“ Fundamentals of Thermodynamic Modelling of Materials ”

November 15-19, 2010
INSTN – CEA Saclay, France

PROFESSOR & TOPIC

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*Thermodynamics from
lattice dynamics with DFT*

[02001]

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density-functional perturbation theory for quasi-harmonic calculations

Stefano Baroni

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lecture given at the INSTN-CEA Winter school on *Fundamentals of Thermodynamic Modeling of Materials*
CEA-INSTN, Saclay, November 15-19, 2010

Sunday, November 14, 2010

the quasi-harmonic approximation

$$F(V, T, \lambda) = \begin{cases} -k_B T \log \left[\int e^{-\frac{v_\lambda(R)}{k_B T}} dR \right] \\ -k_B T \log \left[\sum_n e^{-\frac{E_n(V, \lambda)}{k_B T}} \right] \end{cases}$$

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$$\begin{array}{lll} B_T & = & V \left(\frac{\partial^2 F}{\partial V^2} \right)_T \\ B_S & = & V \left(\frac{\partial^2 U}{\partial V^2} \right)_S \end{array} \quad \begin{array}{lll} C_V & = & -T \left(\frac{\partial^2 F}{\partial T^2} \right)_V \\ C_p & = & -T \left(\frac{\partial^2 G}{\partial T^2} \right)_p \end{array} \quad \dots$$

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$$\begin{aligned} B_T &= V \left(\frac{\partial^2 F}{\partial V^2} \right)_T & C_V &= -T \left(\frac{\partial^2 F}{\partial T^2} \right)_V & \dots \\ B_S &= V \left(\frac{\partial^2 U}{\partial V^2} \right)_S & C_p &= -T \left(\frac{\partial^2 G}{\partial T^2} \right)_p \end{aligned}$$

$$F(V, T, \lambda) = U_0(V, \lambda) + \frac{1}{2} \sum_{\mathbf{q}\nu} \hbar \omega(\mathbf{q}, \nu | V, \lambda) + k_B T \sum_{\mathbf{q}\nu} \log \left(1 - e^{-\frac{\hbar \omega(\mathbf{q}, \nu | V, \lambda)}{k_B T}} \right)$$

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why ab initio

scientific insight stems from the ability to extrapolate our understanding
from simple models to a very complex physical world

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much more so when the extrapolation implies dramatic changes of physical conditions (temperature, pressure, atomic coordination ...)

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density functional theory

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$$\rho(\mathbf{r}) = \sum_v |\psi_v(\mathbf{r})|^2 \quad \int \psi_u^*(\mathbf{r}) \psi_v(\mathbf{r}) d\mathbf{r} = \delta_{uv}$$

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$$\frac{\delta E_{KS}}{\delta \psi_v^*(\mathbf{r})} = \sum_{uv} \Lambda_{vu} \psi_u(\mathbf{r})$$

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + v_{KS}[\rho](\mathbf{r}) \right) \psi_v(\mathbf{r}) = \epsilon_v \psi_v(\mathbf{r})$$

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$$v_{KS}[\rho](\mathbf{r}) = V(\mathbf{r}, \mathbf{R}) + e^2 \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + v_{XC}[\rho](\mathbf{r})$$

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lattice dynamics from perturbation theory

$$V(\mathbf{r}) = V_0(\mathbf{r})$$

$$E = E_0$$

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$$+ \sum_{\mathbf{R}} \mathbf{u}(\mathbf{R}) \cdot \frac{\partial v(\mathbf{r} - \mathbf{R})}{\partial \mathbf{R}}$$

$$E = E_0$$

$$+ \frac{1}{2} \sum_{\mathbf{R}, \mathbf{R}'} \mathbf{u}(\mathbf{R}) \cdot \frac{\partial^2 E}{\partial \mathbf{u}(\mathbf{R}) \partial \mathbf{u}(\mathbf{R}')} \cdot \mathbf{u}(\mathbf{R}') + \dots$$

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$$\det \left[\frac{\partial^2 E}{\partial \mathbf{u}(\mathbf{R}) \partial \mathbf{u}(\mathbf{R}')} - \omega^2 M(\mathbf{R}) \delta_{\mathbf{R}, \mathbf{R}'} \right] = 0$$

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density-functional perturbation theory

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linear response is needed!

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calculating the response

$$n(\mathbf{r}) = \sum_v |\phi_v(\mathbf{r})|^2$$

$$n'(\mathbf{r}) = 2\text{Re} \sum_v \phi_v^{\text{o}*}(\mathbf{r}) \phi'_v(\mathbf{r})$$

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calculating the response

$$n(\mathbf{r}) = \sum_v |\phi_v(\mathbf{r})|^2$$

$$\begin{aligned} n'(\mathbf{r}) &= 2\text{Re} \sum_v \phi_v^{\circ*}(\mathbf{r}) \phi'_v(\mathbf{r}) \\ &= 2\text{Re} \sum_{cv} \rho'_{vc} \phi_v^{\circ*}(\mathbf{r}) \phi_c^{\circ}(\mathbf{r}) \end{aligned}$$

$$\phi'_v = \sum_c \phi_c^{\circ} \frac{\langle \phi_c^{\circ} | V' | \phi_v^{\circ} \rangle}{\epsilon_v^{\circ} - \epsilon_c^{\circ}}$$

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$$(H^{\circ} - \epsilon_v^{\circ}) \phi'_v = -P_c V' \phi_v^{\circ}$$

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DFPT: the equations

DFT

$$V_0(\mathbf{r}) \Leftrightarrow n(\mathbf{r})$$

$$V_{SCF}(\mathbf{r}) = V_0(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \mu_{xc}(\mathbf{r})$$

$$n(\mathbf{r}) = \sum_{\epsilon_v < E_F} |\phi_v(\mathbf{r})|^2$$

$$(-\Delta + V_{SCF}(\mathbf{r})) \phi_v(\mathbf{r}) = \epsilon_v \phi_v(\mathbf{r})$$

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DFPT

$$V'(\mathbf{r}) \Leftrightarrow n'(\mathbf{r})$$

$$V'_{SCF}(\mathbf{r}) = V'(\mathbf{r}) + \int \frac{n'(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \mu'_{xc}(\mathbf{r})$$

$$n'(\mathbf{r}) = 2 \operatorname{Re} \sum_{\epsilon_v < E_F} \phi_v^*(\mathbf{r}) \phi'_v(\mathbf{r})$$

$$(-\Delta + V_{SCF}(\mathbf{r}) - \epsilon_v)\phi'_v(\mathbf{r}) = P_c V'_{SCF}(\mathbf{r}) \phi_v(\mathbf{r})$$

SB, P. Giannozzi, and A. Testa, Phys. Rev. Lett. **58**, 1861 (1987)

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monochromatic perturbations

DFPT rhs:

$$-P_c V'^{\mathbf{q}} \phi_v^{\mathbf{k}}(\mathbf{r})$$

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monochromatic perturbations

$$(H_0 - \epsilon_v^{\mathbf{k}}) \phi_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r}) = -P_c V'^{\mathbf{q}} \phi_v^{\mathbf{k}}(\mathbf{r})$$

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$$(H_0 - \epsilon_v^{\mathbf{k}}) \phi_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r}) = -P_c V'^{\mathbf{q}} \phi_v^{\mathbf{k}}(\mathbf{r})$$

$$n'^{\mathbf{q}}(\mathbf{r}) = e^{i\mathbf{q} \cdot \mathbf{r}} \sum_{v, \mathbf{k}} u_v'^{\mathbf{k}*}(\mathbf{r}) u_v^{\mathbf{k}+\mathbf{q}}(\mathbf{r})$$

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$$V'^{\mathbf{q}}(\mathbf{r}) = V_{ext}'^{\mathbf{q}}(\mathbf{r}) + \int \left(\frac{e^2}{|\mathbf{r} - \mathbf{r}'|} + \kappa_{xc}(\mathbf{r}, \mathbf{r}') \right) n'^{\mathbf{q}}(\mathbf{r}') d\mathbf{r}'$$

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phonons in polar materials

$$E(\mathbf{u}, \mathbf{E}) = \frac{1}{2} M \omega_0^2 u^2 - \frac{\Omega}{8\pi} \epsilon_\infty \mathbf{E}^2 - e Z^* \mathbf{u} \cdot \mathbf{E}$$

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$$\mathbf{F} \equiv -\frac{\partial E}{\partial \mathbf{u}} = -M \omega_0^2 \mathbf{u} + Z^* \mathbf{E}$$

$$\mathbf{D} \equiv -\frac{4\pi}{\Omega} \frac{\partial E}{\partial \mathbf{E}} = \frac{4\pi}{\Omega} Z^* \mathbf{u} + \epsilon_\infty \mathbf{E}$$

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$$\mathbf{F}_T = -M \omega_0^2 \mathbf{u}$$

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$$\mathbf{F}_T = -M \omega_0^2 \mathbf{u} \qquad \mathbf{F}_L = -M \left(\omega_0^2 + \frac{4\pi Z^*}{M \Omega \epsilon_\infty} \right) \mathbf{u}$$

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interatomic force constants

$$\Phi_{st}^{\alpha\beta}(\mathbf{R} - \mathbf{R}') = -\frac{\partial^2 E}{\partial u_s^\alpha(\mathbf{R}) \partial u_t^\beta(\mathbf{R}')}$$

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interatomic force constants

$$\begin{aligned}\Phi_{st}^{\alpha\beta}(\mathbf{R} - \mathbf{R}') &= - \frac{\partial^2 E}{\partial u_s^\alpha(\mathbf{R}) \partial u_t^\beta(\mathbf{R}')} \\ &= \frac{\Omega}{(2\pi)^3} \int e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{R}')} D_{st}^{\alpha\beta}(\mathbf{q}) d\mathbf{q}\end{aligned}$$

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$$D_{st}^{\alpha\beta}(\mathbf{q}) = \bar{D}_{st}^{\alpha\beta}(\mathbf{q}) + \frac{4\pi e^2}{\Omega \epsilon_\infty} Z_s^* Z_t^* \frac{q^\alpha q^\beta}{q^2}$$

short ranged +
dipole-dipole

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interatomic force constants

$$\begin{aligned}
 \Phi_{st}^{\alpha\beta}(\mathbf{R} - \mathbf{R}') &= - \frac{\partial^2 E}{\partial u_s^\alpha(\mathbf{R}) \partial u_t^\beta(\mathbf{R}')} \\
 &= \frac{\Omega}{(2\pi)^3} \int e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{R}')} D_{st}^{\alpha\beta}(\mathbf{q}) d\mathbf{q} \\
 D_{st}^{\alpha\beta}(\mathbf{q}) &= \bar{D}_{st}^{\alpha\beta}(\mathbf{q}) + \frac{4\pi e^2}{\Omega \epsilon_\infty} Z_s^* Z_t^* \frac{q^\alpha q^\beta}{q^2}
 \end{aligned}$$

short ranged +
dipole-dipole

- remove singularities in D(q)

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$$\begin{aligned}
 \Phi_{st}^{\alpha\beta}(\mathbf{R} - \mathbf{R}') &= - \frac{\partial^2 E}{\partial u_s^\alpha(\mathbf{R}) \partial u_t^\beta(\mathbf{R}')} \\
 &= \frac{\Omega}{(2\pi)^3} \int e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{R}')} D_{st}^{\alpha\beta}(\mathbf{q}) d\mathbf{q} \\
 D_{st}^{\alpha\beta}(\mathbf{q}) &= \bar{D}_{st}^{\alpha\beta}(\mathbf{q}) + \frac{4\pi e^2}{\Omega \epsilon_\infty} Z_s^* Z_t^* \frac{q^\alpha q^\beta}{q^2}
 \end{aligned}$$

short ranged +
dipole-dipole

- remove singularities in D(q)
- do FFT's (# R's = # q's - the shorter the range, the coarser the grid)

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interatomic force constants

$$\begin{aligned}\Phi_{st}^{\alpha\beta}(\mathbf{R} - \mathbf{R}') &= -\frac{\partial^2 E}{\partial u_s^\alpha(\mathbf{R}) \partial u_t^\beta(\mathbf{R}')} \\ &= \frac{\Omega}{(2\pi)^3} \int e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{R}')} D_{st}^{\alpha\beta}(\mathbf{q}) d\mathbf{q} \\ D_{st}^{\alpha\beta}(\mathbf{q}) &= \bar{D}_{st}^{\alpha\beta}(\mathbf{q}) + \frac{4\pi e^2}{\Omega \epsilon_\infty} Z_s^* Z_t^* \frac{q^\alpha q^\beta}{q^2}\end{aligned}$$

short ranged +
dipole-dipole

- remove singularities in $D(\mathbf{q})$
- do FFT's (# R's = # q's - the shorter the range, the coarser the grid)
- store information

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interatomic force constants

$$\begin{aligned}\Phi_{st}^{\alpha\beta}(\mathbf{R} - \mathbf{R}') &= -\frac{\partial^2 E}{\partial u_s^\alpha(\mathbf{R}) \partial u_t^\beta(\mathbf{R}')} \\ &= \frac{\Omega}{(2\pi)^3} \int e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{R}')} D_{st}^{\alpha\beta}(\mathbf{q}) d\mathbf{q} \\ D_{st}^{\alpha\beta}(\mathbf{q}) &= \bar{D}_{st}^{\alpha\beta}(\mathbf{q}) + \frac{4\pi e^2}{\Omega \epsilon_\infty} Z_s^* Z_t^* \frac{q^\alpha q^\beta}{q^2}\end{aligned}$$

short ranged +
dipole-dipole

- remove singularities in $D(\mathbf{q})$
- do FFT's (# R's = # q's - the shorter the range, the coarser the grid)
- store information
- interpolate $D(\mathbf{q})$ on any finer mesh (pad Φ with 0's and do FFT⁻¹: # q's = # R's)

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interatomic force constants

$$\begin{aligned}\Phi_{st}^{\alpha\beta}(\mathbf{R} - \mathbf{R}') &= - \frac{\partial^2 E}{\partial u_s^\alpha(\mathbf{R}) \partial u_t^\beta(\mathbf{R}')} \\ &= \frac{\Omega}{(2\pi)^3} \int e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{R}')} D_{st}^{\alpha\beta}(\mathbf{q}) d\mathbf{q}\end{aligned}$$

$$D_{st}^{\alpha\beta}(\mathbf{q}) = \bar{D}_{st}^{\alpha\beta}(\mathbf{q}) + \frac{4\pi e^2}{\Omega \epsilon_\infty} Z_s^* Z_t^* \frac{q^\alpha q^\beta}{q^2}$$

short ranged +
dipole-dipole

- remove singularities in $D(\mathbf{q})$
- do FFT's (# R's = # q's - the shorter the range, the coarser the grid)
- store information
- interpolate $D(\mathbf{q})$ on any finer mesh (pad Φ with 0's and do FFT⁻¹: # q's = # R's)
- calculate phonon bands

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phonons from DFPT

P. Giannozzi, S. de Gironcoli, P. Pavone, and SB, Phys. Rev. B **43**, 7231 (1991)

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DFPT phonons in metals

Stefano de Gironcoli,
Phys. Rev. B **51**, 6773 (1995)

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applications done so far

- Dielectric properties
- Piezoelectric properties
- Elastic properties
- Phonon in crystals and alloys
- Phonon at surfaces, interfaces, superlattices, and nano-structures
- Raman and infrared activities
- Anharmonic couplings and vibrational line widths
- Mode softening and structural transitions
- Electron-phonon interaction and superconductivity
- Thermal expansion
- Isotopic effects on structural and dynamical properties
- Thermo-elasticity and other thermal properties of minerals
- ...

SB, A. Dal Corso, S. de Gironcoli, and P. Giannozzi, *Phonons and related crystal properties from density-functional perturbation theory*, Rev. Mod. Phys. **73**, 515 (2001)

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a sampler of recent applications

VOLUME 90, NUMBER 3

PHYSICAL REVIEW LETTERS

week ending
24 JANUARY 2003

First-Principles Calculation of Vibrational Raman Spectra in Large Systems: Signature of Small Rings in Crystalline SiO₂

Michele Lazzeri and Francesco Mauri

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J|A|C|S

A R T I C L E S

Published on Web 08/17/2007

Vibrational Recognition of Adsorption Sites for CO on Platinum and Platinum–Ruthenium Surfaces

Ismaila Dabo,^{*,†} Andrzej Wieckowski,[‡] and Nicola Marzari[†]

11046 J. AM. CHEM. SOC. • VOL. 129, NO. 36, 2007

atop (CO@Pt₁)

E_{DFT} = +0.10 eV

v_{DFT} = 2050 cm⁻¹

v_{exp} = 2070 cm⁻¹

expt

bridge (CO@Pt₂)

E_{DFT} = +0.03 eV

v_{DFT} = 1845 cm⁻¹

v_{exp} = 1830 cm⁻¹

fcc (CO@Pt₃)

E_{DFT} = 0 eV

v_{DFT} = 1743 cm⁻¹

v_{exp} = 1780 cm⁻¹

DFT

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Dissociation of MgSiO_3 in the Cores of Gas Giants and Terrestrial Exoplanets

Koichiro Umemoto,¹ Renata M. Wentzcovitch,^{1*} Philip B. Allen²

www.sciencemag.org SCIENCE VOL 311 17 FEBRUARY 2006

983

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PRL 100, 257001 (2008)

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week ending
27 JUNE 2008

Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen

P. Cudazzo,¹ G. Profeta,¹ A. Sanna,^{2,3} A. Floris,³ A. Continenza,¹ S. Massidda,² and E. K. U. Gross³

¹CNISM - Dipartimento di Fisica, Università degli Studi dell'Aquila, Via Vetoio 10, I-67010 Coppito (L'Aquila) Italy

²SLACS-INFM/CNR—Dipartimento di Fisica, Università degli Studi di Cagliari, I-09124 Monserrato (CA), Italy

³Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany
(Received 7 December 2007; published 23 June 2008; corrected 27 June 2008)

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PRL 100, 257001 (2008)

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week ending
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(Received 7 December 2007; published 23 June 2008; corrected 27 June 2008)

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thermal expansion

$$P(V, T) = - \frac{\partial F}{\partial V}$$

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thermal expansion

$$\begin{aligned}
 P(V, T) &= -\frac{\partial F}{\partial V} \\
 &= -\frac{\partial U_0}{\partial V} + \frac{1}{V} \sum_{\mathbf{q}\nu} \hbar \omega(\mathbf{q}, \nu) \gamma(\mathbf{q}, \nu) \left(\frac{1}{2} + \frac{1}{e^{\frac{\hbar \omega(\mathbf{q}, \nu)}{k_B T}} - 1} \right)
 \end{aligned}$$

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thermal expansion

$$\begin{aligned}
 P(V, T) &= -\frac{\partial F}{\partial V} \quad -\frac{V}{\omega(\mathbf{q}, \nu)} \frac{\partial \omega(\mathbf{q}, \nu)}{\partial V} \\
 &= -\frac{\partial U_0}{\partial V} + \frac{1}{V} \sum_{\mathbf{q}\nu} \hbar \omega(\mathbf{q}, \nu) \gamma(\mathbf{q}, \nu) \left(\frac{1}{2} + \frac{1}{e^{\frac{\hbar \omega(\mathbf{q}, \nu)}{k_B T}} - 1} \right)
 \end{aligned}$$

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thermal expansion

$$\begin{aligned}
 P(V, T) &= -\frac{\partial F}{\partial V} - \frac{V}{\omega(\mathbf{q}, \nu)} \frac{\partial \omega(\mathbf{q}, \nu)}{\partial V} \\
 &= -\frac{\partial U_0}{\partial V} + \frac{1}{V} \sum_{\mathbf{q}\nu} \hbar \omega(\mathbf{q}, \nu) \gamma(\mathbf{q}, \nu) \left(\frac{1}{2} + \frac{1}{e^{\frac{\hbar \omega(\mathbf{q}, \nu)}{k_B T}} - 1} \right)
 \end{aligned}$$

$$\beta = V^{-1} \left(\frac{\partial V}{\partial T} \right)_P$$

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thermal expansion

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 P(V, T) &= -\frac{\partial F}{\partial V} - \frac{V}{\omega(\mathbf{q}, \nu)} \frac{\partial \omega(\mathbf{q}, \nu)}{\partial V} \\
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 \end{aligned}$$

$$\begin{aligned}
 \beta &= V^{-1} \left(\frac{\partial V}{\partial T} \right)_P \\
 &= -\frac{1}{V} \frac{(\partial P / \partial T)_V}{(\partial P / \partial V)_T} \\
 &= \frac{1}{B_T} \sum_{\mathbf{q}\nu} \hbar \omega(\mathbf{q}, \nu) \gamma(\mathbf{q}, \nu) n'(\mathbf{q}, \nu),
 \end{aligned}$$

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thermal expansion in semiconductors

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thermal expansion in semiconductors

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thermal expansion in semiconductors

P. Pavone, SISSA PhD thesis (1991)
<http://www.sissa.it/cm/thesis/1991/pavone.ps.gz>

Sunday, November 14, 2010

validity of the QHA

J.J. Xie, S.P. Chen, J.S. Tse, S. de Gironcoli, and SB, Phys. Rev. B **60**, 9444 (1999)

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phase boundaries

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phase boundaries

$$G_{A/B}(p, T) = \min_{\lambda_{A/B}} g_{A/B}(p, T | \lambda_{A/B})$$

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phase boundaries

$$G_{A/B}(p, T) = \min_{\lambda_{A/B}} g_{A/B}(p, T | \lambda_{A/B})$$

$$g(p, T | \lambda) = f(V, T | \lambda) + pV$$

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phase boundaries in Mg_2SiO_4

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phase boundaries in Mg_2SiO_4

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phase boundaries in Mg_2SiO_4

+

=

YG Yu, Z Wu, and RM Wentzcovitch,
Earth Planet Sc Lett, **273**, 115 (2008)

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thermo-elastic properties

$$C_{ij,kl}^T(p, T) = \frac{1}{V} \frac{\partial^2 G}{\partial \epsilon_{ij} \partial \epsilon_{kl}}$$

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thermo-elastic properties

$$C_{ij,kl}^T(p, T) = \frac{1}{V} \frac{\partial^2 G}{\partial \epsilon_{ij} \partial \epsilon_{kl}} \qquad C^S = C^T + \frac{T}{c_V} \frac{\partial S}{\partial \epsilon_{ij}} \frac{\partial S}{\partial \epsilon_{kl}}$$

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thermo-elastic properties

$$C_{ij,kl}^T(p, T) = \frac{1}{V} \frac{\partial^2 G}{\partial \epsilon_{ij} \partial \epsilon_{kl}} \quad C^S = C^T + \frac{T}{c_V} \frac{\partial S}{\partial \epsilon_{ij}} \frac{\partial S}{\partial \epsilon_{kl}}$$

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thermo-elastic properties

$$C_{ij,kl}^T(p, T) = \frac{1}{V} \frac{\partial^2 G}{\partial \epsilon_{ij} \partial \epsilon_{kl}} \quad C^S = C^T + \frac{T}{c_V} \frac{\partial S}{\partial \epsilon_{ij}} \frac{\partial S}{\partial \epsilon_{kl}}$$

$$G(p, T|\epsilon) = F(V, T|\epsilon) + pV$$

$$F = F(V, T|\epsilon_{ij}) = \min_{\lambda} f(V, \epsilon_{ij}, T|\epsilon_{ij}, \lambda) \quad p = -\frac{\partial F}{\partial V}$$

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thermo-elastic properties

$$C_{ij,kl}^T(p, T) = \frac{1}{V} \frac{\partial^2 G}{\partial \epsilon_{ij} \partial \epsilon_{kl}} \quad C^S = C^T + \frac{T}{c_V} \frac{\partial S}{\partial \epsilon_{ij}} \frac{\partial S}{\partial \epsilon_{kl}}$$

$$G(p, T|\epsilon) = F(V, T|\epsilon) + pV$$

$$F = F(V, T|\epsilon_{ij}) = \min_{\lambda} f(V, \epsilon_{ij}, T|\epsilon_{ij}, \lambda) \quad p = -\frac{\partial F}{\partial V}$$

$$f(V, T|\epsilon, \lambda) = U_0(V|\epsilon, \lambda) + \frac{1}{2} \sum_{\mathbf{q}\nu} \hbar \omega(\mathbf{q}, \nu|V, \epsilon, \lambda) + k_B T \sum_{\mathbf{q}\nu} \log \left(1 - e^{-\frac{\hbar \omega(\mathbf{q}, \nu|V, \epsilon, \lambda)}{k_B T}} \right)$$

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thermoelastic properties

R.M. Wentzcovitch, B.B. Karki, M. Cococcioni, and S. de Gironcoli,
Phys. Rev. Lett. **92**, 18501 (2004)

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What I cannot **compute**, I do not understand [adapted from Richard P. Feynman]

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JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **21** (2009) 395502 (19pp)

doi:10.1088/0953-8984/21/39/395502

QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials

Paolo Giannozzi^{1,2}, Stefano Baroni^{1,3}, Nicola Bonini⁴,
Matteo Calandra⁵, Roberto Car⁶, Carlo Cavazzoni^{7,8},
Davide Ceresoli⁴, Guido L Chiarotti⁹, Matteo Cococcioni¹⁰,
Ismaila Dabo¹¹, Andrea Dal Corso^{1,3}, Stefano de Gironcoli^{1,3},
Stefano Fabris^{1,3}, Guido Fratesi¹², Ralph Gebauer^{1,13},
Uwe Gerstmann¹⁴, Christos Gougoussis⁵, Anton Kokalj^{1,15},
Michele Lazzeri⁵, Layla Martin-Samos¹, Nicola Marzari⁴,
Francesco Mauri⁵, Riccardo Mazzarello¹⁶, Stefano Paolini^{3,9},
Alfredo Pasquarello^{17,18}, Lorenzo Paulatto^{1,3}, Carlo Sbraccia^{1,†},
Sandro Scandolo^{1,13}, Gabriele Sclauszero^{1,3}, Ari P Seitsonen⁵,
Alexander Smogunov¹³, Paolo Umari¹ and
Renata M Wentzcovitch^{10,19}

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That's all Folks!

these slides at
<http://talks.baroni.me>

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