

Neutron star crusts beyond the Wigner-Seitz approximation

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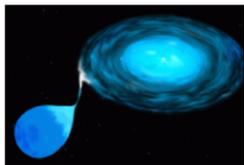
EXOCT 2007

Plan

- 1 Introduction
- 2 Band theory and Wigner-Seitz approximation
- 3 Comparison near neutron drip
- 4 Conclusion and perspectives

Neutron star crust and observations

Many observational phenomenae are related to the physics of the crust



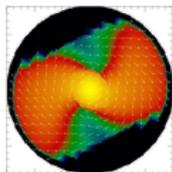
Explosions thermonucléaires et sursauts X dans les binaires X



Effondrement d'étoiles massives et supernova



Sursauts gamma et oscillations des magnétars



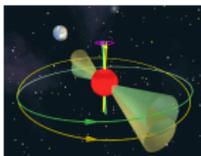
Déformations non axiales, oscillations et émission d'ondes gravitationnelles



Tremblements de croûte et irrégularités de la période de rotation des pulsars

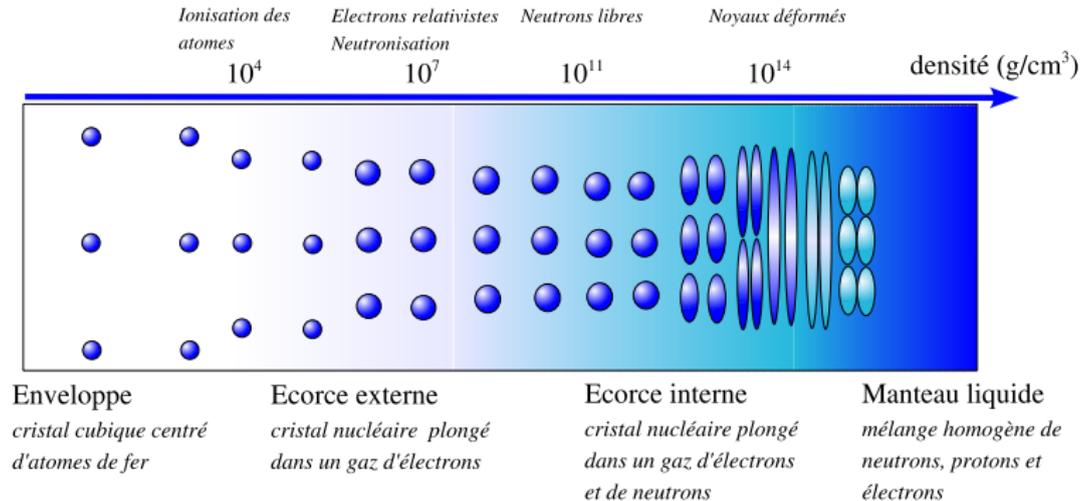


Refroidissement des étoiles à neutrons et émission X thermique



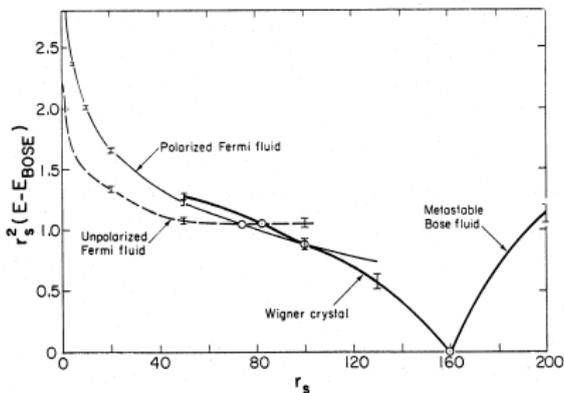
Précession libre dans les pulsars

Structure of neutron star crust



Electronic structure

The electronic properties in the crust are much simpler than in terrestrial matter!



Ceperley et al., PRL45(1980) 566.

$$r_s \equiv d/a_0$$

$$a_0 \equiv \hbar^2/m_e e^2$$

$$d \equiv (3/4\pi n_e)^{1/3}$$

metals $r_s \sim 2 - 6$

neutron star crust

$r_s \sim 10^{-5} - 10^{-2}$

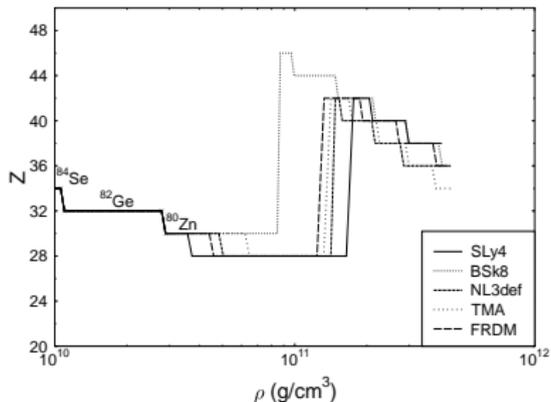
Composition of the outer crust (T=0)

The composition of the outer crust is completely determined by the experimental atomic masses except in the bottom layers above $\sim 6 \times 10^{10} \text{ g.cm}^{-3}$

μ [MeV]	μ_e [MeV]	ρ_{max} [g/cm ³]	P [dyne/cm ²]	n_b [cm ⁻³]	Element	Z	N
930.60	0.95	8.02×10^6	5.22×10^{23}	4.83×10^{30}	⁵⁶ Fe	26	30
931.32	2.61	2.71×10^8	6.98×10^{25}	1.63×10^{32}	⁶² Ni	28	34
932.04	4.34	1.33×10^9	5.72×10^{26}	8.03×10^{32}	⁶⁴ Ni	28	36
932.09	4.46	1.50×10^9	6.44×10^{26}	9.04×10^{32}	⁶⁶ Ni	28	38
932.56	5.64	3.09×10^9	1.65×10^{27}	1.86×10^{33}	⁸⁶ Kr	36	50
933.62	8.38	1.06×10^{10}	8.19×10^{27}	6.37×10^{33}	⁸⁴ Se	34	50
934.75	11.43	2.79×10^{10}	2.85×10^{28}	1.68×10^{34}	⁸² Ge	32	50
935.89	14.61	6.07×10^{10}	7.63×10^{28}	3.65×10^{34}	⁸⁰ Zn	30	50
936.44	16.17	8.46×10^{10}	1.15×10^{29}	5.08×10^{34}	⁸² Zn	30	52
936.63	16.81	9.67×10^{10}	1.32×10^{29}	5.80×10^{34}	¹²⁸ Pd	46	82
937.41	19.16	1.47×10^{11}	2.23×10^{29}	8.84×10^{34}	¹²⁶ Ru	44	82
938.12	21.35	2.11×10^{11}	3.45×10^{29}	1.26×10^{35}	¹²⁴ Mo	42	82
938.78	23.47	2.89×10^{11}	5.05×10^{29}	1.73×10^{35}	¹²² Zr	40	82
939.47	25.77	3.97×10^{11}	7.36×10^{29}	2.38×10^{35}	¹²⁰ Sr	38	82
939.57	26.09	4.27×10^{11}	7.74×10^{29}	2.56×10^{35}	¹¹⁸ Kr	36	82

Composition of the outer crust (T=0)

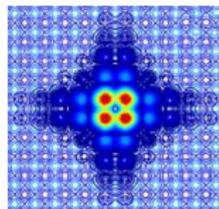
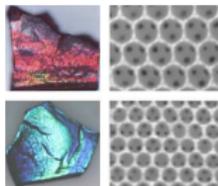
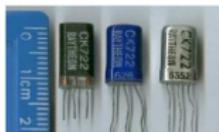
Comparison between different theoretical mass tables



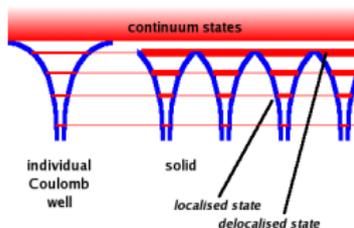
Rüster et al., PRC73 (2006) 035804.

“Neutronic” crystals

The inner crust of neutron stars is the nuclear analog of periodic systems in condensed matter : electrons in solids, photonic and phononic crystals, cold atomic Bose gases in optical lattice



⇒ neutron star crust can thus be viewed as a “**neutronic**” crystal



new approach by applying the band theory of solids at the nuclear scale

Chamel, Nucl.Phys.A747(2005)109.

Chamel, Nucl.Phys.A773(2006)263.

Band theory

Floquet-Bloch theorem

« I found to my delight that the wave differed from the plane wave of free electrons only by a periodic modulation. »

Bloch, Physics Today 29 (1976), 23-27.



$$\varphi_{\alpha\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\alpha\mathbf{k}}(\mathbf{r})$$

$$u_{\alpha\mathbf{k}}(\mathbf{r} + \mathbf{T}) = u_{\alpha\mathbf{k}}(\mathbf{r})$$

- α → rotational symmetry around the lattice sites
- \mathbf{k} → translational symmetry of the crystal

Mean field approximation

In the Hartree-Fock approximation with Skyrme forces, the single particle states are the solutions of

$$h_0^{(q)} \varphi_{\alpha\mathbf{k}}^{(q)}(\mathbf{r}) = \varepsilon_{\alpha\mathbf{k}}^{(q)} \varphi_{\alpha\mathbf{k}}^{(q)}(\mathbf{r})$$

$$h_0^{(q)} \equiv -\nabla \cdot \frac{\hbar^2}{2m_q^\oplus(\mathbf{r})} \nabla + U_q(\mathbf{r}) - i\mathbf{W}_q(\mathbf{r}) \cdot \nabla \times \sigma$$

$$\frac{\hbar^2}{2m_q^\oplus(\mathbf{r})} = \frac{\delta\mathcal{E}(\mathbf{r})}{\delta\tau_q(\mathbf{r})}, \quad U_q(\mathbf{r}) = \frac{\delta\mathcal{E}(\mathbf{r})}{\delta n_q(\mathbf{r})}, \quad \mathbf{W}_q(\mathbf{r}) = \frac{\delta\mathcal{E}(\mathbf{r})}{\delta\mathbf{J}_q(\mathbf{r})}$$

Mean field approximation

Equivalently the HF equations can be solved for $u_{\alpha\mathbf{k}}(\mathbf{r})$

$$(h_0^{(q)} + h_{\mathbf{k}}^{(q)})u_{\alpha\mathbf{k}}^{(q)}(\mathbf{r}) = \varepsilon_{\alpha\mathbf{k}}^{(q)} u_{\alpha\mathbf{k}}^{(q)}(\mathbf{r})$$

$$h_{\mathbf{k}}^{(q)} \equiv \frac{\hbar^2 k^2}{2m_q^\oplus(\mathbf{r})} + \mathbf{v}_q \cdot \hbar\mathbf{k},$$

$$\mathbf{v}_q \equiv \frac{1}{i\hbar}[\mathbf{r}, h_0^{(q)}]$$

Symmetries

By symmetry, the crystal lattice can be partitioned into identical primitive cells. The HF equations need to be solved only inside one cell.

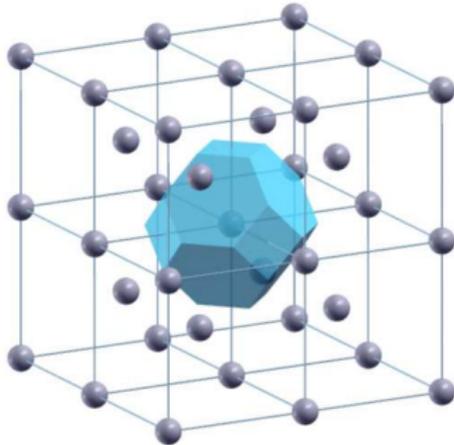
- The shape of the cell depends on the crystal symmetry
- The boundary conditions are fixed by the Floquet-Bloch theorem

$$\varphi_{\alpha\mathbf{k}}(\mathbf{r} + \mathbf{T}) = e^{i\mathbf{k}\cdot\mathbf{T}} \varphi_{\alpha\mathbf{k}}(\mathbf{r}) \leftrightarrow u_{\alpha\mathbf{k}}(\mathbf{r} + \mathbf{T}) = u_{\alpha\mathbf{k}}(\mathbf{r})$$

Wigner-Seitz cell

In particular the Wigner-Seitz or Voronoi cell is very useful since it reflects the local symmetry the lattice.

Example : body centered cubic lattice



Wigner-Seitz approximation

Approximation proposed by Wigner&Seitz in 1933 in the study of metallic sodium (only one valence electron per site) :



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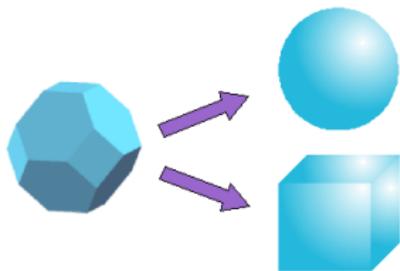
- Neglect the contribution of $h_{\mathbf{k}}^{(q)}$

Wigner-Seitz approximation

Approximation proposed by Wigner&Seitz in 1933 in the study of metallic sodium (only one valence electron per site) :



- Neglect the contribution of $h_{\mathbf{k}}^{(q)}$
- Replace the W-S cell by a simpler cell of same volume



Boundary conditions ?

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- Neumann boundary conditions with the vanishing of the normal derivative of φ as suggested by Wigner-Seitz

Boundary conditions ?

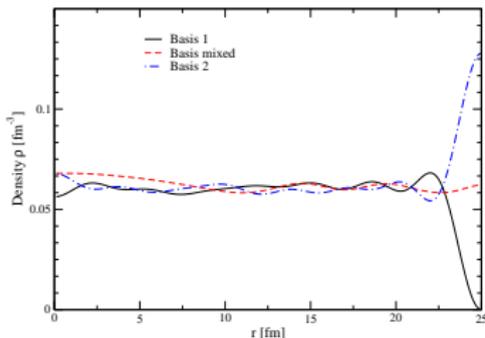
- Neumann boundary conditions with the vanishing of the normal derivative of φ as suggested by Wigner-Seitz
- Dirichlet boundary conditions with the vanishing of φ

Boundary conditions ?

- **Neumann boundary conditions** with the vanishing of the normal derivative of φ as suggested by Wigner-Seitz
- **Dirichlet boundary conditions** with the vanishing of φ
- **mixed boundary conditions** proposed by Negele&Vauherin
 - vanishing of φ for even ℓ
 - vanishing of the normal derivative of φ for odd ℓ
 - or *vice versa* as suggested by Baldo and coworkers

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Validity of the W-S approximation

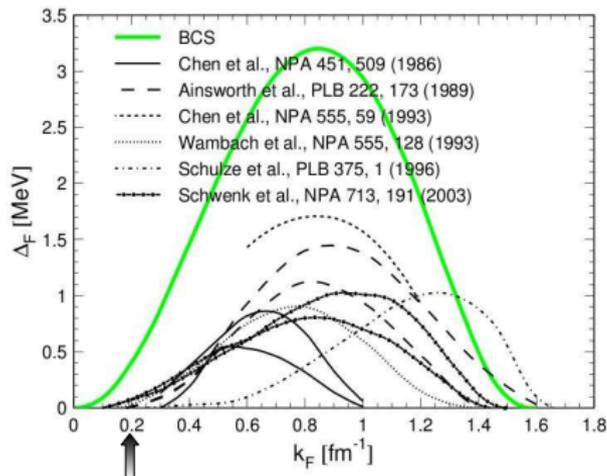
Comparison between the W-S approximation and the band theory near neutron drip

- assuming spherical nuclear clusters
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Baldo et al., Nucl.Phys.A749(2005),42c.

Validity of the W-S approximation

Comparison between the W-S approximation and the band theory near neutron drip

- assuming spherical nuclear clusters
- neglecting neutron pairing effects.

Due to proximity effects the neutron pairing field is smaller than its value in infinite matter and of order of a few ~ 10 keV.

Baldo et al. (2007), arXiv :nucl-th/0703099

Monrozeau et al. (2007), arXiv :nucl-th/0703064

Validity of the W-S approximation

Comparison between the W-S approximation and the band theory near neutron drip

- assuming spherical nuclear clusters
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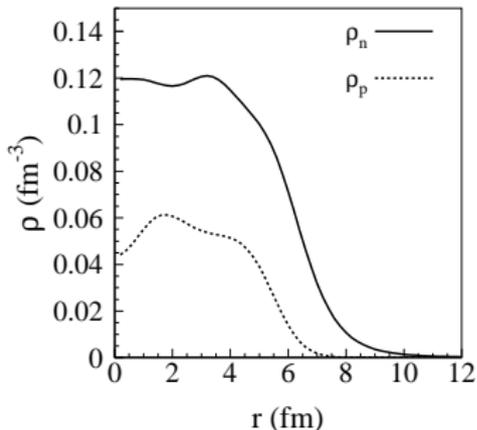
Body centered cubic crystal of zirconium like clusters

$$\rho = 7 \times 10^{11} \text{ g.cm}^{-3}$$

$$R_{\text{cell}} = 49 \text{ fm}$$

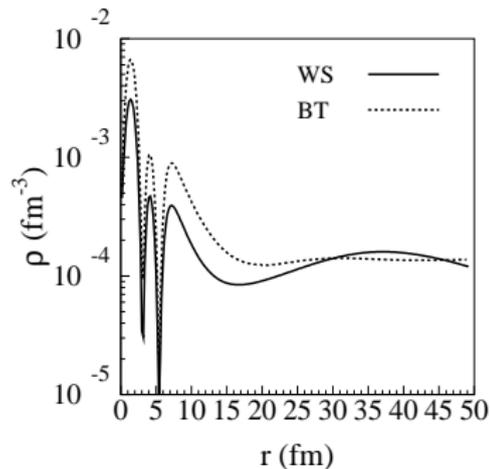
$$Z = 40$$

$$N = 90 \text{ bound} + 70 \text{ unbound}$$



W-S approximation vs band theory

Density of unbound neutrons in the W-S cell with ^{200}Zr .



W-S approx. (thick line)

band theory (dashed line)

Chamel et al, Phys.Rev.C75 (2007), 055806

\Rightarrow the W-S approximation leads to spurious fluctuations due to box size effects

W-S approximation vs band theory (II)

W-S approximation



full spherical symmetry

band theory



discrete rotational symmetry

W-S approximation vs band theory (II)

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full spherical symmetry

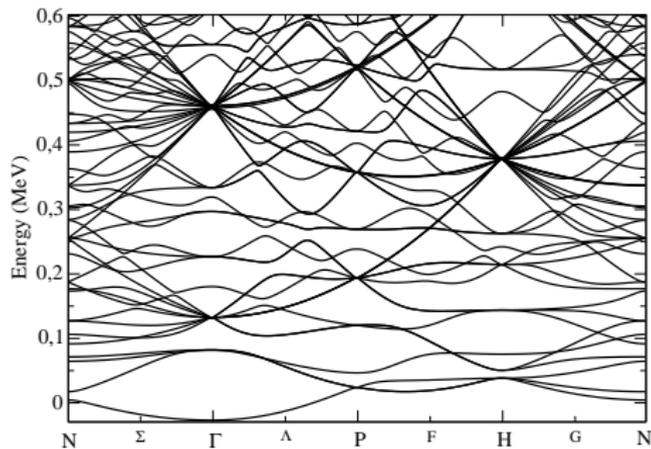
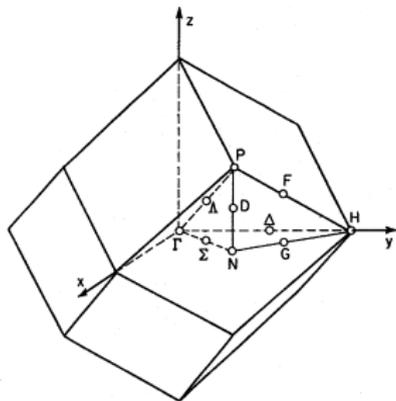
band theory



discrete rotational symmetry

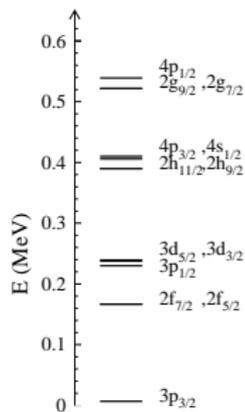
⇒ the W-S approximation overestimates the neutron shell effects

Neutron energy spectrum

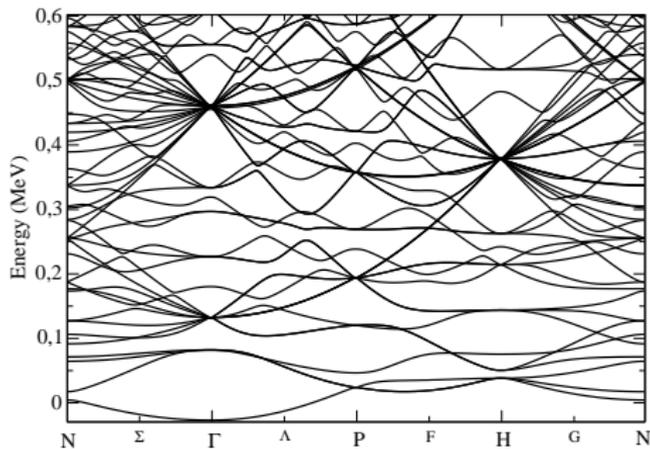


Neutron energy spectrum

W-S approximation



band theory



W-S approximation vs band theory (II)

Density of unbound neutron single particle states

W-S approximation vs band theory (II)

Density of unbound neutron single particle states
in the W-S approximation

$$\mathcal{N}(\mathcal{E}) = \frac{1}{V_{\text{cell}}} \sum_{n,\ell} (2\ell + 1) \delta(\mathcal{E} - \mathcal{E}_{n,\ell})$$

W-S approximation vs band theory (II)

Density of unbound neutron single particle states
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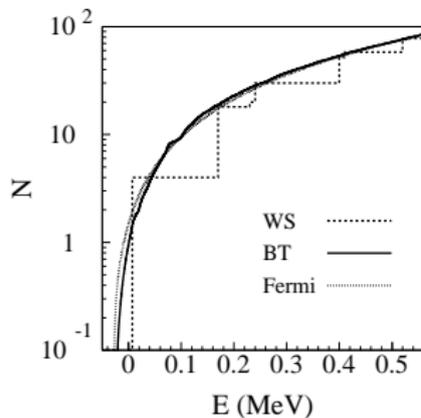
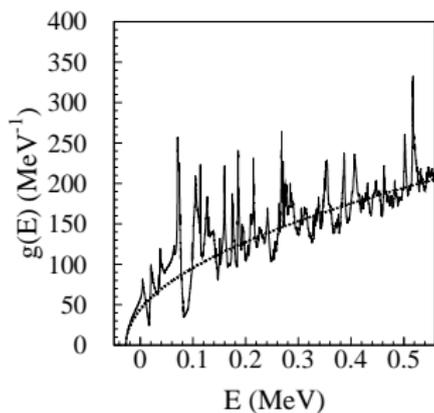
$$\mathcal{N}(\mathcal{E}) = \frac{1}{\mathcal{V}_{\text{cell}}} \sum_{n,l} (2l+1) \delta(\mathcal{E} - \mathcal{E}_{n,l})$$

in the band theory

$$\mathcal{N}(\mathcal{E}) = \frac{1}{4\pi^3} \sum_{\alpha} \int d^3k \delta(\mathcal{E} - \mathcal{E}_{\alpha\mathbf{k}}) = \frac{1}{4\pi^3} \oint_{\mathcal{E}_{\mathbf{k}}=\mathcal{E}} \frac{dS}{|\nabla_{\mathbf{k}}\mathcal{E}_{\mathbf{k}}|}$$

W-S approximation vs band theory (II)

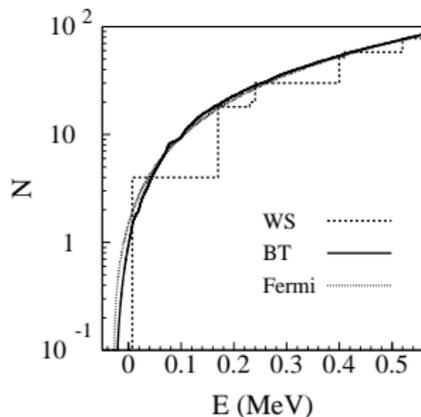
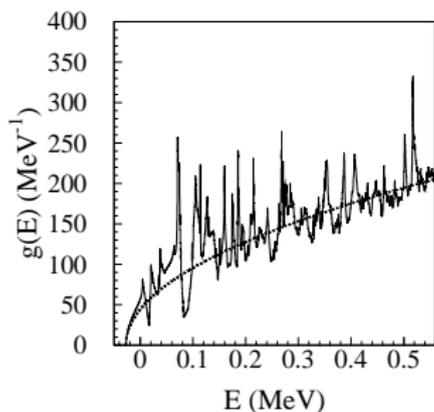
Density of unbound neutron single particle states



Chamel et al, Phys.Rev.C75 (2007), 055806

W-S approximation vs band theory (II)

Density of unbound neutron single particle states



Chamel et al, Phys.Rev.C75 (2007), 055806

\Rightarrow The average density of states is well reproduced by that of the Fermi gas

Neutron Fermi surface

At low temperatures the transport properties depend on the topology of the Fermi surface



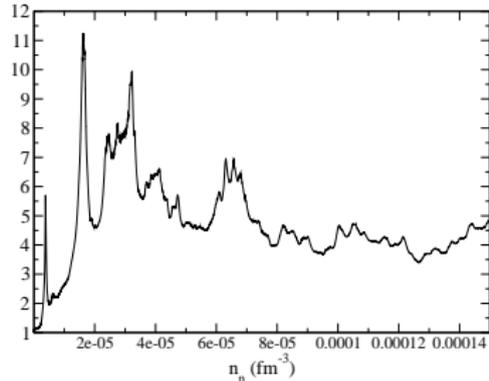
Chamel et al. Phys.Rev.C75(2007), 055806

The Fermi surface is spherical (\sim alkali metals) at densities below $n_n \lesssim \sqrt{2\pi}/3\nu_{\text{cell}}$ but non spherical at higher densities (\sim transition metals).

Optical effective mass

$$m_{\star} = n_n / \mathcal{K}$$

$$\mathcal{K} = \frac{1}{12\pi^3 \hbar^2} \int |\nabla_{\mathbf{k}} \mathcal{E}_{\mathbf{k}}| dS_{\mathbf{F}}$$

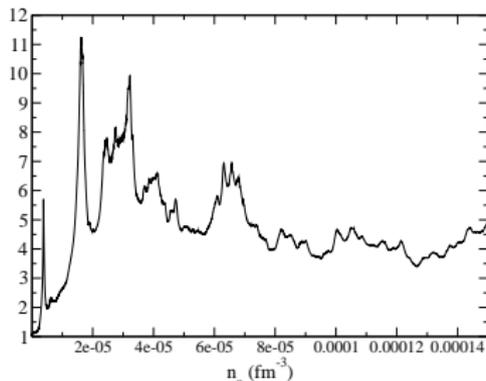


Chamel, *Nucl.Phys.A773(2006)263-278*.

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Chamel, Nucl.Phys.A773(2006)263-278.

why “optical” ?

dielectric constant
of metals ($\omega_T \gg 1$)

Cohen, Phil.Mag.49(1958)762

$$\varepsilon\{\omega\} \simeq 1 - \omega_{p_{\star}}^2 / \omega^2 + \varepsilon_{\text{inter}}$$
$$\omega_{p_{\star}}^2 = 4\pi e^2 n_e / m_{\star}$$

Macroscopic vs microscopic effective mass

m_* is the average over all occupied states

$$m_* = \frac{n_n}{\mathcal{K}} \quad \mathcal{K} = \frac{1}{3} \int_F \frac{d^3k}{(2\pi)^3} \text{Tr} \frac{1}{m_*(\mathbf{k})}$$

of the local effective mass tensor defined by

$$\left(\frac{1}{m_*(\mathbf{k})} \right)^{ij} = \frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}_{\mathbf{k}}}{\partial k_i \partial k_j}$$

usually introduced in neutron diffraction.

Zeilinger et al., PRL57 (1986), 3089.

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⇒ **macroscopic** effective mass relevant for hydrodynamics

Effective mass and entrainment effects

m_* governs the dynamics of the free neutrons.

In the crust rest frame

$$\mathbf{p}_n = m_* \mathbf{v}_n$$

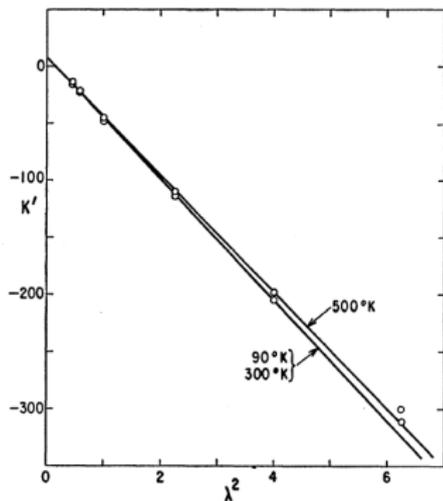
therefore in another frame, the momentum and the velocity are not aligned

$$\mathbf{p}_n = m_* \mathbf{v}_n + (m - m_*) \mathbf{v}_c$$

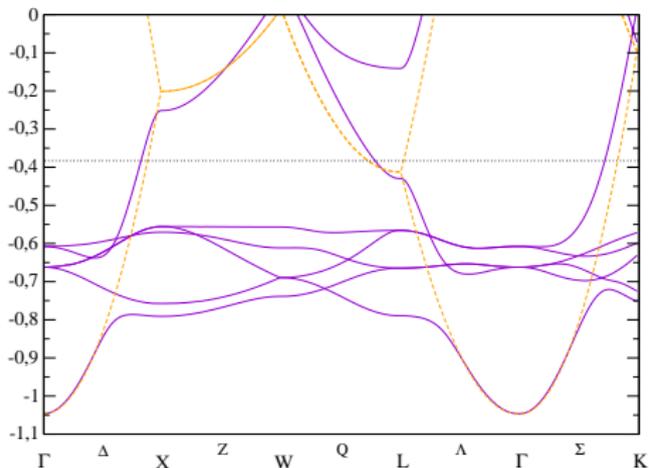
\Rightarrow entrainment effects (non dissipative)

For electrons in solids $m_* \sim 1 - 2m_e$.

Example in solid state physics : copper



$m_{\star} = (1.44 \pm 0.01)m_e$
Roberts, Phys. Rev. 118 (1960), 1509.



Chodorow's model

$m_{\star} = 1.285m_e$
Chamel, Nucl.Phys. A773 (2006) 263.

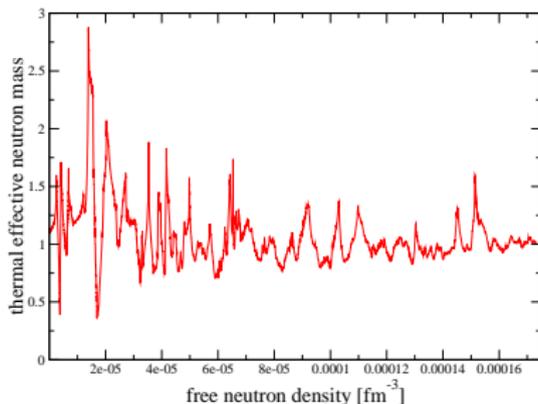
Neutron specific heat at high temperatures

At high temperatures, the free neutrons behave almost like an ideal Fermi gas

preliminary calculations

Neutron specific heat at low temperatures

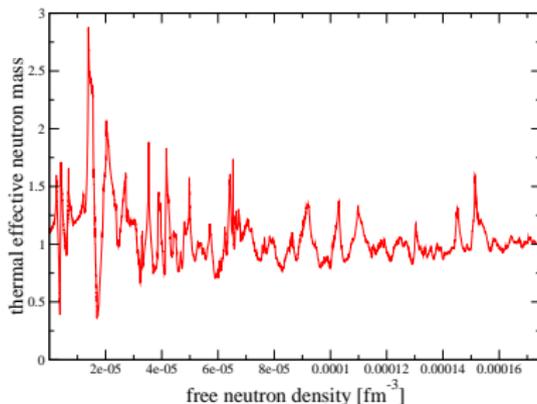
At low temperatures, the specific heat vary like $C_v \propto (m_\Theta/m)T$ where m_Θ is a thermal effective mass



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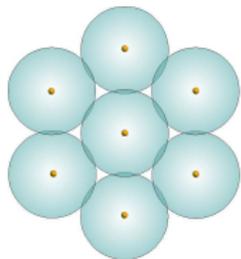
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preliminary calculations

⇒ very sensitive to the presence of the clusters !

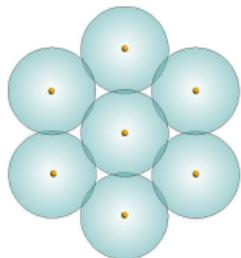
Conclusion



The validity of the W-S approximation depends on the energy scale $\delta\mathcal{E}$:

- reasonable if $\delta\mathcal{E} \gtrsim \hbar^2/2mR_{\text{cell}}^2 \sim 0.1 \text{ MeV}$
- otherwise the full band theory is required.

Conclusion

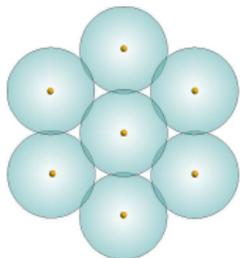


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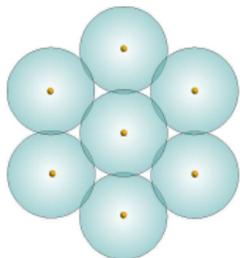
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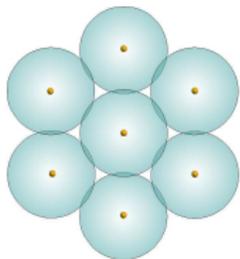
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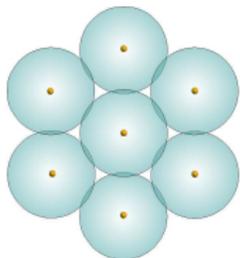
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- **restricted to spherical clusters** \Rightarrow cannot describe pastas

Conclusion



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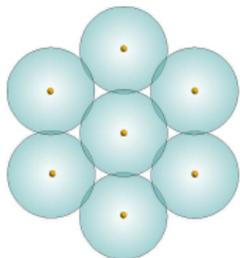
- reasonable if $\delta\mathcal{E} \gtrsim \hbar^2/2mR_{\text{cell}}^2 \sim 0.1 \text{ MeV}$
- otherwise the full band theory is required.

\Rightarrow hot ($T \gtrsim 10^9 \text{ K}$) dense matter in young neutron stars and in supernovae.

Main limitations for application to cold dense matter :

- **choice of boundary conditions** \Rightarrow uncertainties on the structure, spurious fluctuations of observables
- **restricted to spherical clusters** \Rightarrow cannot describe pastas
- **finite box size** \Rightarrow impossible to study transport properties.

Conclusion



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Validity of the W-S approximation for pairing effects ?