Physics of a neutron star crust Lecture 2.

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Nuclear Dynamics: from Stars to Colliders

June 29 – July 10, 2026

BLTR, JINR, Dubna, Russia

Physics of a neutron star crust

Selection of topics and plan

"Everything should be made as simple as possible, but not simpler"

Attributed to Albert Einstein

According to Robinson [*Nature* **557**, 30 (2018)], it can be a compressed version of lines from a 1933 lecture by Einstein:
"*It can scarcely be denied that the supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience*."

My preference in these lectures: *models, which can be solved analytically*

Lecture 1: Introduction and basic models of outer crust at T=0

Lecture 2: Outer crust: thermodynamics and elasticity

Lecture 3: Inner crust

+ Mass-radius relation (without crust EOS)

Thermodynamics of the outer crust

(school topic: theoretical description of interacting fermion systems)

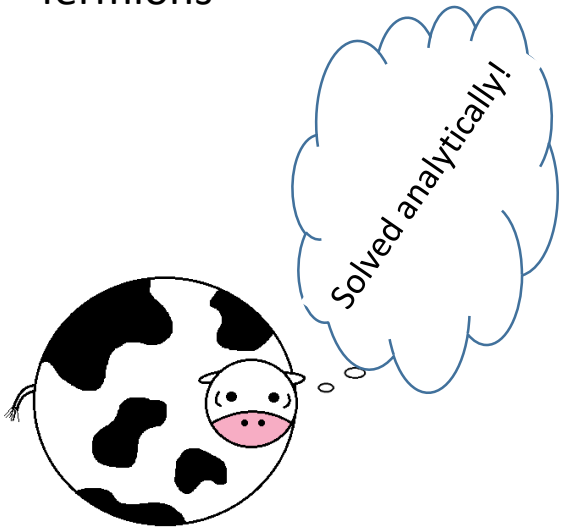
$$F = F_{\rm e} + F_{\rm i} + F_{\rm ie} + \sum_i M_i N_i$$

Nuclei mass (nuclear physics)



Model system
Ideal degenerate gas of electrons

Electrons: relativistic noninterracting fermions





Model system
Nuclei on the **uniform** neutralizing background of electrons

Static lattice:

$$\epsilon = \zeta \frac{Z^2 e^2}{a} n$$

$$\zeta = \begin{cases} -0.895929255682 & \text{bcc} \\ -0.895873615195 & \text{fcc} \\ -0.895838120459 & \text{hcp} \end{cases}$$

Ion sphere

$$\zeta = -0.9$$

$$P_{\rm i} \approx -4.6 \times 10^{-3} Z^{2/3} P_{\rm e}$$

What about thermal effects?

Thermodynamics of nuclei in outer crust
Classical nuclei

It is convenient to consider system at given *N, V, T* => Helmholtz free energy

$$F = -T \ln Z$$

$$Z = \sum_s \exp\left(-\frac{E_s}{T}\right) = \frac{g^N}{N!} \int\int \exp\left(-\frac{E}{T}\right) \prod_{i=1}^{N} \frac{\mathrm{d}^3 r_j \mathrm{d}^3 p_j}{(2\pi\hbar)^3}$$

$$= \frac{g^N}{N!} \int \exp\left(-\sum_j \frac{p_j^2}{2mT}\right) \prod_{i=1}^{N} \frac{V \mathrm{d}^3 p_i}{(2\pi\hbar)^3} \cdot \frac{1}{V^N} \int \exp\left(-\frac{V}{T}\right) \prod_{i=1}^{N} \mathrm{d}^3 r_i$$

Z_{id} — Partion function of Ideal classical gas!

Z_{nid} — Coulomb corrections (nonideal)

Well known (analytical)

Next slides

$$F = -T \ln\left(Z_{\mathrm{id}} Z_{\mathrm{nid}}\right) = F_{\mathrm{id}} + F_{\mathrm{nid}}$$

Partition function in a classical limit can be factorized and thermodynamic functions becomes a sum of ideal and nonideal contributions

Thermodynamics of nuclei in outer crust
Classical nuclei, nonideal part

Dimensional analysis

$T = 0$

We have:

Ze Charge

a Distance

Energy scale $\dfrac{Z^2e^2}{a}$

Density $n = \dfrac{3}{4\pi a^3}$

Energy density $\epsilon = \zeta \dfrac{Z^2e^2}{a} n$

We need to calculate a constant!

$T > 0$

We have:

Ze Charge

a Distance

T Energy

Energy scale $\dfrac{Z^2e^2}{a}$

Density $n = \dfrac{3}{4\pi a^3}$

Dimensionless $\Gamma = \dfrac{Z^2e^2}{aT}$

Helmholtz free energy density $\mathfrak{f} = f(\Gamma)\dfrac{Z^2e^2}{a} n$

We need to calculate one-parameter function!

Thermodynamics of nuclei in outer crust
Classical nuclei

Known

Calculated numerically (MC, MD)
(approximations: Potekhin&Chabrier 2000)

$$F = -T\ln\left(Z_{\rm id}Z_{\rm nid}\right) = F_{\rm id} + F_{\rm nid}; \quad F_{\rm nid} = NTf_0(\Gamma)$$

Partition function in a classical limit can be factorized and thermodynamic functions becomes a sum of ideal and nonideal contributions

$$S_{\rm nid} = -\left(\frac{\partial F_{\rm nid}}{\partial T}\right) = N\left(\Gamma\frac{\partial f_0}{\partial\Gamma} - f_0\right)$$

$$U_{\rm nid} = F_{\rm nid} + S_{\rm nid}T = NT\Gamma\frac{\partial f_0}{\partial\Gamma}, \quad u_0 \equiv \Gamma\frac{\partial f_0}{\partial\Gamma}$$

$$P_{\rm nid} = -\frac{\partial F_{\rm nid}}{\partial V} = \frac{u_0}{3}n$$

← Accurate for classical ions!

Rather simple thermodynamics: everything is given by one function of Γ

No complicated chemistry (complicated dependence on *Z*)

Thermodynamics of nuclei in outer crust
Quantum effects

Dimensional analysis

$$T > 0, \quad \hbar \to 0$$

We have:

Ze	Charge
a	Distance
T	Energy

Energy scale $\dfrac{Z^2e^2}{a}$

Density $n = \dfrac{3}{4\pi a^3}$

Dimensionless $\Gamma = \dfrac{Z^2e^2}{aT}$

Helmholtz free energy density $\mathfrak{f} = f(\Gamma)\dfrac{Z^2e^2}{a}n$

We need to calculate one-parameter function!

$$T > 0, \quad \hbar \neq 0$$

We have:

Ze	Charge
a	Distance
$T,\ T_p = \hbar\sqrt{\frac{4\pi n_i Z_i^2 e^2}{m_i}}$	Energy

Energy scale $\dfrac{Z^2e^2}{a}$

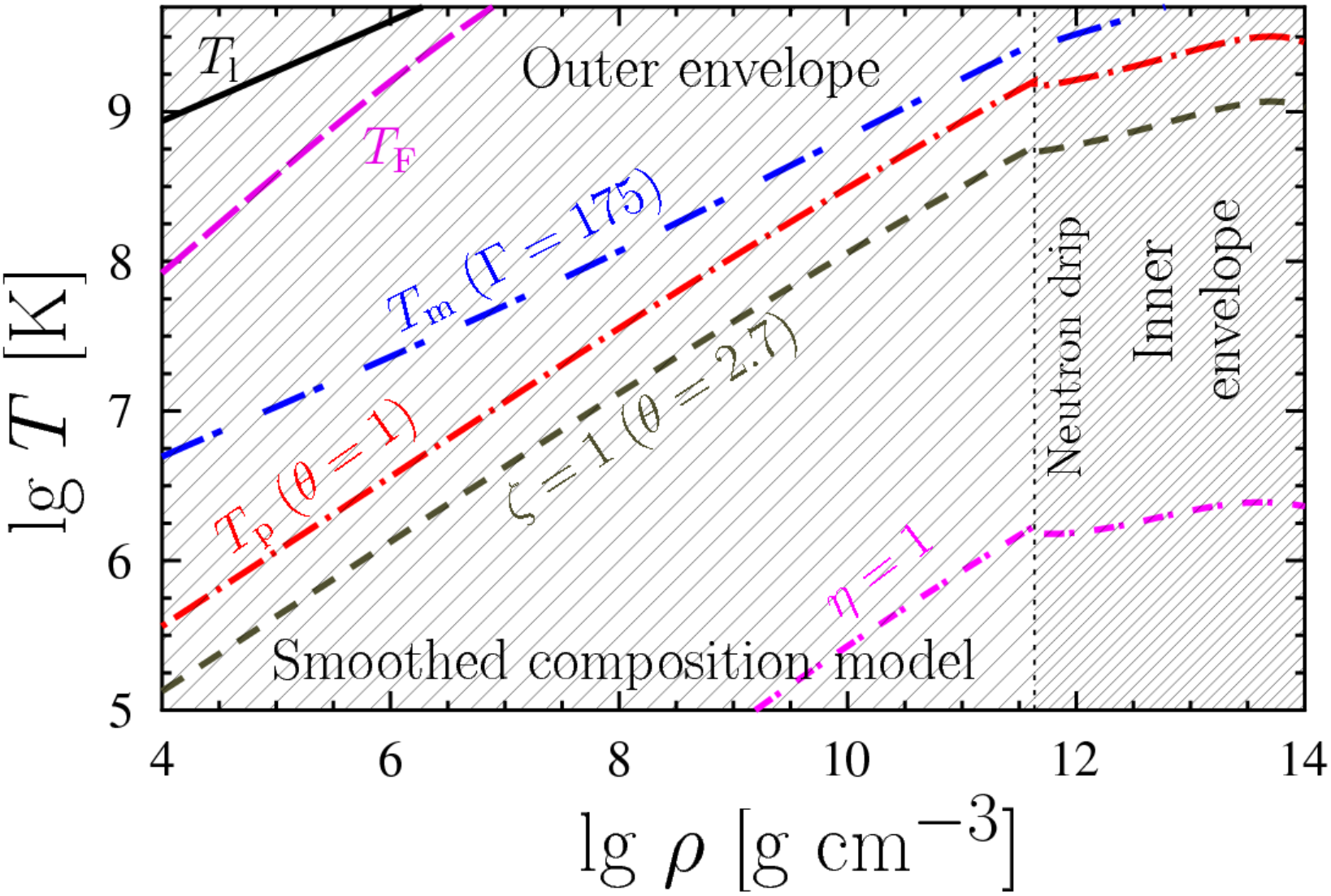
Density $n = \dfrac{3}{4\pi a^3}$

Dimensionless $\Gamma = \dfrac{Z^2e^2}{aT},\ \theta = \dfrac{T_p}{T}$

Helmholtz free energy density $\mathfrak{f} = f(\Gamma,\theta)\dfrac{Z^2e^2}{a}n$

We need to calculate two-parameter function!

Thermodynamics of nuclei in outer crust T(ρ) diagram



Thermodynamics of nuclei in outer crust
Quantum effects

Typical frequency of ion motion

$$\omega_{\rm p} = \sqrt{\frac{4\pi n_i Z_i^2 e^2}{m_i}}$$

Quantum effects are important if

$$T \lesssim T_{\rm p} = \hbar\omega_{\rm p}$$

Path Integral Monte-Carlo

Quantum corrections
Physically motivated approximations
(harmonic oscillator thermodynamics)
(Baiko&AIC, 2022)

$$\frac{F_{\rm i}}{NT} = f_{\rm id} + f_{\rm cl} + f_{\rm q}$$

Ideal part
(textbook)

Classical nonideal part
(approximations: Potekhin&Chabrier 2000)

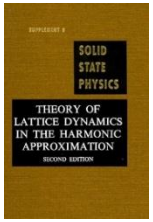
Thermodynamics of nuclei in outer crust Solid

$$\frac{F_\mathrm{i}}{N} = \zeta\frac{Z^2e^2}{a} + E_\mathrm{h}(\theta) + E_\mathrm{ah}(r_s,\theta)$$

$$r_s = a/a_\mathrm{B}$$

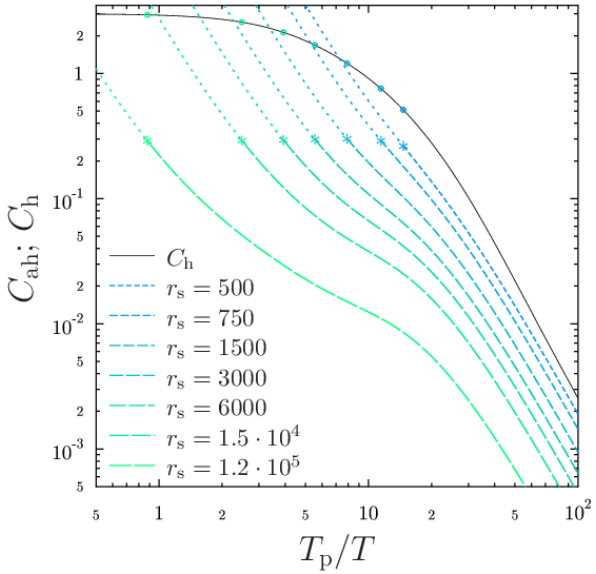
$$a_\mathrm{B} = \hbar^2/(m_\mathrm{i}Z_\mathrm{i}^2e^2)$$

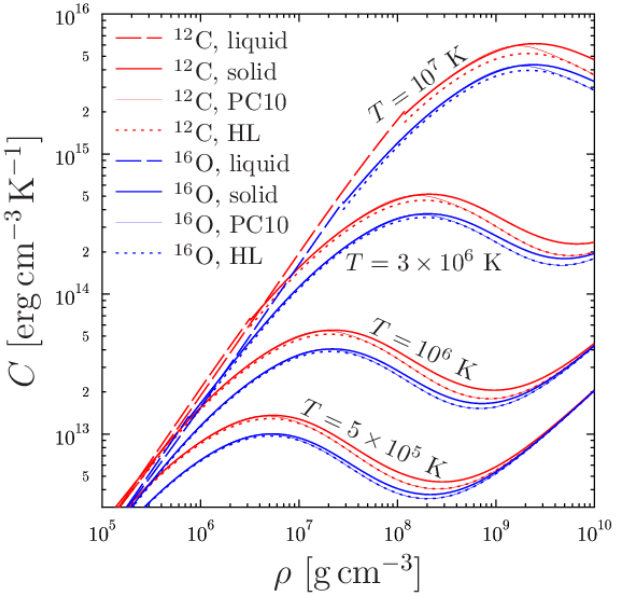
Static lattice
(known exactly)

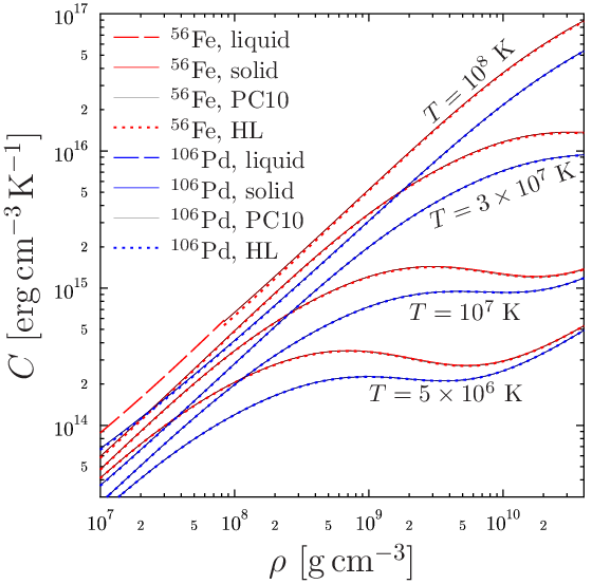


Harmonic energy
(Baiko et al., 2001)

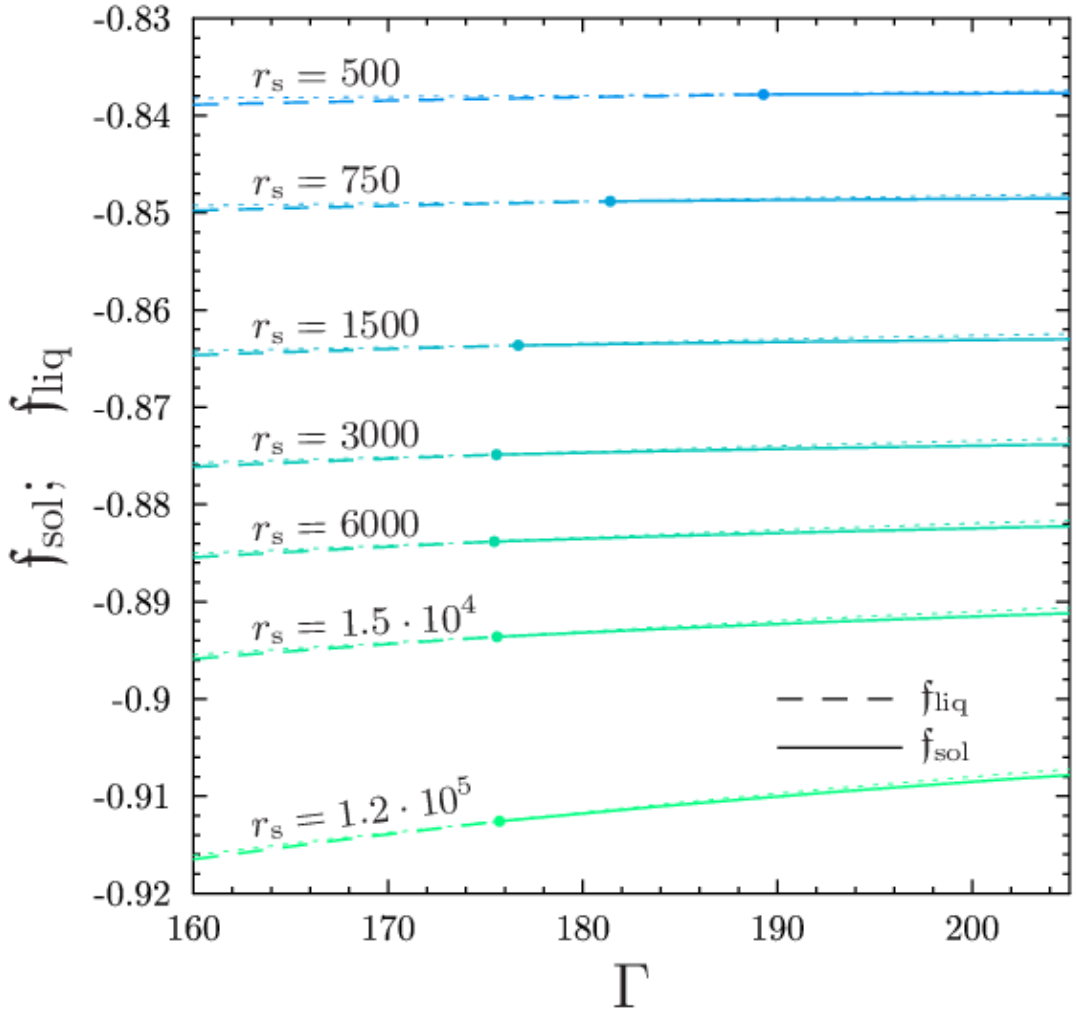
Approximation of
PIMC calculations
(Baiko&AIC, 2022)







Thermodynamics of nuclei in outer crust Melting



Free energies per ion are normalized for $\frac{Z^2e^2}{a}$

- Very sensitive for small errors in approximations
- The coupling parameter for melting increases with increase of the density

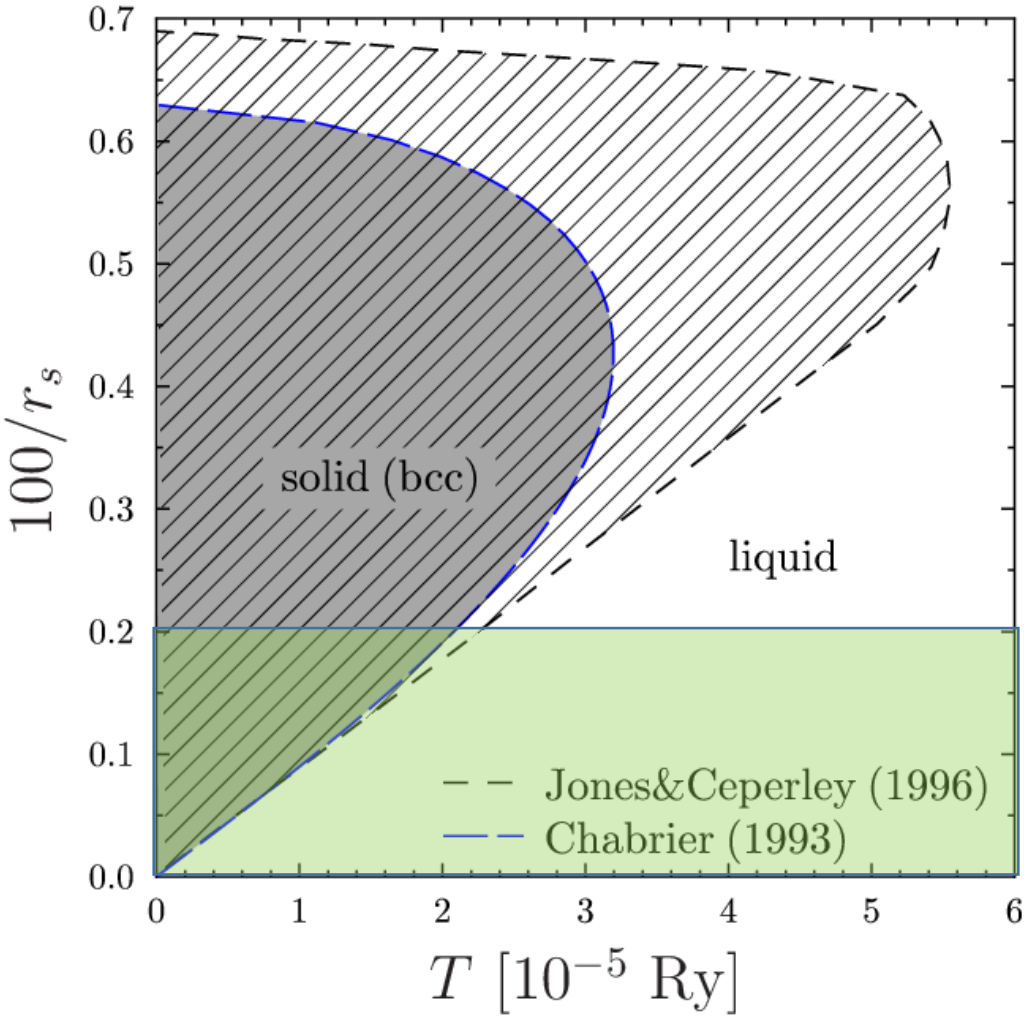
Dimensionless density

$$r_s = a/a_{\mathrm{B}}$$

$$a_{\mathrm{B}} = \hbar^2/(m_{\mathrm{i}}Z_{\mathrm{i}}^2e^2)$$

Nuclei in outer crust on OCP phase diagram

OCP phase diagram



Astrophysical applications

$$r_s \gtrsim 500$$

Fusion reactions are not to fast in pycnonuclear regime
[Baiko 2021]

$$R = \frac{n_i^2}{\pi} \frac{a_B}{\hbar} S(E_{\rm pk}) g(0)$$

Contact probability
(function of r_s and Γ)

The sign problem is not significant for ions at astrophysically relevant parameter range (if wave functions overlap, fusion starts)
D.A. Baiko (2011?)

Thermodynamics of nuclei in outer crust (one component Coulomb plasma)



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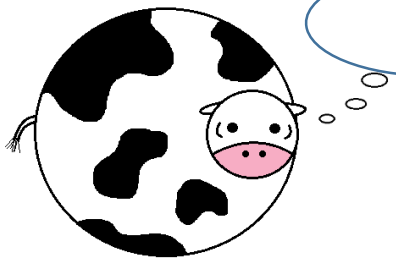
Accurate quantitative description:
fits of ab-initio simulations





What is that we (NS crust microphysicists) want to do!

Provide accurate and reliable description of the crust properties, which can be safely used in astrophysical applications.

Something like tables of density and specific heat for terrestrial materials – one can solve problems without dealing electrodynamics and quantum mechanics etc., which, in fact, determine these values

"The more you look, the less you see"

But… We want describe NS crust, this slide is about OCP….

Thermodynamics of outer crust Melting: do we solve correct problem?



Two slides before:

Melting at fixed density (Helmholtz free energies were compared)

Any textbook on phase transitions:

The pressure should be equal in the phases => Compare the Gibbs free energies!!!

The problem, which you solve, was about spherical cows, not about neutron star crust!

Should we reanalyze melting?



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Thermodynamics of outer crust Melting: do we solve correct problem?

Three slides before:

Melting at fixed density (Helmholtz free energies were compared)

Any textbook on phase transitions:

The pressure should be equal in the phases => Compare the Gibbs free energies!!
The problem, which you solve, was about spherical cows, not about neutron star crust!

Should we reanalyze melting?

Generally yes, but $$P_{\rm i} \approx -4.6 \times 10^{-3} Z^{2/3} P_{\rm e} \quad (\rho \gg 10^6 \ {\rm g/cm^3})$$

Melting was considered in a correct formulation, but the result is almost unaffected

There is a density jump between liquid and solid state, but it is only about 0.05%!!!

$$\frac{\delta \Gamma_m}{\Gamma_m} = -\frac{\delta a}{a} = \frac{1}{3}\frac{\delta n}{n}$$

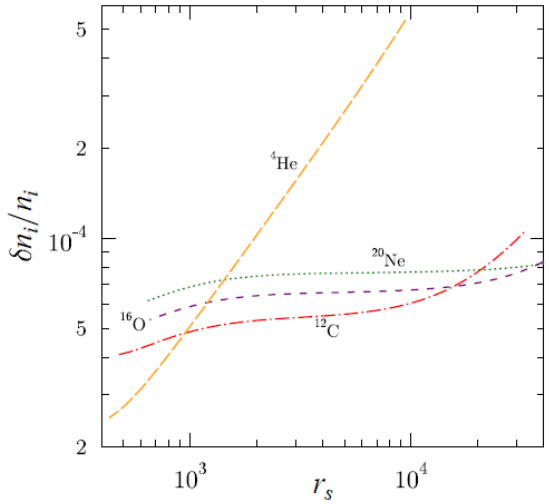


Figure from Baiko&AIC, 2022

Thermodynamics of nuclei in outer crust

Mixtures

$F(T, \{n_i, Z_i, A_i\})$

Number of parameters increases: require huge number of simulations + complicated approximations. Not fully realized yet

$$\frac{F_\mathrm{i}}{NT} = f_\mathrm{id} + f_\mathrm{nid}^\mathrm{cl} + f_\mathrm{q}$$

Ideal free energy
(any appropriate textbook)

Quantum corrections
Linear mixing rule (intuitive)

Classical nonideal free energy:

Linear mixing rule [based on MC simulations, see corrections in liquid phase in Potekhin et al. (2009)]

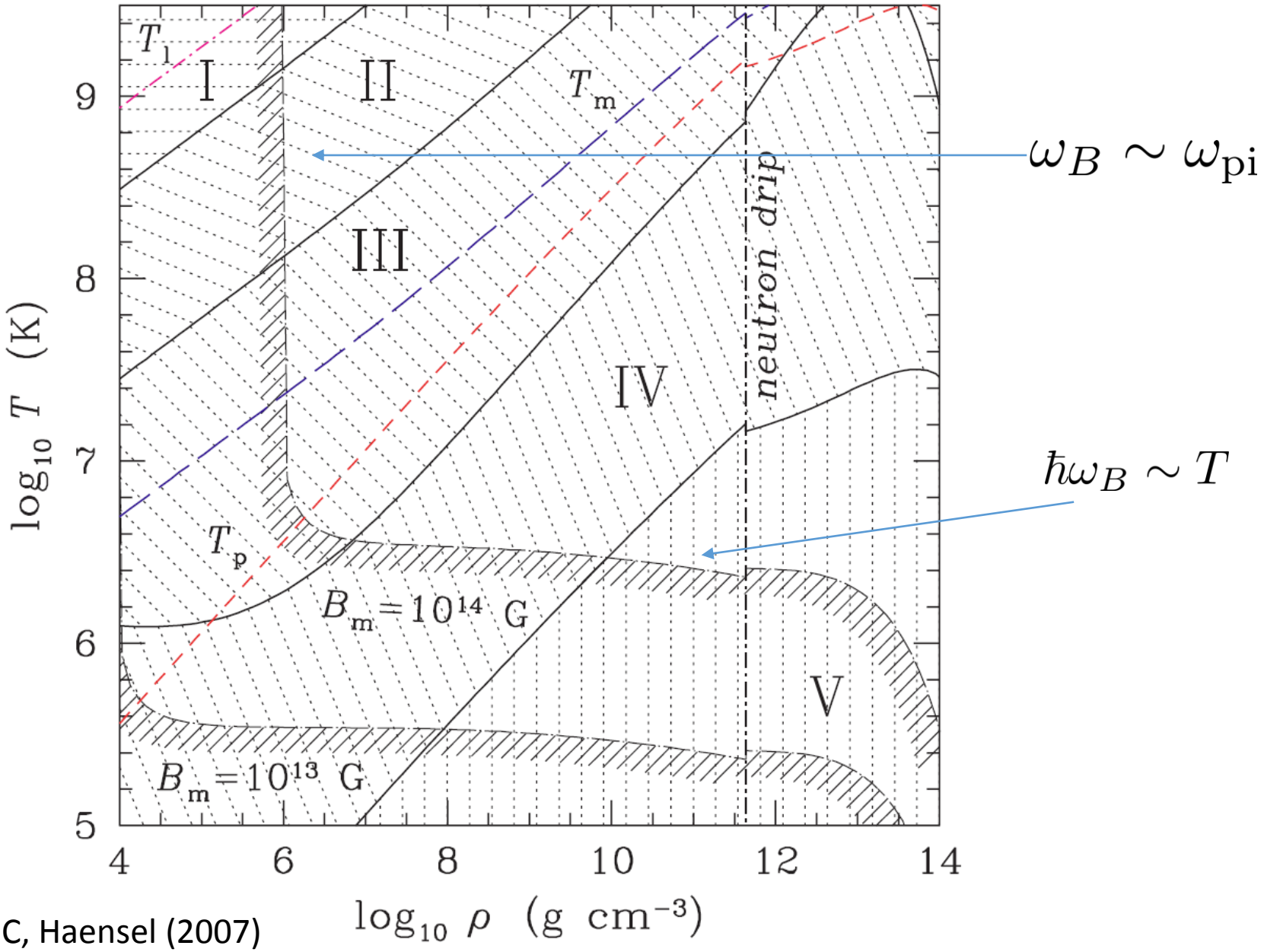
$$f_\mathrm{i} = \frac{F_\mathrm{i}}{NT} = \sum_i \frac{N_i\, f_i^\mathrm{OCP}(\Gamma_i)}{N}, \quad \Gamma_i = \frac{Z^2 e^2}{a_i}, \quad a_i = (4\pi Z_i n_\mathrm{e}/3)^{-1/3}$$

<u>Uniform phase or separation (phases with different compositions)</u>

«Competition» of (ideal) mixing entropy and nonideal parts
(=correction to the linear mixing)

In crystallized phase correction to the linear mixing are strong and can lead to separation, as in a terrestrial conditions (Baiko 2022-2025; applications for WD cooling)

Effects of magnetic field on nuclei



AIC, Haensel (2007)

Thermodynamics of nuclei in outer crust (multicomponent Coulomb plasma)

Approximate formulae for quantitative description, based on ab-initio simulations for OCP + limited simulation for mixtures+ physical intuition

User-friendly: Skye code (Jermin+2021)



Complex physics, as in a case of terrestrial multicomponent materials

Thermodynamics of the outer crust

(school topic: theoretical description of interacting fermion systems)

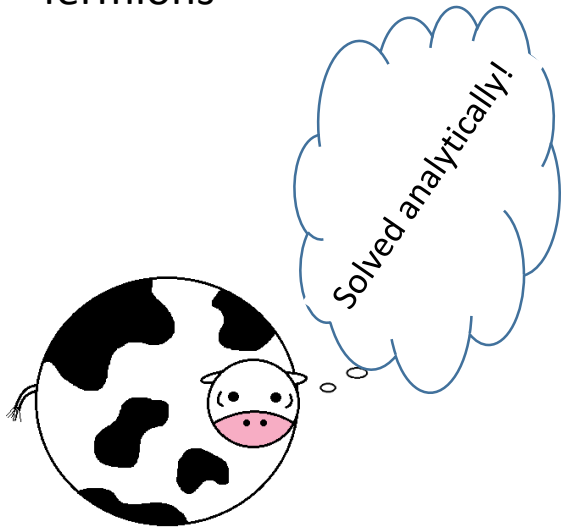
$$F = F_{\rm e} + F_{\rm i} + F_{\rm ie} + \sum_i M_i N_i$$

Nuclei mass (nuclear physics)



Model system
Ideal degenerate gas of electrons

Electrons: relativistic noninterracting fermions





Model system
Nuclei on the **uniform** neutralizing background of electrons



Corrections

- No uniform electron background (screening)

Liquid:
Potekhin & Chabrier (2000)
Crystall: Baiko (2002)

The corrections, as predicted today, affects melting temperature. BUT it can be byproduct of different approaches, applied to calculate these corrections….

- ….

Elasticity of (outer) crust

Some key questions

[from INT workshop INT-18-71W, Astro-Solids, Dense Matter, and Gravitational Waves, April 16-20, 2018]

- What is the minimum, typical, and maximum ellipticity one should expect?

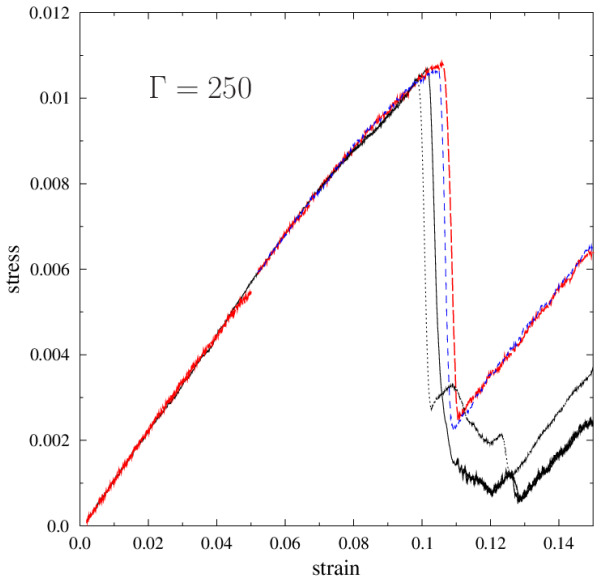
What is the strength (breaking strain) of the crust?

- How does strain evolve in the crust and how does it break?

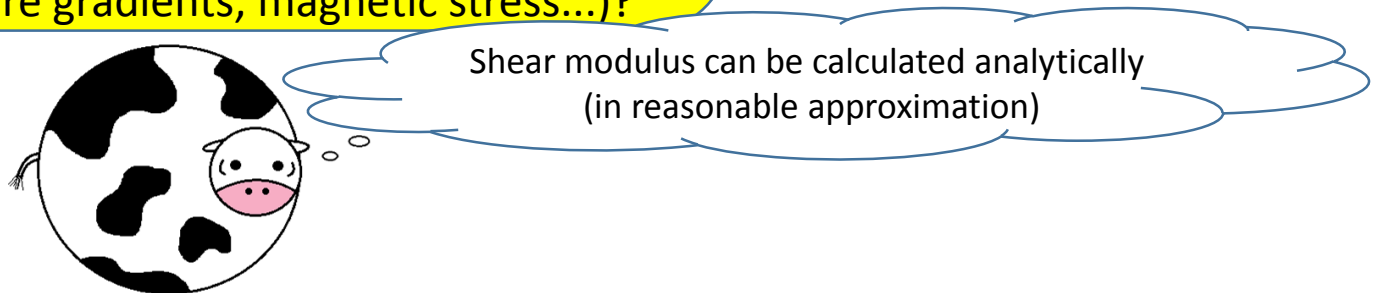
- What are the implications of observed upper limits on the ellipticity?

- At what point do upper limits become “interesting” (e.g. constrain theory)?

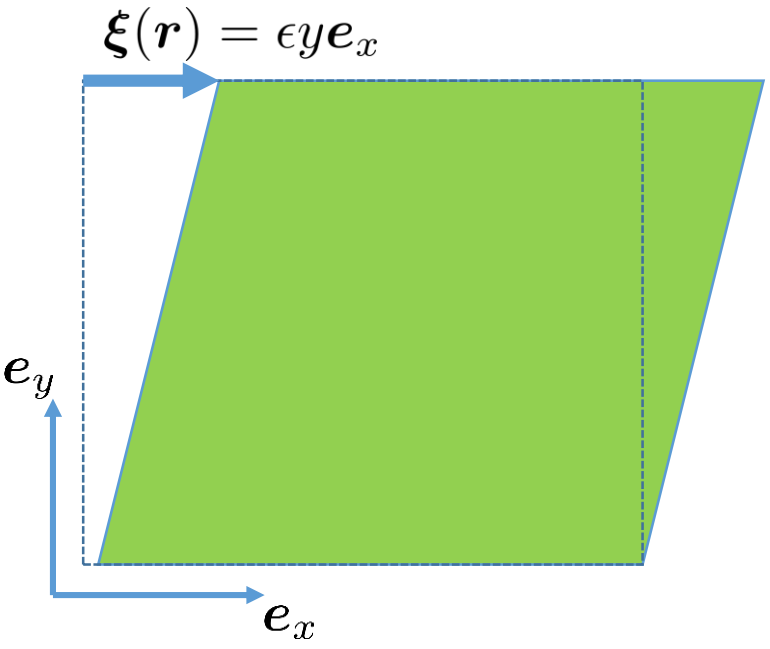
- What are possible mountain building mechanisms (such as asymmetric accretion, temperature gradients, magnetic stress...)?



Typical stress-strain curves
[MD simulations]



Introduction: Theory of Elasticity



Deformation: $\boldsymbol{r} \to \boldsymbol{r} + \boldsymbol{\xi}(\boldsymbol{r})$

Displacement gradient $u_{ij} = \dfrac{\partial \xi_i}{\partial x_j}$

$$f_i = \frac{\partial \sigma_{ij}}{\partial x_j}$$

Forces

(to volume element from nearby elements)

In the crust $\sigma_{ij} = -P\delta_{ij} + \delta\sigma_{ij}$

EOS

(electrons+undeformed lattice)

Elastic part $\delta\sigma_{ij}(u_{ij})$

Elastic part of stress tensor

Microphysics: $\delta\sigma_{ij} = \delta\sigma_{ij}(u_{ij}, \ldots)$

$$\delta\sigma_{ij} \lesssim 10^{-3} P_e$$

Reminder: Traditional case $P = 0$

Taylor expansion for energy: $\delta^{(2)}\mathcal{E} = \frac{1}{2} S_{ijkl} u_{ij} u_{kl}$

$$\mathcal{E} = \rho_0 E$$

Density at not deformed state, i.e. corresponding to $\boldsymbol{\xi} = 0 \;\Rightarrow u_{ij} = 0$

Energy per unit mass at given deformation

Generally, $\mathcal{E}$ is not equal to the energy density

Elastic part of stress tensor

Microphysics: $\delta\sigma_{ij} = \delta\sigma_{ij}(u_{ij}, \ldots)$

$$\delta\sigma_{ij} \lesssim 10^{-3} P_e$$

Reminder: Traditional case $P = 0$

$$\delta^{(2)}\mathcal{E} = \frac{1}{2} S_{ijkl} u_{ij} u_{kl}$$

$$\sigma_{ij} = \frac{1}{2} B_{ijkl} \left(u_{kl} + u_{lk}\right)$$

$$P = 0 \Rightarrow \qquad S_{ijkl} = B_{ijkl}$$

Voigt symmetry: $S_{ijkl} = S_{jikl} = S_{klij}$ - up to 21 coefficients

Elastic part of stress tensor

Microphysics: $\delta\sigma_{ij} = \delta\sigma_{ij}(u_{ij}, \ldots)$

$$\delta\sigma_{ij} \lesssim 10^{-3} P_e$$

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$$\delta^{(2)}\mathcal{E} = \frac{1}{2} S_{ijkl} u_{ij} u_{kl}$$

$$\sigma_{ij} = \frac{1}{2} B_{ijkl} \left(u_{kl} + u_{lk}\right)$$

For cubic crystal 3 independent coefficients:

$$c_{11} = B_{xxxx}, \quad c_{12} = B_{xxyy}, \quad c_{44} = B_{xyxy}$$

Isotropic material: $\delta^{(2)}\mathcal{E} = \mu \left(u_{ik} - \frac{1}{3}\delta_{ik} u_{ll}\right)^2 + \frac{K}{2} u_{ll}^2$

Elastic part of stress tensor

Microphysics: $\delta\sigma_{ij} = \delta\sigma_{ij}(u_{ij}, \ldots)$

$$\delta\sigma_{ij} \lesssim 10^{-3} P_e$$

Neutron star crust: $P \neq 0$ [Wallace (1967), Baiko (2011), see also Marcus & Qiu (2009)]

$$\delta\mathcal{E} = -P\delta_{ij}u_{ij} + \frac{1}{2}S_{ijkl}u_{ij}u_{kl}$$

$$\delta\sigma_{ij} = \frac{1}{2}B_{ijkl}\left(u_{kl} + u_{lk}\right)$$

$$P \neq 0 \Rightarrow \quad S_{iklm} \neq B_{iklm}$$

Voigt symmetry: $B_{ijkl} = B_{jikl} = B_{klij}$ - up to 21 coefficients

Elasticity under finite pressure

[Wallace (1967), Baiko (2011), see also Marcus & Qiu (2009)]

$$\delta\mathcal{E} = -P\delta_{ij}u_{ij} + \frac{1}{2}S_{ijkl}u_{ij}u_{kl}$$

Associated with $\delta E = -P\delta V$

$$\tilde{R}_i^\alpha = R_j^\alpha\left(\delta_{ij} + u_{ij}\right)$$

$$\tilde{V} = \det\left(\delta_{ij} + u_{ij}\right) V$$

$$\delta\sigma_{ij} = \frac{1}{2}B_{ijkl}\left(u_{kl} + u_{lk}\right)$$

$$B_{ijkl} = S_{ijkl} - P\left(\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl}\right)$$

Associated with $-P\delta^{(2)}V$, i.e. change of the volume (compression) in the second order of strain (deformation); it does not associated with perturbation of the stress

The elastic stresses are linear over displacements

Elasticity under finite pressure

Example: isotropic elastic material

$$B_{ijkl} = K\delta_{ij}\delta_{kl} + \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \tfrac{2}{3}\delta_{ij}\delta_{kl}\right)$$

The same form as for $P = 0$

$$\begin{aligned} S_{ijkl} &= B_{ijkl} + P\left(\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl}\right) \\ &= \left(K - P\right)\delta_{ij}\delta_{kl} + \mu\delta_{ik}\delta_{jl} \\ &+ \left(\mu + P\right)\delta_{il}\delta_{jk} - \frac{2\mu}{3}\delta_{ij}\delta_{kl} \end{aligned}$$

Elasticity under finite pressure

Example: isotropic elastic material

$$B_{ijkl} = K\delta_{ij}\delta_{kl} + \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \tfrac{2}{3}\delta_{ij}\delta_{kl}\right)$$

$$\begin{aligned}\delta\sigma_{ij} &= \frac{1}{2}B_{ijkl}\left(u_{kl} + u_{lk}\right) \\ &= K\delta_{ij}u_{ll} + \frac{\mu}{2}\left(u_{ik} + u_{ki} - \frac{2}{3}\delta_{ik}u_{ll}\right)\end{aligned}$$

Equation for variation of the stress tensor have standard form (same as for vanishing pressure at non-deformed state)

B_{ijkl} Is the most useful for neutron star applications (allows to calculate stresses, but not the energies!!!)

S_{ijkl} Is useful for microphysical calculations

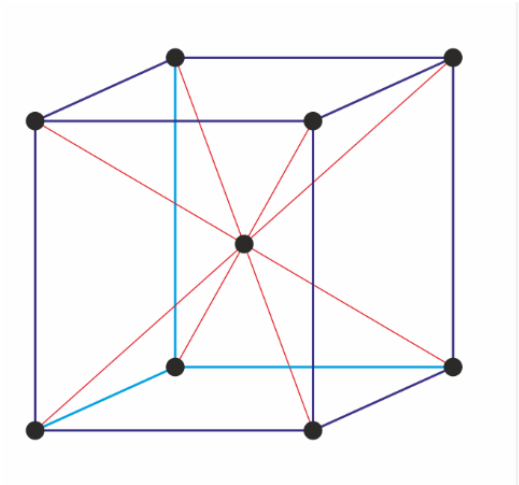
Basic model and scaling

[one component crust – all ions are equal]

$$\delta\sigma_{ij} = \frac{Z^2e^2}{a} n\,\delta\tilde{\sigma}_{ij}\left(u_{ij}, \Gamma = \frac{Z^2e^2}{aT}, \frac{T}{\hbar\omega_P}, ak_{\mathrm{TF}}, \ldots\right)$$

Point charges, TF screening: $a = (4\pi n/3)^{-1/3}$

Ions form BCC lattice



(Arbitrary) uniform compression/expansion does not lead to breaking
(but can initiate nuclear reactions)

Beyond scope:

Realistic (Jancovici 1962) electron screening [Baiko 2002]

Hidden symmetry of elasticity tensor

Uniform deformation at microphysical level

$$\boldsymbol{R} \to \boldsymbol{R}' = \boldsymbol{R} + \boldsymbol{\xi}(\boldsymbol{R}), \quad \xi_i = u_{ij} R_j$$

Change in energy (ion-ion interaction for example)

$$\delta\mathcal{E}'_{ion} = \frac{1}{2}\sum_{ions} Z_a Z_b e^2 \left(\frac{1}{|\boldsymbol{R} + \boldsymbol{\xi}(\boldsymbol{R})|} - \frac{1}{|\boldsymbol{R}|} \right)$$

Agrees with numerical results by Kozhberov (2019)

$$\frac{R_i}{R^3}\xi_i + \frac{3R_iR_k - R^2\delta_{ik}}{R^5}\xi_i\xi_k = \frac{R_iR_j}{R^3}u_{ij} + \frac{3R_iR_k - R^2\delta_{ik}}{R^5}R_jR_l u_{ij}u_{kl}$$

Contributes to S_{ijkl} , but note:

$$S_{ijil} = 0$$

For any Coulomb crystal (arbitrary structure and composition), neglecting ion motion

After summation over ions lead to term

$$-\sigma^0_{ij} V_0 \, u_{ij} = -P\mathrm{d}V$$

(if nondeformed lattice had symmetric stress tensor)

Hidden symmetry of elasticity tensor

Uniform deformation at microphysical level

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Change in energy (ion-ion interaction for example)

$$\delta\mathcal{E}'_{ion} = \frac{1}{2}\sum_{ions} Z_a Z_b e^2 \left(\frac{1}{|\boldsymbol{R} + \boldsymbol{\xi}(\boldsymbol{R})|} - \frac{1}{|\boldsymbol{R}|} \right)$$

$$\frac{R_i}{R^3}\xi_i + \frac{3R_iR_k - R^2\delta_{ik}}{R^5}\xi_i\xi_k = \frac{R_iR_j}{R^3}u_{ij} + \frac{3R_iR_k - R^2\delta_{ik}}{R^5}R_jR_l u_{ij}u_{kl}$$

Agrees with numerical results by Kozhberov (2019)

Contributes to S_{ijkl} , but note:

$$B_{ijil} = S_{ijil} = 0$$

For any Coulomb crystal (arbitrary structure and composition), neglecting ion motion

After summation over ions lead to term

$$-\sigma^0_{ij} V_0 \, u_{ij} = -P\mathrm{d}V$$

(if nondeformed lattice had symmetric stress tensor)

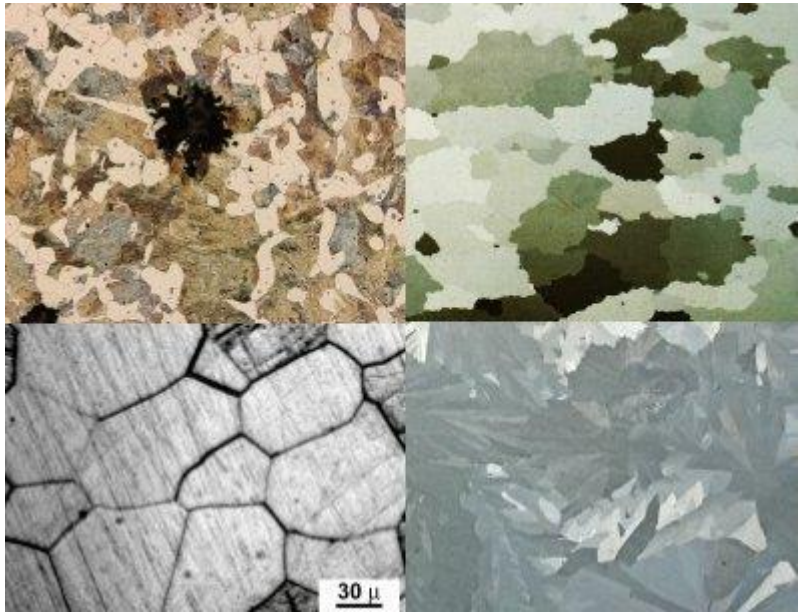
Small deformations: Polycrystal

Polycrystalline matter, made of large number of single crystals, should be isotropic.

$$\delta\sigma_{ij} = \mu_{\text{eff}}\left(u_{ik} + u_{ki} - \frac{2}{3}\delta_{ij}u_{ll}\right) + K u_{ll}\delta_{ij}$$

Shear modulus

Compression modulus



[From Wikipedia]

Landau&Lifshitz, vol. 7: "The relation between the elastic properties of the whole crystal and those of components crystallites depends on actual form of the latter and the amount of correlation of their mutual orientation."

Ogata&Ichimaru (1990):
(Uniform deformation=Voigt average)

$$\mu_{\text{eff}}^{\text{V}} = 0.120\frac{Z^2e^2}{a}n$$

Kobyakov&Pethick (2015):
(self consistent theory by Eshelby 1961)

$$\mu_{\text{eff}}^{\text{sc}} = 0.093\frac{Z^2e^2}{a}n$$

28% difference

Polycrystalline crust: Voigt average

Assumptions:
(1) uniform distribution of crystallite orientations
(2) uniform deformation within whole polycrystalline matter

$$\delta^{(2)}\mathcal{E} = \sum_c \frac{V_c}{2V} S^c_{ijkl} u_{ij} u_{kl} = \sum_c \frac{V_c}{2V} S_{mnop} R^c_{im} R^c_{jn} R^c_{ko} R^c_{lp} u_{ij} u_{kl} = S^V_{ijkl} u_{ij} u_{kl}$$

$$S^V_{ijkl} = \left\langle S_{mnop} R^c_{im} R^c_{jn} R^c_{ko} R^c_{lp} \right\rangle$$

$$R_{ik} R_{il} = \delta_{kl}$$

Rotation matrix, required to rotate crystal axis to the lab system

Following convolutions are invariants (see, e.g. D. Blaschke 2017)

$$S^V_{iijj} = \langle S_{mnop} R_{im} R_{in} R_{jo} R_{jp} \rangle = \langle S_{mnop} \delta_{mn} \delta_{op} \rangle = S_{iijj}$$

$$S^V_{ijij} = \langle S_{mnop} R_{im} R_{jn} R_{io} R_{jp} \rangle = \langle S_{mnop} \delta_{mo} \delta_{np} \rangle = S_{ijij}$$

Voigt average gives an upper limit for elastic tensor
(nonunifrom deformation of crystallites, in principle, can reduce the energy)

Polycrystalline crust: Voigt average

Assumptions:
(1) uniform distribution of crystallite orientations
(2) uniform deformation within polycrystalline

$$\delta^{(2)}\mathcal{E} = \sum_c \frac{V_c}{2V} S^c_{ijkl} u_{ij} u_{kl} = \sum_c \frac{V_c}{2V} S_{mnop} R^c_{im} R^c_{jn} R^c_{ko} R^c_{lp} u_{ij} u_{kl} = S^V_{ijkl} u_{ij} u_{kl}$$

$$S^V_{ijkl} = \langle S_{mnop} R_{im} R_{jn} R_{ko} R_{lp} \rangle$$

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$$S^V_{ijij} = \langle S_{mnop} R_{im} R_{jn} R_{io} R_{jp} \rangle = \langle S_{mnop} \delta_{mo} \delta_{np} \rangle = S_{ijij}$$

For Coulomb crystals (neglecting ion motion): $S_{ijij} = 0 \Rightarrow S^V_{ijij} = 0$

(can be also shown in the same way as for monocrystal, by uniform deformation of polycrystal)

Polycrystalline crust: Voigt average

Isotropic elastic tensor:

$$B^V_{ijkl} = \lambda\delta_{ij}\delta_{kl} + 2\mu^V_{\rm eff}\left(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}\right), \quad K = \lambda + \frac{2}{3}\mu^V_{\rm eff}$$

$$B^V_{ijij} = 3\lambda + 12\mu^V_{\rm eff}$$

For Coulomb crystals (neglecting ion motion):

$$B^V_{ijij} = S^V_{ijij} = 0 \;\Rightarrow\; \lambda = -4\,\mu^V_{\rm eff};\; K = -\frac{10}{3}\mu^V_{\rm eff}$$

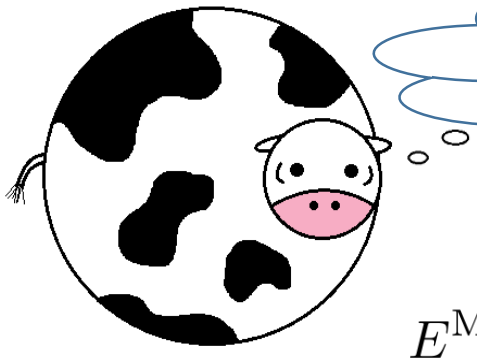
$$E^M \propto \frac{n}{a_{\rm e}} \propto n^{4/3} \Rightarrow P = \frac{1}{3}E,\; K = n\frac{{\rm d}P}{{\rm d}n} = \frac{4}{9}E^M$$

AIC (2021)

$$\mu^V_{\rm eff} = -\frac{2}{15}E^M$$

For any Coulomb crystal
(arbitrary structure and composition)

Polycrystalline crust: Voigt average



Some problems can be solved analytically!

$$E^{\mathrm{M}} = -\zeta \frac{Z^2 e^2}{a} n, \quad a = \left(\frac{3}{4\pi n}\right)^{1/3}, \quad \zeta = 0.89592925568$$

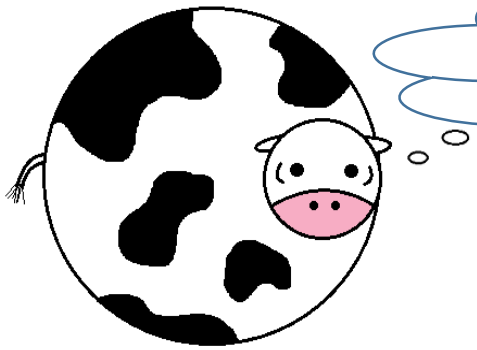
0.1194572 [Baiko 2011]

$$\mu_{\mathrm{eff}}^{\mathrm{V}} = \frac{2\zeta}{15} \frac{Z^2 e^2}{a} n = 0.11945723409 \frac{Z^2 e^2}{a} n$$

$$\mu_{\mathrm{eff}}^{V} = -\frac{2}{15} E^{M}$$

For any Coulomb crystal
(arbitrary structure and composition)

Polycrystalline crust: Voigt average



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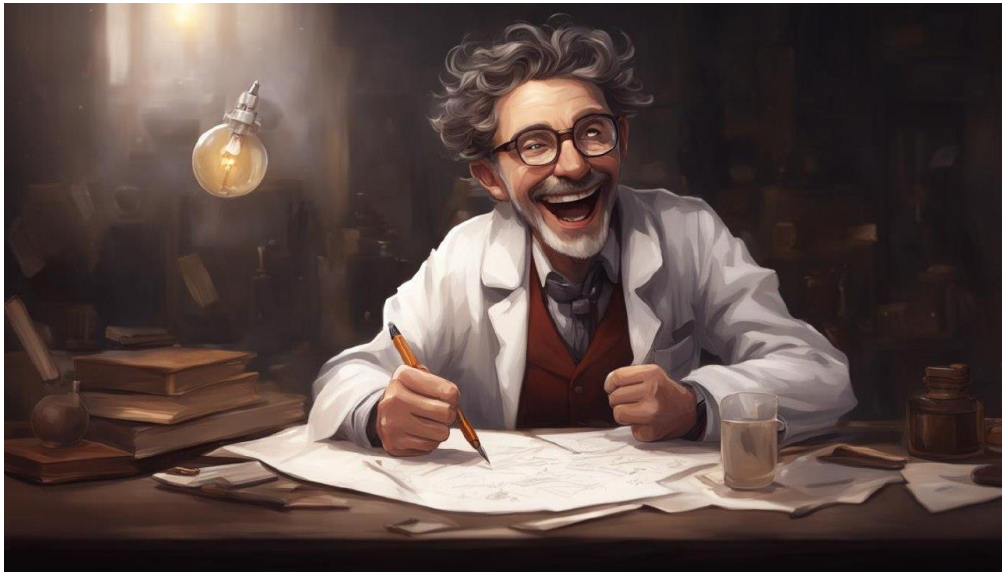
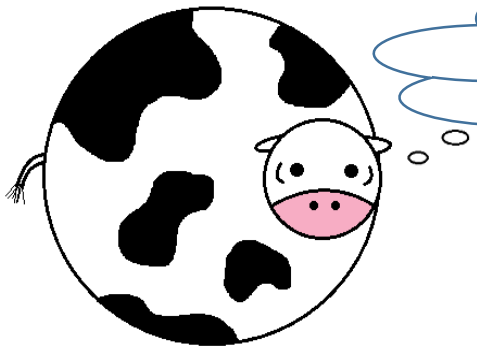


$$\mu_{\rm eff}^{V} = -\frac{2}{15} E^{M}$$

For any Coulomb crystal
(arbitrary structure and composition)

Polycrystalline crust: Voigt average



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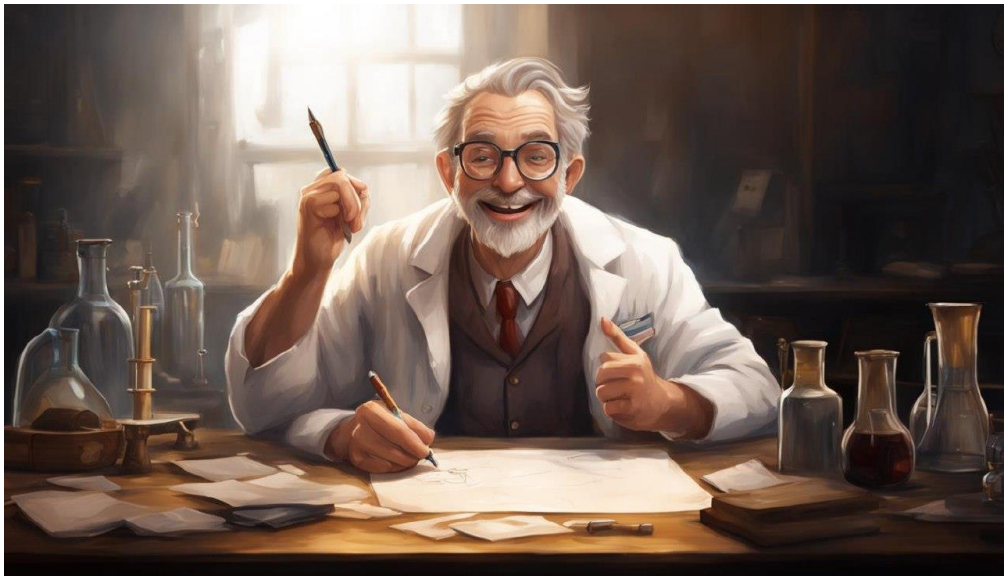


$$\mu_{\text{eff}}^{V} = -\frac{2}{15} E^{M}$$

For any Coulomb crystal
(arbitrary structure and composition)

Note for students

If you calculate two quantities and they coincide up to several digits without any known reason

- Try to understand why
- Report to scientific advisor

If the same holds true for two functions – you are lucky. Almost for sure there are something behind it.
Probably, it allows to make theory even simpler (or you localize an error in the code…).

> "Everything should be made as simple as possible, but not simpler"

Attributed to Albert Einstein

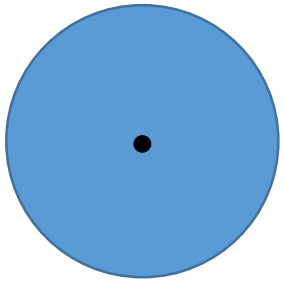
Elasticity: analytical formulae

$$\mu_{\rm eff}^{V} = -\frac{2}{15} E^{M}$$

For any Coulomb crystal
(arbitrary structure and composition)

Ion sphere model:

$$E^{\rm M} = -\frac{9}{10}\frac{Z^2 e^2}{a} n, \quad a = \left(\frac{3}{4\pi n}\right)^{1/3}$$



$$\mu_{\rm eff}^{\rm V} = \frac{3}{25}\frac{Z^2 e^2}{a} n = 0.12\frac{Z^2 e^2}{a} n$$

Multicomponent crystal: Linear mixing rule

$$E^{\rm M} = -\frac{9}{10}\sum_i \frac{Z_i^{5/3} e^2}{a_e} n_i, \quad a_e = \left(\frac{3}{4\pi n_e}\right)^{1/3}$$

$$\mu_{\rm eff}^{\rm V} = \frac{3}{25}\sum_i \frac{Z_i^{5/3} e^2}{a_e} n_i = 0.12\sum_i \frac{Z_i^{5/3} e^2}{a_e} n_i$$

For arbitrary structure and composition of crystallites (no metallurgy for the crust!)

Screening corrections for elasticity

Thomas-Fermi approximation

Energy density $$\epsilon = \epsilon_C + \kappa^2 a_e^2 \epsilon_{\rm scr}$$

Uniform background

Screening wave number

$$\mu_{\rm eff}^V = -\frac{2}{15}\epsilon_C + \frac{4}{15}\kappa^2 a_e^2 \epsilon_{scr}$$

Ion sphere model:

$$\epsilon_C = -\frac{9}{10}\sum_i \frac{Z_i^{5/3} e^2}{a_e} n_i; \quad \epsilon_{\rm scr} \approx -0.103 \sum_i \frac{Z_i^{7/3} e^2}{a_e} n_i$$

$$\mu_{\rm eff}^{\rm V} = 0.12 \sum_i \frac{Z_i^{5/3} e^2}{a_e} n_i - 9.4 \times 10^{-4} \frac{\sqrt{1+x^2}}{x} \sum_i \frac{Z_i^{7/3} e^2}{a_e} n_i$$

Physics of a neutron star crust
Summary of lecture 2.

- ➢ Thermodynamics of the outer crust: $F = F_{\rm e} + F_{\rm i} + F_{\rm ie} + \sum_i M_i N_i$
- ✓ Electrons: analytical Sommerfeld expansion
- ✓ Nuclei (ions):
- Done, within one component approximation (fits of ab initio simulations)
- Extrapolations to many components, based on limited ab initio simulations
- ❑ Corrections: a bit controversially in liquid and solid state. Is it real?
- ➢ Crust elasticity
- ✓ Finite pressure should be taken into account
- ✓ Effective shear modulus can be calculated analytically (within static Voigt approximation)
- ○ Corrections for quantum and thermal motion of nuclei (Baiko 2012)

Lecture 3

- ➢ Inner crust
- Extended Thomas-Fermi calculations and pasta phases
- Compressible liquid drop model
- Mass-radius relation (without crust EOS)