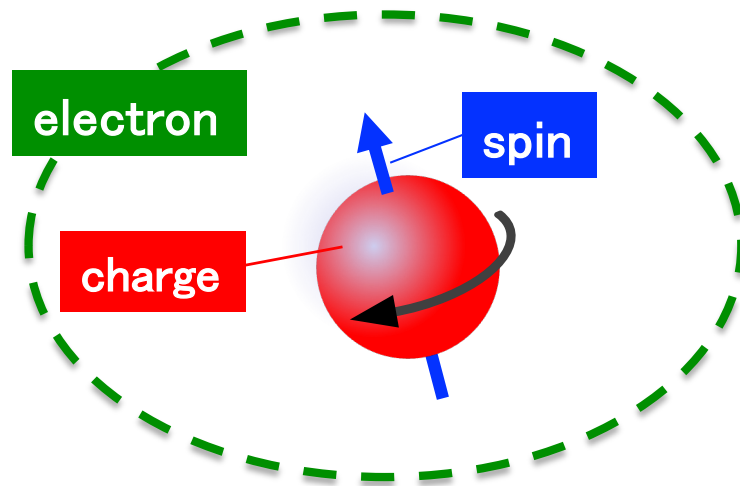
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In collaboration with

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E. Saitoh, Univ. Tokyo**

Electronics, spintronics, and “ferronics”



Electronics

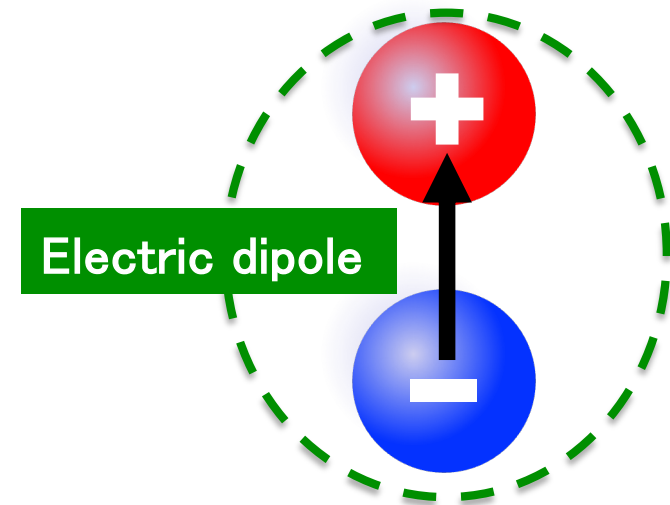
Charge: monopole

Charge current
= monopole current

Spintronics

Spin: dipole

Spin current
= dipole current



Electric “dipole”
→ electric dipole current

Can we construct a new electronics
making use of the electric dipole current?

Background (1)

Journal of Magnetism and Magnetic Materials 541 (2022) 168468

Magnonics vs. Ferronics

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A B S T R A C T

Magnons are the elementary excitations of the magnetic order that carry spin, momentum, and energy. Here we compare the magnon with the *ferron*, i.e. the elementary excitation of the electric dipolar order, that transports polarization, momentum, and energy in ferroelectrics.

Background (2)

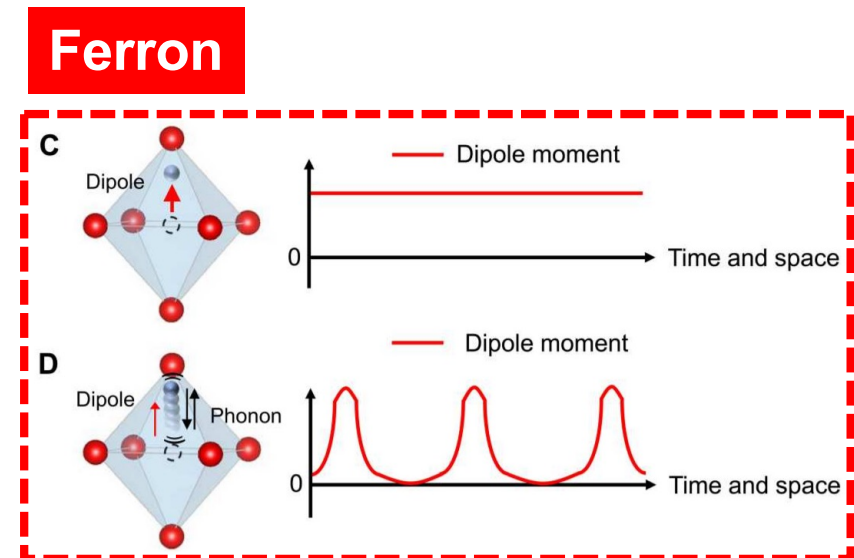
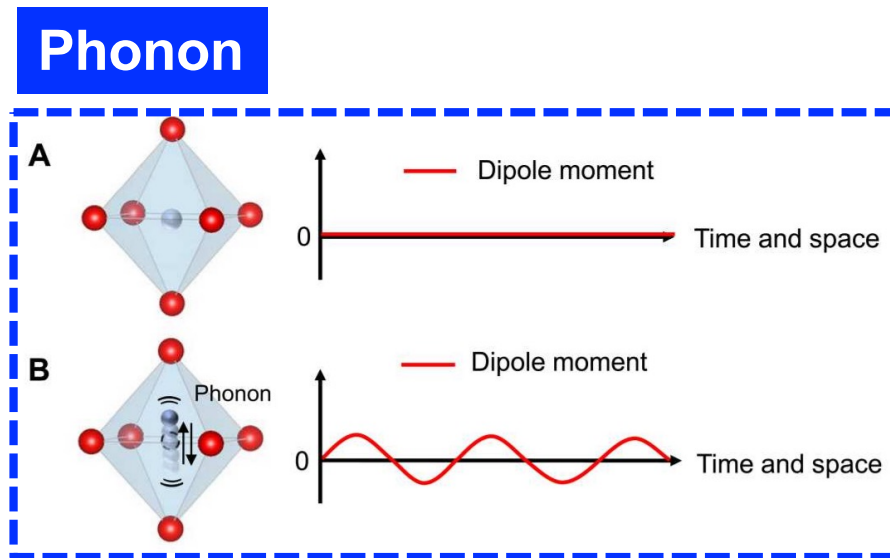
SCIENCE ADVANCES | RESEARCH ARTICLE

Sci. Adv. 9, eadd7194 (2023)

PHYSICS

Electric field–dependent phonon spectrum and heat conduction in ferroelectrics

Brandi L. Wooten¹, Ryo Iguchi², Ping Tang³, Joon Sang Kang⁴, Ken-ichi Uchida^{2,5},
Gerrit E. W. Bauer^{3,5,6,7,8}, Joseph P. Heremans^{1,4,9*}



Wooten et al.,
Sci. Adv. 9, eadd7194 (2023)

Pb(Zr, Ti)O₃

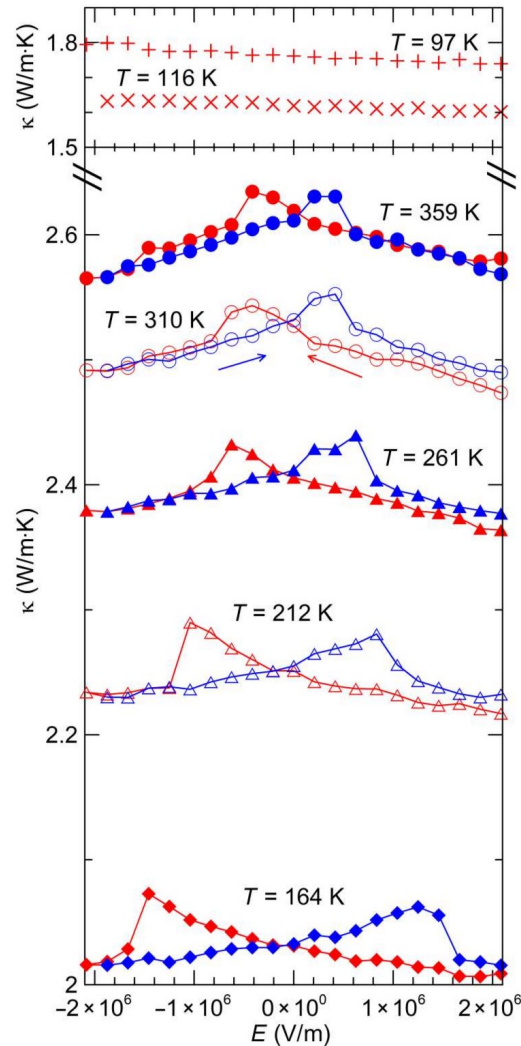


Fig. 5. Electric field dependence of the thermal conductivity $\kappa(E, T)$ through the hysteresis loops. The coercive field exceeds the maximum field that could safely be applied to the sample at $T < 160$ K so that only one branch of the hysteresis loop is shown at 116 K and below, which still allows for the determination of κ'/κ .

Specific heat: $C \sim 3N$ (Dulong-Petit @ high temp.)

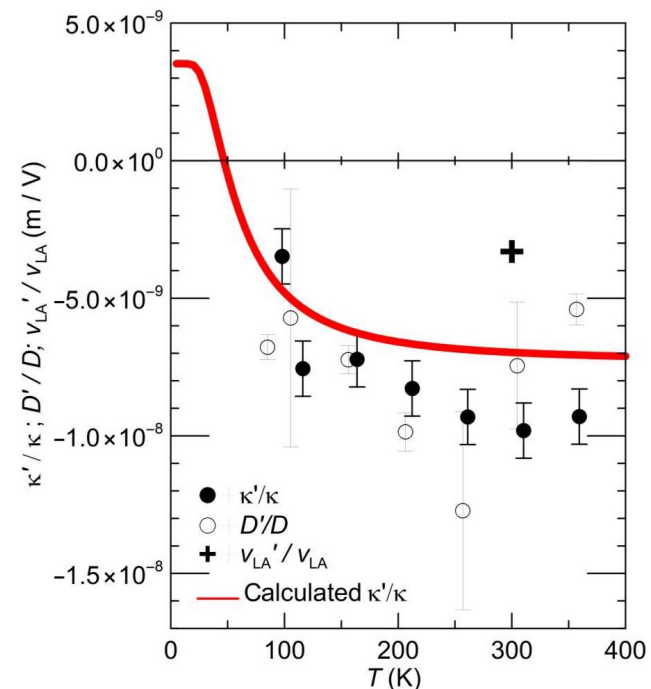
Thermal conductivity: $\kappa = \frac{1}{3} C v^2 \tau \propto v^2$

Assume E-dependence comes solely from v , then

$$\frac{\kappa'}{\kappa} = 2 \frac{v'}{v}$$

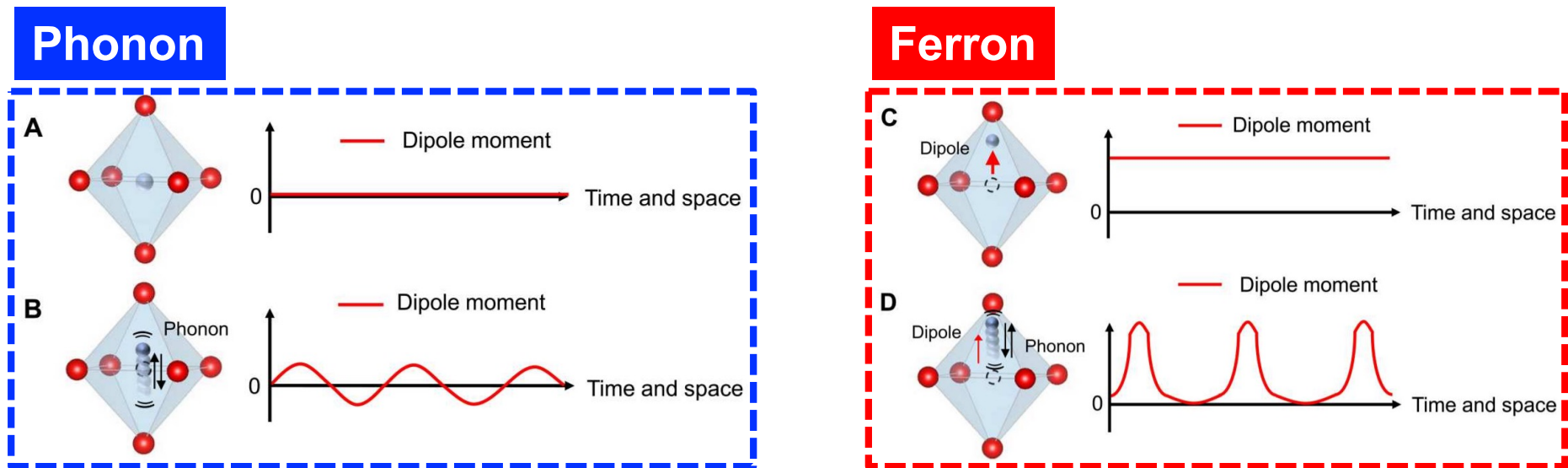
(E dependence, not due to the decreasing domain walls)

E-dependent κ means
“phonon+dipole = ferron”!!



Motivation & Purpose

The system discussed so far is a ferroelectricity of **ion-displacement type**.



In the case of the displacement-type ferroelectrics, distinction between “phonon” and “ferron” is elusive.

We would like to pursue the possibility of defining the polarization current purely electronically, by considering a model of **electronic ferroelectricity**.

Electronic ferroelectricity

nature

Vol 436|25 August 2005|doi:10.1038/nature04039

Ferroelectricity from iron valence ordering in the charge-frustrated system LuFe_2O_4

Naoshi Ikeda¹, Hiroyuki Ohsumi¹, Kenji Ohwada², Kenji Ishii², Toshiya Inami², Kazuhisa Kakurai³, Youichi Murakami⁴, Kenji Yoshii², Shigeo Mori⁵, Yoichi Horibe⁵ & Hijiri Kitô⁶

Scientific Reports | (2021) 11:4277



Direct evidence of electronic ferroelectricity in YbFe_2O_4 using neutron diffraction and nonlinear spectroscopy

K. Fujiwara^{1,2}, Y. Fukada¹, Y. Okuda¹, R. Seimiya¹, N. Ikeda¹, K. Yokoyama³, H. Yu³, S. Koshihara³ & Y. Okimoto³✉



Magnetodielectric phenomena in a charge- and spin-frustrated system of layered iron oxide

Makoto Naka, Aya Nagano,* and Sumio Ishihara

Department of Physics, Tohoku University, Sendai 980-8578, Japan

(Received 3 March 2008; revised manuscript received 24 April 2008; published 27 June 2008)

Dielectric and magnetic phenomena in spin- and charge-frustrated system $R\text{Fe}_2\text{O}_4$ (R is a rare-earth metal ion) are studied. An electronic model for charge, spin, and orbital degrees in a pair of triangular-lattice planes is derived. We analyze this model by utilizing the mean-field approximation and the Monte Carlo simulation in a finite size cluster. A threefold-type charge-ordered structure with charge imbalance between the planes is stabilized in finite temperatures. This polar charge order is reinforced by spin ordering of Fe ions. This magnetodielectric phenomenon is caused by spin frustration and charge-spin coupling in the exchange interaction. We show cross-correlation effect in magnetic- and electric-field responses. Oxygen-deficiency effect as an impurity effect in a frustrated charge-spin coupled system is also examined.

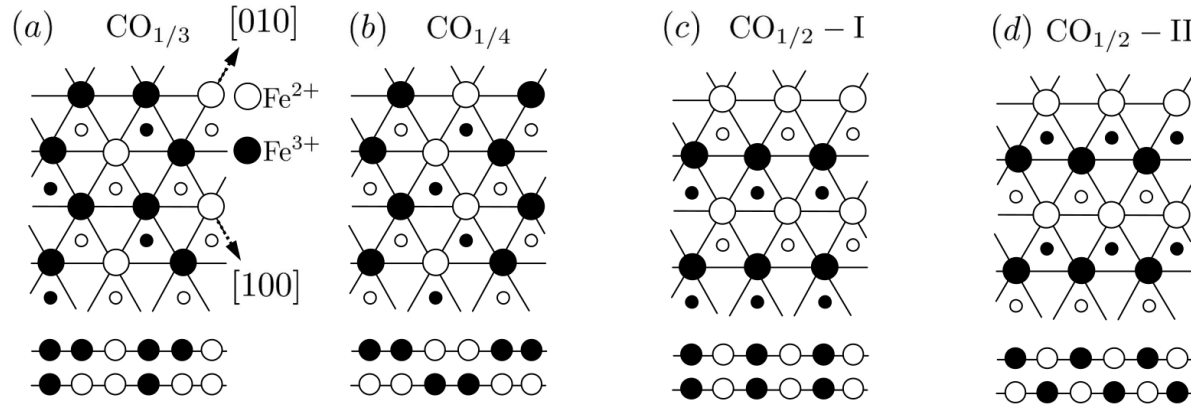


FIG. 5. Charge structures in a W layer: (a) $\text{CO}_{1/3}$, (b) $\text{CO}_{1/4}$, (c) $\text{CO}_{1/2}$ -I, and (d) $\text{CO}_{1/2}$ -II. The filled and open circles represent Fe^{3+} and Fe^{2+} , respectively, and large and small circles are for Fe ions in the upper and lower planes, respectively. Lower panel in each figure is a side view from $[1\bar{1}0]$.

We use much simpler model.

Excitonic insulator model of ferroelectricity

Excitonic insulator as a ferroelectric material

É. G. Batyev and V. A. Borisjuk

Institute of Semiconductor Physics, USSR Academy of Sciences, Siberian Branch

(Submitted 16 July 1980)

Pis'ma Zh. Eksp. Teor. Fiz. **32**, No. 6, 419–422 (20 September 1980)

It is shown that an excitonic dielectric with a resolved dipole transition is a ferroelectric material.

PACS numbers: 77.80. — e

The purpose of this paper is to focus attention on the fact that an excitonic dielectric with an allowed dipole transition is polarized. The known mechanisms for ferroelectricity are in some way associated with a lattice; however, here we have a new, purely electronic mechanism: polarization occurs as a result of transition to the excitonic dielectric state caused by an attraction between electrons and holes.

The effective Hamiltonian of an excitonic dielectric with an allowed dipole transition in a two-band approximation has the form¹

$$H = \begin{pmatrix} \xi & \Delta \\ \Delta^* & -\xi \end{pmatrix}, \quad \Delta = \Delta_0 + \mathbf{p}\mathbf{v}_{12}. \quad (1)$$

Our Model Theory of electronic ferroelectricity

Phys. Rev. B 54, 17452 (1996)

T. Portengen,* Th. Östreich,† and L. J. Sham

See also Batyev & Borisjuk,
JETP Lett. 32, 395 (1980)

Department of Physics, University of California San Diego, La Jolla, California 92093-0319

(Received 28 May 1996; revised manuscript received 20 September 1996)

We present a theory of the linear and nonlinear optical characteristics of the insulating phase of the Falicov-Kimball model within the self-consistent mean-field approximation.

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1,$$

$$\epsilon_p = \epsilon_{min} + \frac{W}{6}(3 - \cos p_x - \cos p_y - \cos p_z)$$

$$\mathcal{H}_0 = \sum_{\mathbf{p}} \begin{pmatrix} d_{\mathbf{p}}^\dagger & f_{\mathbf{p}}^\dagger \end{pmatrix} \begin{pmatrix} \epsilon_{\mathbf{p}} & V_{\mathbf{p}} \\ V_{\mathbf{p}}^* & E_0 \end{pmatrix} \begin{pmatrix} d_{\mathbf{p}} \\ f_{\mathbf{p}} \end{pmatrix} = \sum_{\mathbf{p}} \psi_{\mathbf{p}}^\dagger \hat{h}_0(\mathbf{p}) \psi_{\mathbf{p}}$$

$$V_p = iV(\sin p_x + \sin p_y + \sin p_z)$$

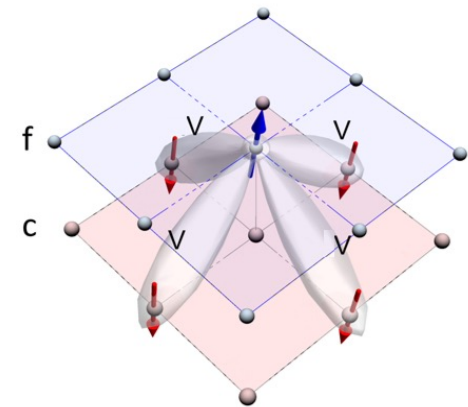
[see also Sandu, PRB 72, (2005)]

$$\mathcal{H}_1 = \frac{U}{N} \sum_{\mathbf{k}} \left(\sum_{\mathbf{p}} d_{\mathbf{p}}^\dagger d_{\mathbf{p}-\mathbf{k}} \right) \left(\sum_{\mathbf{p}'} f_{\mathbf{p}'}^\dagger f_{\mathbf{p}'+\mathbf{k}} \right)$$

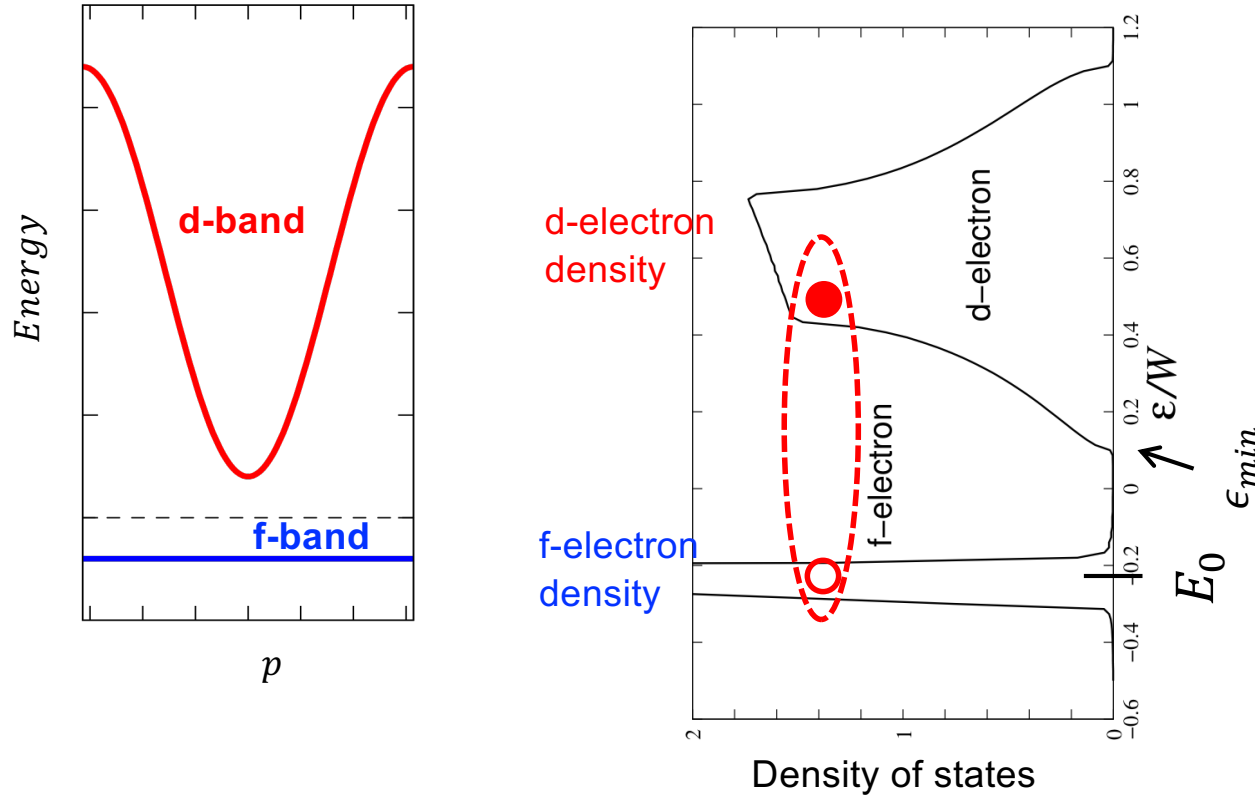
d-electron density f-electron density

Possible application:
SmB₆, Sm₃Se₄, etc

From Alexandrov et al.,
PRL 114, 177202 (2015),
with minor modification.



Density of states



Possible application:
SmB₆, Sm₃Se₄, etc

$$\langle \Delta_q \rangle = -\frac{1}{\sqrt{N}} \sum_p \langle f_p^\dagger d_{p+q} \rangle$$

$$\epsilon_p = \epsilon_{min} + \left(\frac{W}{6}\right)(3 - \cos p_x - \cos p_y - \cos p_z)$$

FIG. 1. An example of the density of states considered in this work as a function of energy in the non-interacting case ($U = 0$) for $\epsilon_{min}/W = 0.1$, $V/W = 0.1$, and $E_0/W = -0.2$, where W is the d -electron bandwidth.

Green's function

$$\mathcal{H}_0 = \sum_{\mathbf{p}} (d_{\mathbf{p}}^\dagger, f_{\mathbf{p}}^\dagger) \begin{pmatrix} \varepsilon_{\mathbf{p}}, & V_{\mathbf{p}} \\ V_{\mathbf{p}}^*, & E_0 \end{pmatrix} \begin{pmatrix} d_{\mathbf{p}} \\ f_{\mathbf{p}} \end{pmatrix} = \sum_{\mathbf{p}} \psi_{\mathbf{p}}^\dagger \hat{h}_0(\mathbf{p}) \psi_{\mathbf{p}}$$

$$\hat{G} = - \left(\partial_\tau + \hat{h}_0 \right)^{-1}$$

$$\begin{aligned} \hat{G}(\mathbf{p}, i\varepsilon_n) &= \begin{pmatrix} G_1(\mathbf{p}, i\varepsilon_n), & G_2(\mathbf{p}, i\varepsilon_n) \\ G_3(\mathbf{p}, i\varepsilon_n), & G_4(\mathbf{p}, i\varepsilon_n) \end{pmatrix} \\ &= \frac{1}{D(\mathbf{p}, i\varepsilon_n)} \begin{pmatrix} i\varepsilon_n - E_0, & V_{\mathbf{p}} \\ V_{\mathbf{p}}^*, & i\varepsilon_n - \epsilon_{\mathbf{p}} \end{pmatrix} \end{aligned}$$

$$D(\mathbf{p}, i\varepsilon_n) = (i\varepsilon_n - \lambda_{\mathbf{p}}^+)(i\varepsilon_n - \lambda_{\mathbf{p}}^-)$$

$$\lambda_{\mathbf{p}}^\pm = Q_{\mathbf{p}} \pm R_{\mathbf{p}},$$

$$Q_{\mathbf{p}} = \frac{\varepsilon_{\mathbf{p}} + E_0}{2},$$

$$R_{\mathbf{p}} = \sqrt{\left(\frac{\varepsilon_{\mathbf{p}} - E_0}{2} \right)^2 + |V_{\mathbf{p}}|^2}.$$

$$G_1 \text{ —————}$$

$$G_2 \text{ —————} \times \text{-----}$$

$$G_3 \text{ -----} \times \text{—————}$$

$$G_4 \text{ -----}$$

Effective (bosonic) action by functional integral

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1,$$

$$\mathcal{H}_1 = \frac{U}{N} \sum_{\mathbf{k}, \mathbf{p}, \mathbf{p}'} \left(d_{\mathbf{p}}^\dagger d_{\mathbf{p}-\mathbf{k}} \right) \left(f_{\mathbf{p}'}^\dagger f_{\mathbf{p}'+\mathbf{k}} \right) = -\frac{U}{N} \sum_{\mathbf{q}} \left(\sum_{\mathbf{p}} d_{\mathbf{p}+\mathbf{q}}^\dagger f_{\mathbf{p}} \right) \left(\sum_{\mathbf{p}'} f_{\mathbf{p}'}^\dagger d_{\mathbf{p}'+\mathbf{q}} \right)$$

Introduce new momentum q by
 $k = p - p' - q$
 $p \rightarrow p + q$
 $\equiv B_q^\dagger$
 $\equiv B_q$

Action

$$\mathcal{S} = \int_0^\beta d\tau \left\{ \psi_{\mathbf{p}}^\dagger \partial_\tau \psi_{\mathbf{p}} + \mathcal{H} \right\} = \int_0^\beta d\tau \left\{ \sum_{\mathbf{p}} \psi_{\mathbf{p}}^\dagger (\partial_\tau + \hat{h}_0(\mathbf{p})) \psi_{\mathbf{p}} - \frac{U}{N} \sum_{\mathbf{q}} B_q^\dagger B_q \right\}$$

$$1 = \int \mathcal{D}[\xi, \xi^*] \exp \left(-\frac{1}{U} \sum_{\mathbf{q}} \int_0^\beta d\tau \xi_{\mathbf{q}}^* \xi_{\mathbf{q}} \right)$$

Insert the identity of unity

$$\xi_{\mathbf{q}} = \Delta_{\mathbf{q}} + \frac{U}{\sqrt{N}} B_{\mathbf{q}}$$

Shift transformation

$$\langle \Delta_{\mathbf{q}} \rangle = -\frac{1}{\sqrt{N}} \sum_{\mathbf{p}} \langle f_{\mathbf{p}}^\dagger d_{\mathbf{p}+\mathbf{q}} \rangle$$

$$\mathcal{Z} = \int \mathcal{D}[\psi, \psi^\dagger] e^{-\mathcal{S}} = \int \mathcal{D}[\Delta, \Delta^*] e^{-\frac{1}{U} \int_0^\beta d\tau \sum_{\mathbf{q}} \Delta_{\mathbf{q}}^* \Delta_{\mathbf{q}}} \int \mathcal{D}[\psi, \psi^\dagger] e^{-\mathcal{S}'}$$

New action

$$\mathcal{S}' = \int_0^\beta d\tau \sum_{\mathbf{p}, \mathbf{p}'} \psi_{\mathbf{p}}^\dagger \left([\partial_\tau + \hat{h}_0(\mathbf{p})] \delta_{\mathbf{p}, \mathbf{p}'} + \hat{h}_1(\mathbf{p}, \mathbf{p}') \right) \psi_{\mathbf{p}'}$$

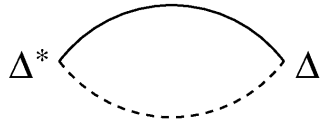
$$\hat{h}_1(\mathbf{p}, \mathbf{p}') = \frac{1}{\sqrt{N}} \begin{pmatrix} 0, & \Delta_{\mathbf{p}-\mathbf{p}'} \\ \Delta_{\mathbf{p}'-\mathbf{p}}^*, & 0 \end{pmatrix}$$

Integrating out electrons $\rightarrow$ Effective action $\mathcal{Z} = \mathcal{Z}_0 \times \int \mathcal{D}[\Delta, \Delta^*] \exp\{-\mathcal{S}_{\text{eff}}\}$

$$\mathcal{S}_{\text{eff}} = \int_0^\beta d\tau \sum_{\mathbf{q}} \frac{1}{U} \Delta_{\mathbf{q}}^* \Delta_{\mathbf{q}} + \text{Tr} \sum_{l=1}^{\infty} \frac{1}{l} \left(\widehat{G} \widehat{h}_1 \right)^l = \mathcal{S}_1 (\text{only when } \mathbf{E} \neq 0) + \mathcal{S}_2 + \mathcal{S}_4 + \dots$$

Quadratic term of the effective action

$$\mathcal{S}_2 = \frac{1}{2} \sum_{\mathbf{q}} \left(a_1(\mathbf{q}) \Delta_{\mathbf{q}}^* \Delta_{\mathbf{q}} + a_2(\mathbf{q}) \Delta_{\mathbf{q}}^* \Delta_{-\mathbf{q}}^* + a_3(\mathbf{q}) \Delta_{\mathbf{q}} \Delta_{-\mathbf{q}} \right)$$



$$a_1(\mathbf{q}) = 2 \left(\frac{1}{U} + \frac{T}{N} \sum_{\mathbf{p}} G_1(\mathbf{p} + \mathbf{q}) G_4(\mathbf{p}) \right)$$



$$a_2(\mathbf{q}) = \frac{T}{N} \sum_{\mathbf{p}} G_2(\mathbf{p} + \mathbf{q}) G_2(\mathbf{p}),$$

$$a_3(\mathbf{q}) = \frac{T}{N} \sum_{\mathbf{p}} G_3(\mathbf{p} + \mathbf{q}) G_3(\mathbf{p}),$$

$$\begin{aligned} a_1(\mathbf{q}, 0) - a_1(\mathbf{0}, 0) &= \xi_1^2 q^2, \\ a_2(\mathbf{q}, 0) - a_2(\mathbf{0}, 0) &= \xi_2^2 q^2, \\ a_3(\mathbf{q}, 0) - a_3(\mathbf{0}, 0) &= \xi_3^2 q^2, \end{aligned}$$

$$\xi_1^2 = 2 \frac{T}{N} \sum_{\mathbf{p}} [G_1(\mathbf{p})]^2 G_4(\mathbf{p}) \left\{ G_1(\mathbf{p}) \frac{v_{\mathbf{p}}^2}{3} + \frac{M_{\mathbf{p}}^2}{3} \right\},$$

$$\xi_2^2 = \frac{T}{N} \sum_{\mathbf{p}} G_1(\mathbf{p}) [G_2(\mathbf{p})]^2 \left\{ G_1(\mathbf{p}) \frac{v_{\mathbf{p}}^2}{3} + \frac{M_{\mathbf{p}}^2}{3} \right\}$$

$$\xi_3^2 = \frac{T}{N} \sum_{\mathbf{p}} G_1(\mathbf{p}) [G_3(\mathbf{p})]^2 \left\{ G_1(\mathbf{p}) \frac{v_{\mathbf{p}}^2}{3} + \frac{M_{\mathbf{p}}^2}{3} \right\}$$

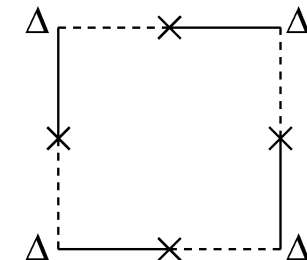
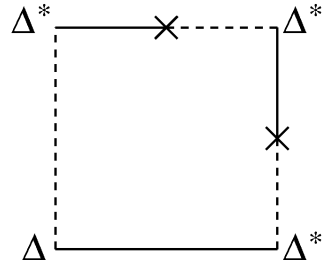
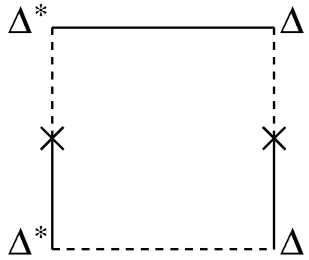
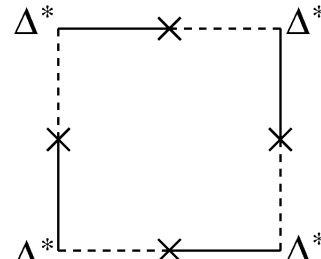
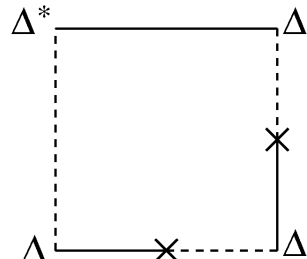
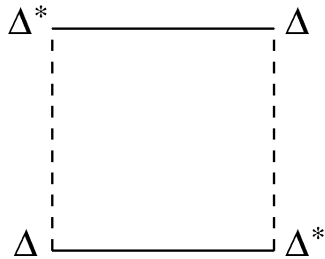
Quartic term of the effective action

$$\mathcal{S}_4 = \frac{T}{4N} \sum_{\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3, \mathbf{q}_4} \delta_{\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3 + \mathbf{q}_4, 0}$$

$$\times \left\{ (b_1 + b_2) \Delta_{-\mathbf{q}_1}^* \Delta_{-\mathbf{q}_2}^* \Delta_{\mathbf{q}_3} \Delta_{\mathbf{q}_4} \right. \\ + b_3 \Delta_{-\mathbf{q}_1}^* \Delta_{\mathbf{q}_2} \Delta_{\mathbf{q}_3} \Delta_{\mathbf{q}_4} + b_4 \Delta_{-\mathbf{q}_1}^* \Delta_{-\mathbf{q}_2}^* \Delta_{-\mathbf{q}_3}^* \Delta_{\mathbf{q}_4} \\ \left. + b_5 \Delta_{-\mathbf{q}_1}^* \Delta_{-\mathbf{q}_2}^* \Delta_{-\mathbf{q}_3}^* \Delta_{-\mathbf{q}_4}^* + b_6 \Delta_{\mathbf{q}_1} \Delta_{\mathbf{q}_2} \Delta_{\mathbf{q}_3} \Delta_{\mathbf{q}_4} \right\}$$

$$\mathbf{p} = (\mathbf{p}, i\epsilon_n)$$

$$\mathbf{q} = (\mathbf{q}, i\omega_m)$$



$$b_1 = 2 \frac{T}{N} \sum_{\mathbf{p}} (G_1(\mathbf{p}))^2 (G_4(\mathbf{p}))^2,$$

$$b_2 = 4 \frac{T}{N} \sum_{\mathbf{p}} G_1(\mathbf{p}) G_2(\mathbf{p}) G_3(\mathbf{p}) G_4(\mathbf{p}),$$

$$b_3 = 4 \frac{T}{N} \sum_{\mathbf{p}} G_1(\mathbf{p} + \mathbf{q}) (G_3(\mathbf{p}))^2 G_4(\mathbf{p}),$$

$$b_4 = 4 \frac{T}{N} \sum_{\mathbf{p}} G_1(\mathbf{p} + \mathbf{q}) (G_2(\mathbf{p}))^2 G_4(\mathbf{p}),$$

$$b_5 = \frac{T}{N} \sum_{\mathbf{p}} (G_2(\mathbf{p}))^4,$$

$$b_6 = \frac{T}{N} \sum_{\mathbf{p}} (G_3(\mathbf{p}))^4.$$

Mean-field approximation & Gaussian fluctuations

$$\Delta_{\mathbf{q}} = \sqrt{\beta N} \delta_{\mathbf{q},0} \Delta_0 + \delta \Delta_{\mathbf{q}}$$

$$a_0 = a_1(0) + a_2(0) + a_3(0) \\ \propto T - T_c$$

$$\mathcal{S}_{\text{GL}} = \mathcal{S}_2 + \mathcal{S}_4 \rightarrow \beta F_{\text{MFA}} + \mathcal{S}_{\text{gauss}}$$

$$b_0 = \sum_{i=1}^6 b_i$$

$$F_{\text{MFA}} = N \left(\frac{a_0}{2} \Delta_0^2 + \frac{b_0}{4} \Delta_0^4 \right)$$

$$\Delta_0^2 = \frac{|a_0|}{b_0}$$

$$\mathcal{S}_{\text{gauss}} = \sum_{\mathbf{q}} (\delta \Delta_{\mathbf{q}}^*, \delta \Delta_{-\mathbf{q}}) \begin{pmatrix} A(\mathbf{q}) & B(\mathbf{q}) \\ B^*(\mathbf{q}) & A(\mathbf{q}) \end{pmatrix} \begin{pmatrix} \delta \Delta_{\mathbf{q}} \\ \delta \Delta_{-\mathbf{q}}^* \end{pmatrix}$$

$$\begin{pmatrix} \alpha_{\mathbf{q}} \\ \beta_{\mathbf{q}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \delta \Delta_{\mathbf{q}} - \delta \Delta_{-\mathbf{q}}^* \\ \delta \Delta_{\mathbf{q}} + \delta \Delta_{-\mathbf{q}}^* \end{pmatrix}$$

$$A(\mathbf{q}) = \frac{a_1(\mathbf{q})}{4} + \frac{4b_1 + 4b_2 + 3b_3 + 3b_4}{8} \Delta_0^2, \\ B(\mathbf{q}) = \frac{a_2(\mathbf{q})}{2} + \frac{b_1 + b_2 + 3b_4 + 6b_5}{4} \Delta_0^2,$$

$$\mathcal{S}_{\text{gauss}} = \sum_{\mathbf{q}} \left(\underbrace{\Lambda_{-}(\mathbf{q}) \alpha_{\mathbf{q}}^* \alpha_{\mathbf{q}}}_{\text{phase mode}} + \underbrace{\Lambda_{+}(\mathbf{q}) \beta_{\mathbf{q}}^* \beta_{\mathbf{q}}}_{\text{amplitude mode}} \right)$$

Numerical evaluation of the model

50 x 50 x 50 cubic lattice

Density of states

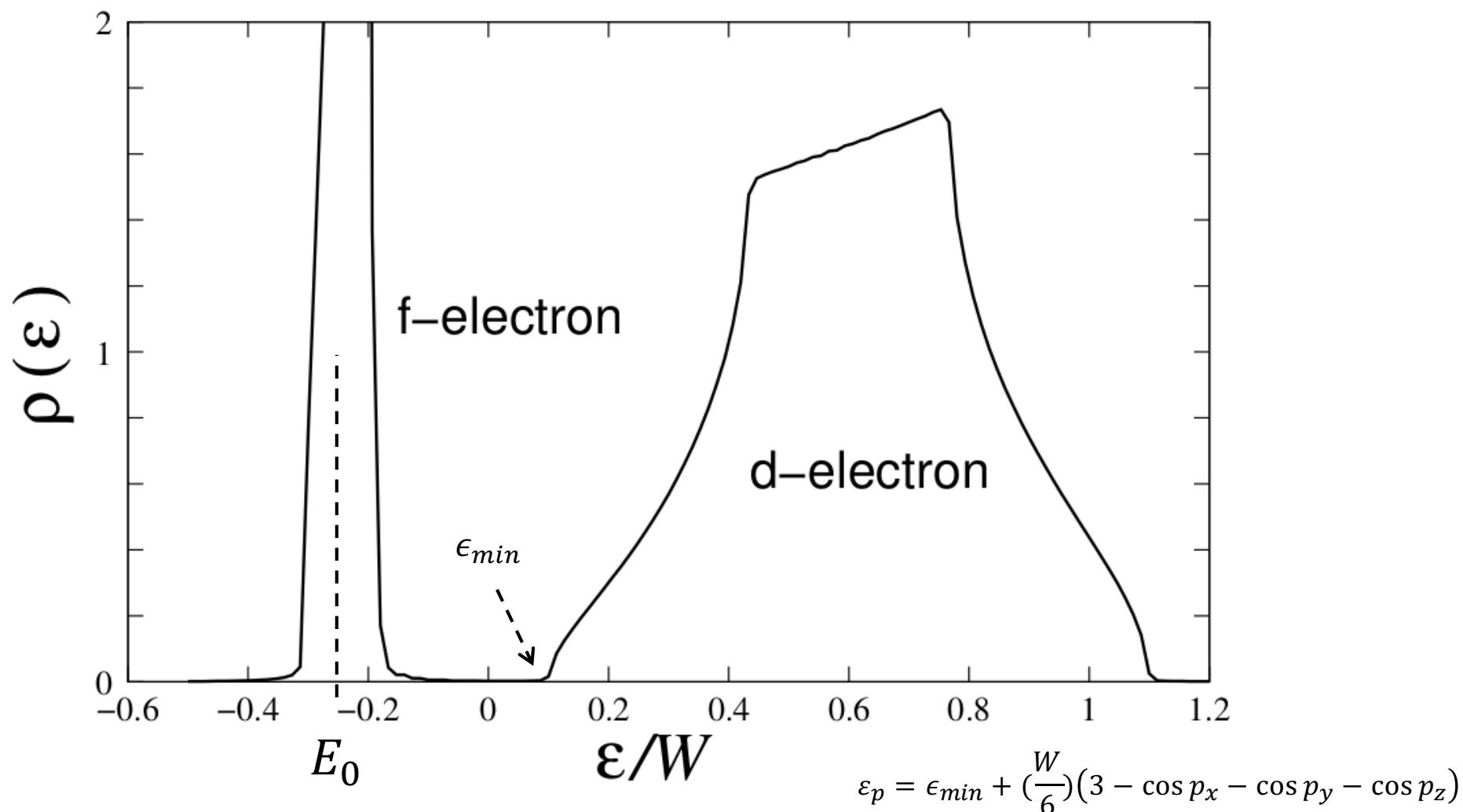
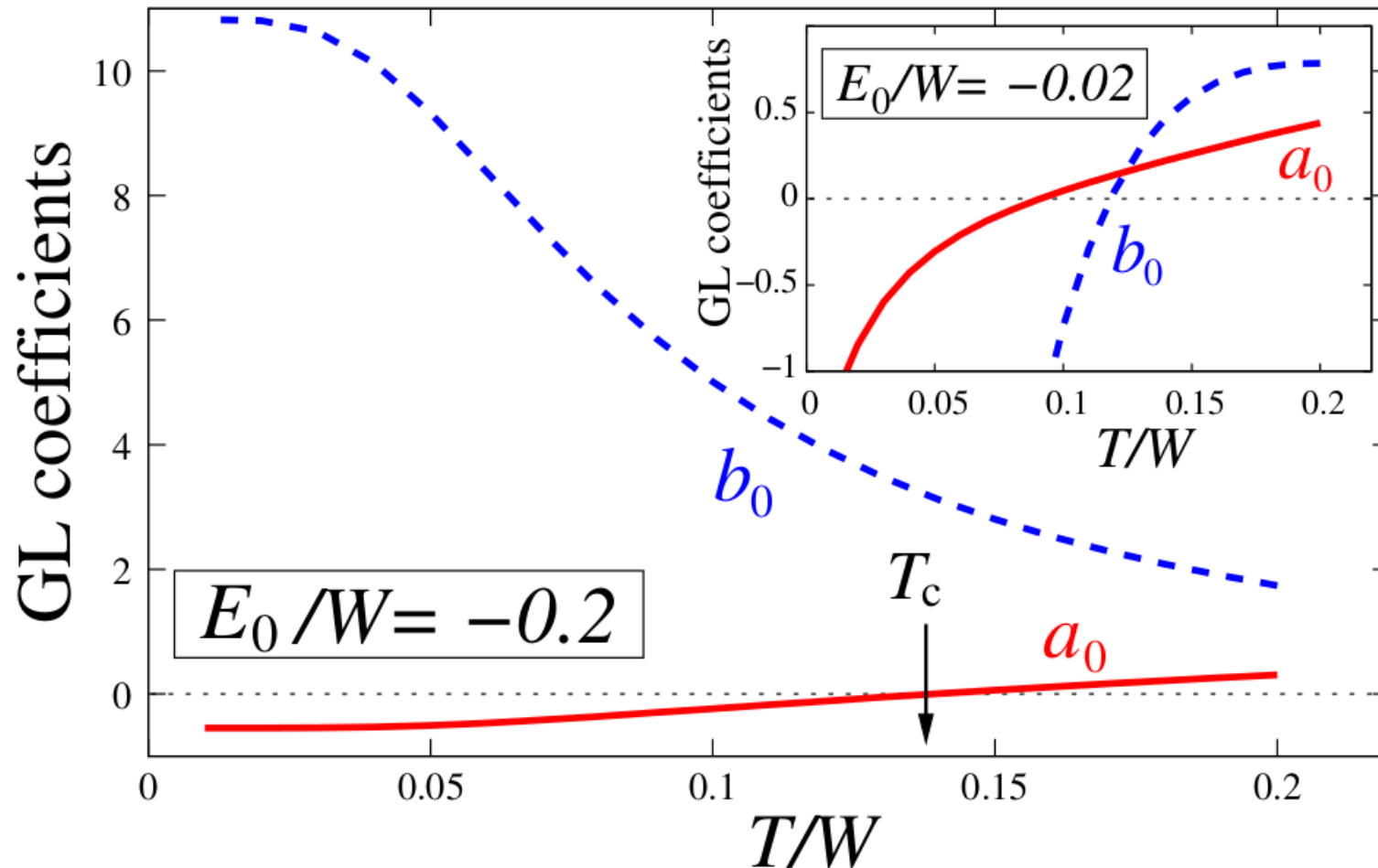


FIG. 1. An example of the density of states considered in this work as a function of energy in the non-interacting case ($U = 0$) for $\epsilon_{\min}/W = 0.1$, $V/W = 0.1$, and $E_0/W = -0.2$, where W is the d -electron bandwidth.

W : d -band width

Evaluation of the GL coefficients

$$F_{\text{MFA}} = N \left(\frac{a_0}{2} \Delta_0^2 + \frac{b_0}{4} \Delta_0^4 \right)$$



W: d-band width

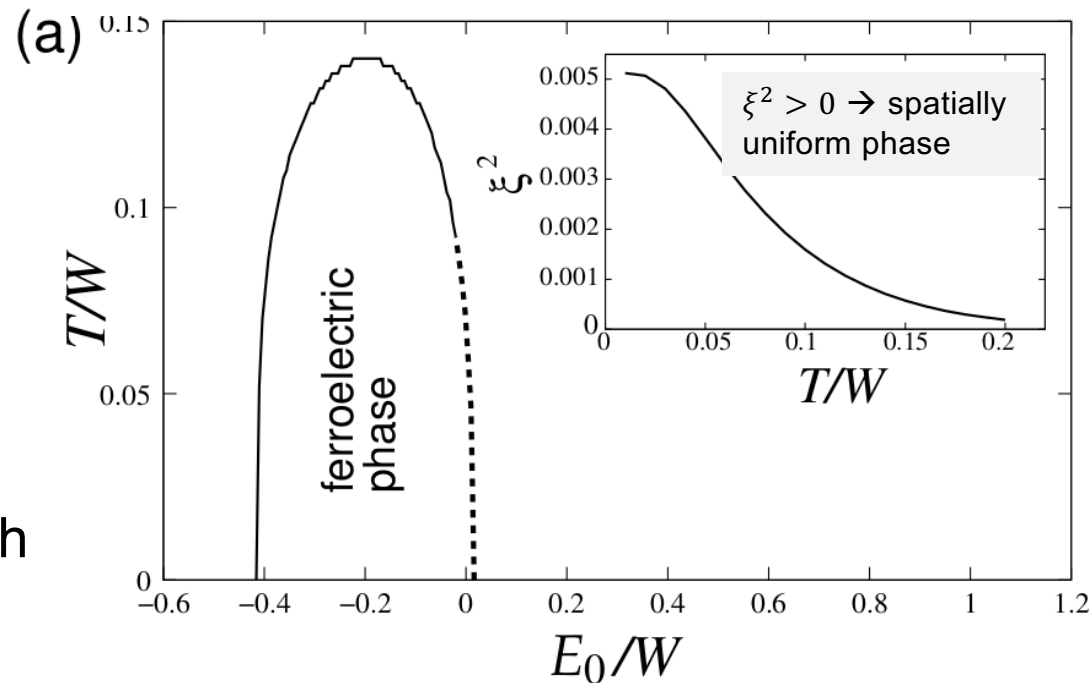
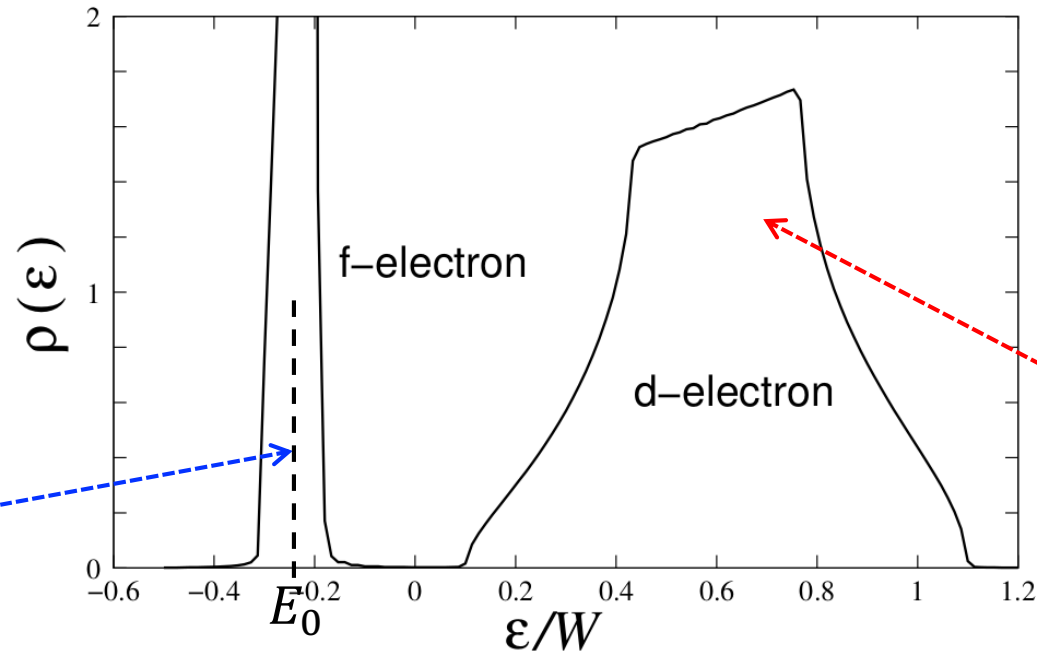
Phase diagram

$$\epsilon_{min} = 0.1,$$

$$\frac{V}{W} = 0.1,$$

$$\frac{U}{W} = 1.0$$

f-band position:
varied



W: d-band width

$$\begin{aligned} a_1(\mathbf{q}, 0) - a_1(\mathbf{0}, 0) &= \xi_1^2 q^2, \\ a_2(\mathbf{q}, 0) - a_2(\mathbf{0}, 0) &= \xi_2^2 q^2, \\ a_3(\mathbf{q}, 0) - a_3(\mathbf{0}, 0) &= \xi_3^2 q^2, \end{aligned}$$

$$\xi^2 = \xi_1^2 + \xi_2^2 + \xi_3^2$$

Collective modes (Gaussian action)

$$\mathcal{S}_{\text{GL}} = \mathcal{S}_2 + \mathcal{S}_4 \rightarrow \beta F_{\text{MFA}} + \mathcal{S}_{\text{gauss}}.$$

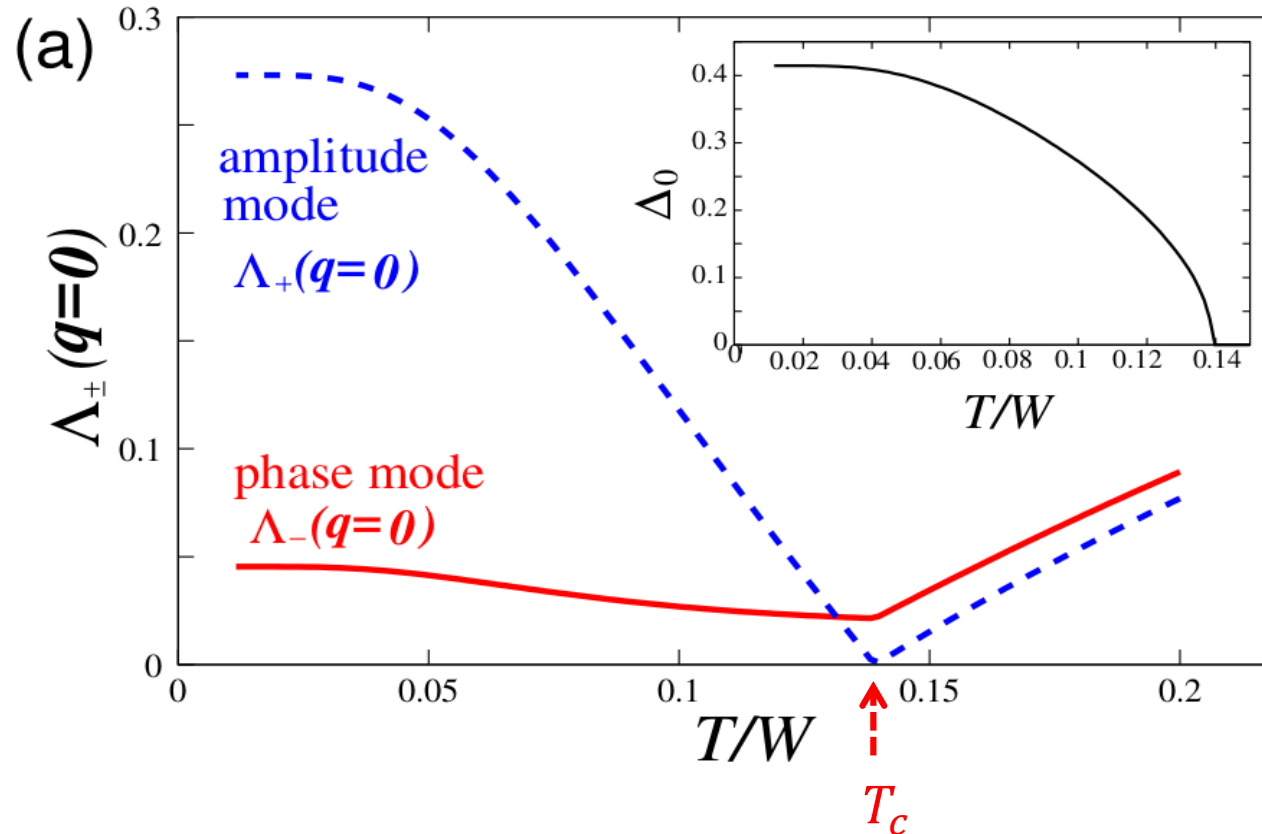
$$\Delta_{\mathbf{q}} = \sqrt{\beta N} \delta_{\mathbf{q},0} \Delta_0 + \delta \Delta_{\mathbf{q}}$$

$$A(\mathbf{q}) = \frac{a_1(\mathbf{q})}{4} + \frac{4b_1 + 4b_2 + 3b_3 + 3b_4}{8} \Delta_0^2,$$

$$B(\mathbf{q}) = \frac{a_2(\mathbf{q})}{2} + \frac{b_1 + b_2 + 3b_4 + 6b_5}{4} \Delta_0^2,$$

$$\begin{pmatrix} \delta \Delta_{\mathbf{q}} \\ \delta \Delta_{-\mathbf{q}}^* \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{q}} \\ \beta_{\mathbf{q}} \end{pmatrix}$$

$$\mathcal{S}_{\text{gauss}} = \sum_{\mathbf{q}} (\delta \Delta_{\mathbf{q}}^*, \delta \Delta_{-\mathbf{q}}) \begin{pmatrix} A(\mathbf{q}) & B(\mathbf{q}) \\ B^*(\mathbf{q}) & A(\mathbf{q}) \end{pmatrix} \begin{pmatrix} \delta \Delta_{\mathbf{q}} \\ \delta \Delta_{-\mathbf{q}}^* \end{pmatrix} = \sum_{\mathbf{q}} \left(\underbrace{\Lambda_{-}(\mathbf{q}) \alpha_{\mathbf{q}}^* \alpha_{\mathbf{q}}}_{\text{phase mode}} + \underbrace{\Lambda_{+}(\mathbf{q}) \beta_{\mathbf{q}}^* \beta_{\mathbf{q}}}_{\text{amplitude mode}} \right)$$



$$\epsilon_{\min} = 0.1,$$

$$\frac{V}{W} = 0.1,$$

$$\frac{U}{W} = 1.0$$

$$\frac{E_0}{W} = -0.2$$

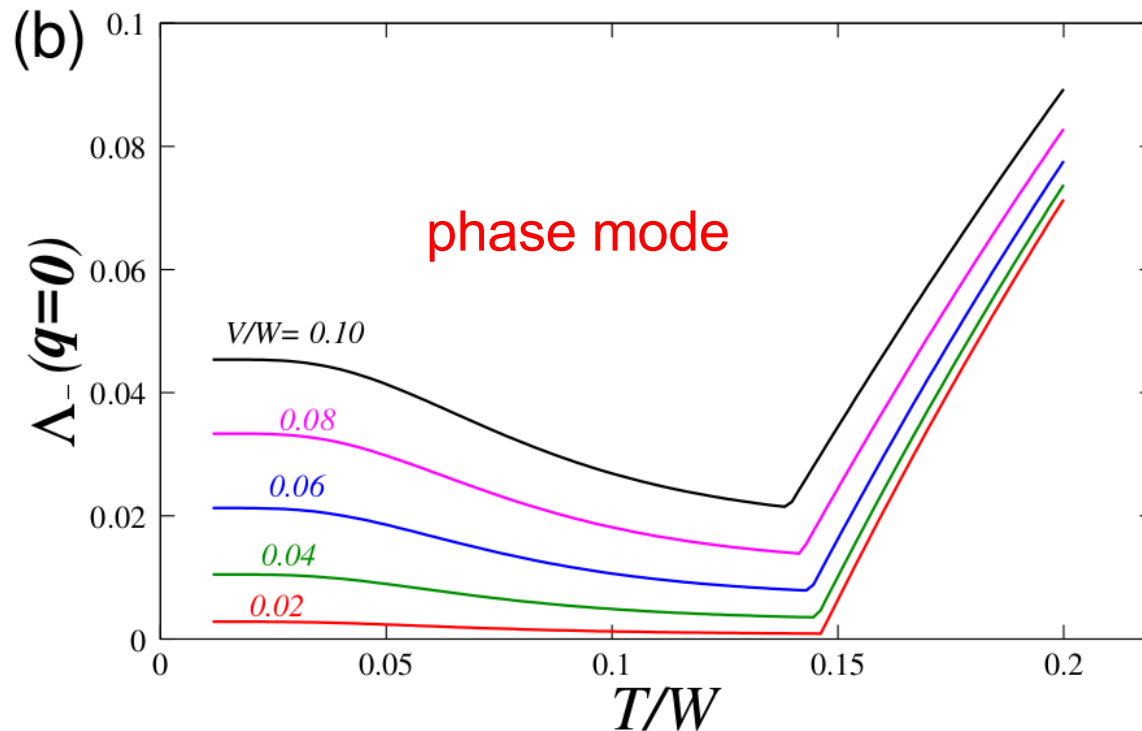
Collective modes (2)

$$\mathcal{S}_{\text{GL}} = \mathcal{S}_2 + \mathcal{S}_4 \rightarrow \beta F_{\text{MFA}} + \mathcal{S}_{\text{gauss}}.$$

$$\Delta_{\mathbf{q}} = \sqrt{\beta N} \delta_{\mathbf{q},0} \Delta_0 + \delta \Delta_{\mathbf{q}}$$

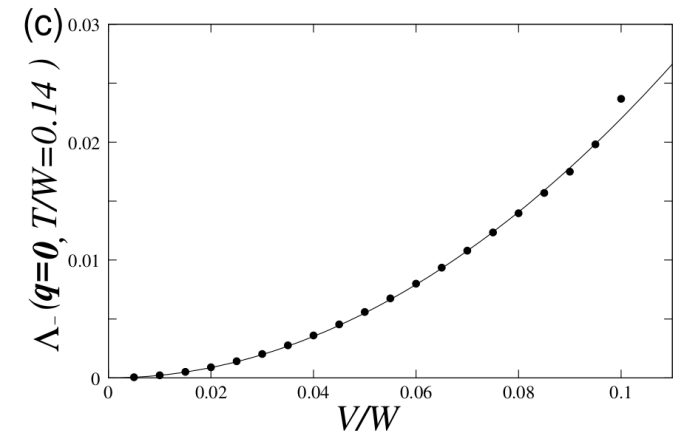
$$\begin{pmatrix} \delta \Delta_{\mathbf{q}} \\ \delta \Delta_{-\mathbf{q}}^* \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{q}} \\ \beta_{\mathbf{q}} \end{pmatrix}$$

$$\mathcal{S}_{\text{gauss}} = \sum_{\mathbf{q}} (\delta \Delta_{\mathbf{q}}^*, \delta \Delta_{-\mathbf{q}}) \begin{pmatrix} A(\mathbf{q}) & B(\mathbf{q}) \\ B^*(\mathbf{q}) & A(\mathbf{q}) \end{pmatrix} \begin{pmatrix} \delta \Delta_{\mathbf{q}} \\ \delta \Delta_{-\mathbf{q}}^* \end{pmatrix} = \sum_{\mathbf{q}} \left(\underbrace{\Lambda_{-}(\mathbf{q}) \alpha_{\mathbf{q}}^* \alpha_{\mathbf{q}}}_{\text{phase mode}} + \underbrace{\Lambda_{+}(\mathbf{q}) \beta_{\mathbf{q}}^* \beta_{\mathbf{q}}}_{\text{amplitude mode}} \right)$$



$$A(\mathbf{q}) = \frac{a_1(\mathbf{q})}{4} + \frac{4b_1 + 4b_2 + 3b_3 + 3b_4}{8} \Delta_0^2,$$

$$B(\mathbf{q}) = \frac{a_2(\mathbf{q})}{2} + \frac{b_1 + b_2 + 3b_4 + 6b_5}{4} \Delta_0^2,$$



Electric polarization

Scalar potential

$$\mathcal{H}_{\text{ext}} = -|e| \sum_{\mathbf{K}} \sum_{\mathbf{p}} \phi_{\mathbf{K}} (d_{\mathbf{p}+\mathbf{K}}^\dagger d_{\mathbf{p}} + f_{\mathbf{p}+\mathbf{K}}^\dagger f_{\mathbf{p}}), \quad \mathbf{E} = -i\mathbf{K} \phi_{\mathbf{K}}$$

Action (free energy) linear in E $S_1 = \beta F_1 = -\beta \sum_{\mathbf{r}_j} \mathbf{P}(\mathbf{r}_j) \cdot \mathbf{E}$

$$\mu = \mu_a + \mu_b,$$

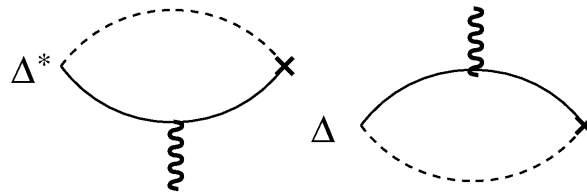
$$\mathbf{P}(\mathbf{r}_j) = \mu \left(\Delta(\mathbf{r}_j) + \Delta^*(\mathbf{r}_j) \right)$$

$$\mu_a = -|e| \frac{T}{N} \sum_{\mathbf{p}} (G_1(\mathbf{p}))^2 G_0(\mathbf{p}) \tilde{V}_p(\mathbf{v}_p \cdot \hat{\mathbf{e}}) \hat{\mathbf{e}},$$

$$\mu_b = -|e| \frac{T}{N} \sum_{\mathbf{p}} G_0(\mathbf{p}) G_1(\mathbf{p}) G_4(\mathbf{p}) \tilde{V}_p(\mathbf{v}_p \cdot \hat{\mathbf{e}}) \hat{\mathbf{e}},$$

$\tilde{V}_p = -iV_p$ is a pure real number

$$\hat{\mathbf{e}} = \mathbf{E}/E$$



In the momentum space, ...

$$P_q^z = P_{eq} + \delta P_q^z$$

The polarization dynamics is described by the amplitude mode

$$\delta P_q^z = \mu^z \left(\delta \Delta_q + \delta \Delta_{-q}^* \right) = \mu^z \sqrt{2} \beta_q$$

$$\begin{pmatrix} \alpha_q \\ \beta_q \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \delta \Delta_q - \delta \Delta_{-q}^* \\ \delta \Delta_q + \delta \Delta_{-q}^* \end{pmatrix}$$

Polarization dynamics

So far, we have constructed the quantum action for the excitonic insulator model of electronic ferroelectricity.

Below, we consider the polarization dynamics by mapping the quantum action to time-dependent Ginzburg-Landau eq.

Time-dependent GL eq. for amplitude mode

$$\mathcal{S}_{\text{gauss}} = \sum_{\mathbf{q}} (\delta\Delta_{\mathbf{q}}^*, \delta\Delta_{-\mathbf{q}}) \begin{pmatrix} A(\mathbf{q}), & B(\mathbf{q}) \\ B^*(\mathbf{q}), & A(\mathbf{q}) \end{pmatrix} \begin{pmatrix} \delta\Delta_{\mathbf{q}} \\ \delta\Delta_{-\mathbf{q}}^* \end{pmatrix} = \sum_{\mathbf{q}} (\Lambda_{-}(\mathbf{q})\alpha_{\mathbf{q}}^*\alpha_{\mathbf{q}} + \Lambda_{+}(\mathbf{q})\beta_{\mathbf{q}}^*\beta_{\mathbf{q}})$$

$$\frac{\partial}{\partial t}\beta_{\mathbf{q}} = -\gamma_{+}(\mathbf{q}) \frac{\partial \mathcal{H}_{\text{gauss}}}{\partial \beta_{\mathbf{q}}^*} = -\gamma_{+}(\mathbf{q})\Lambda_{+}(\mathbf{q})\beta_{\mathbf{q}}$$

$$\mathcal{S}_{\text{gauss}}|_{\text{classical limit}} = \beta\mathcal{H}_{\text{gauss}},$$

$\omega_m = 0$ component only

$$\mathbf{q} = (\mathbf{q}, i\omega_m)$$

C. Dominicis, Lett. Nuovo Cimento 12 (1975)

$$\Lambda_{\pm}(\mathbf{q}) = \Lambda_{\pm}(\mathbf{q}) + \frac{|\omega_m|}{\gamma_{\pm}(\mathbf{q})}$$

In the long-wavelength limit, the damping should be a diffusive form.

$$\gamma_{+}(\mathbf{q}) = \gamma_{+}(0) + D_{+}q^2$$

In the magnetic case, see

Fulde & Luther, PR 175, 337 (1968);

J. Hertz, PRB 14, 1165 (1976),

See also A. Millis, PRL 88, 217204 (2002).

Polarization diffusion eq.

$$\text{Recall } \delta P_{\mathbf{q}}^z = \mu^z (\delta\Delta_{\mathbf{q}} + \delta\Delta_{-\mathbf{q}}^*) = \mu^z \sqrt{2}\beta_{\mathbf{q}}.$$

$$\left(\frac{\partial}{\partial t} + \mathcal{D}_{+}^{\text{eff}} q^2 + \frac{1}{\tau_{+}^{\text{eff}}} \right) \delta P_{\mathbf{q}}^z = 0,$$

$$\mathcal{D}_{+}^{\text{eff}} = D_{+}\Lambda_{+}(0)$$

$$\frac{1}{\tau_{+}^{\text{eff}}} = \gamma_{+}(0)\Lambda_{+}(0)$$

Polarization current

The polarization diffusion eq. can be transformed into the continuity eq.

Polarization diffusion equation

$$\left(\frac{\partial}{\partial t} + \mathcal{D}_+^{\text{eff}} q^2 + \frac{1}{\tau_+^{\text{eff}}} \right) \delta P_q^z = 0 \quad \Rightarrow \quad \frac{\partial}{\partial t} \delta P^z(\mathbf{r}) + \text{div} \mathbf{J}_P + \frac{1}{\tau_+^{\text{eff}}} \delta P^z(\mathbf{r}) = 0$$

$$\mathcal{D}_+^{\text{eff}} = D_+ \Lambda_+(0) \quad \frac{1}{\tau_+^{\text{eff}}} = \gamma_+(0) \Lambda_+(0)$$

Polarization current

$$\mathbf{J}_P = -\mathcal{D}_+^{\text{eff}} \nabla \delta P^z(\mathbf{r})$$

$$P(\mathbf{r}_j) = \mu \left(\Delta(\mathbf{r}_j) + \Delta^*(\mathbf{r}_j) \right)$$

$$\delta P_q^z = \mu^z \left(\delta \Delta_q + \delta \Delta_{-q}^* \right) = \mu^z \sqrt{2} \beta_q$$

This polarization current is defined in terms of the electronic ferroelectricity order parameter Δ

Summary

- We have discussed the possibility of defining the polarization current purely electronically, by considering a model of electronic ferroelectricity.
- We indeed found a polarization current that is defined solely in terms of electronic ferroelectricity order parameter.
- ~~The “ferron” thermal conductivity is shown to exhibit a cusp at T_c .~~

Thank you very much for your attention!