Hartree-Fock phase diagram of the Homogeneous Electron Gas in 2 or 3 Dimensions

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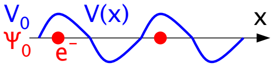
Why Hartree-Fock is still interesting ?

For many body systems : mean field must be done first. But Hartree-Fock ground state of HEG is still unknown !

Iterative Method (Lanczos) for homogeneous system : bi-stable, not converging in general.



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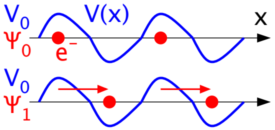

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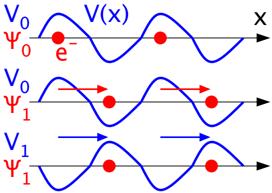

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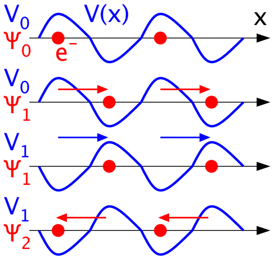

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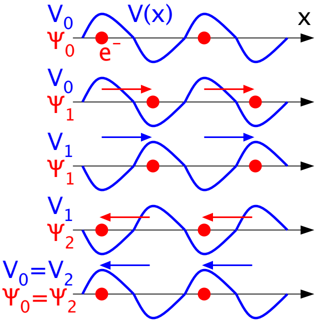
In our study : descent method (conjugate gradient)



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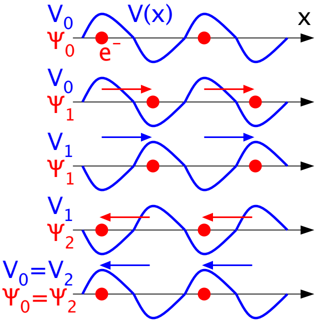
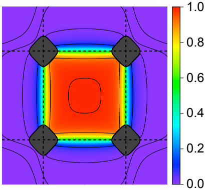
In spite of its "simplicity" : leads to exotic solutions with anisotropic fermi surfaces.

"Cheap" algorithm : great system sizes are available (up to 10^6 e^-). We can get rid of finite size effects.





Jellium Model (HEG)

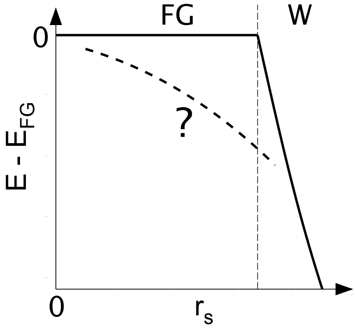
- negative charges : N electrons in a box : $|\Psi_N\rangle$
- positive charges : uniform background
- coulomb interaction : $1/r$

$\rightarrow$ good model for solid sodium (Na) (3D), heterostructures (2D)

One physical parameter

Mean distance between electrons $\sim r_s$

- kinetic energy $\sim 1/r_s^2$
- potential energy $\sim 1/r_s$



Two well known solutions :

- Fermi Gas (FG) : minimise kinetic energy
- Wigner crystal (W) : minimise potential energy

Our study : periodic states

Hartree-Fock : $\Psi_N = \det(\{\phi_{\mathbf{k}}\})$
$\phi_{\mathbf{k}}$: single particle wave function.

The goal is to find the set of $\phi_{\mathbf{k}}$ which give the lowest energy.

Ansatz :

Periodic charge density $\rightarrow \phi_{\mathbf{k}} =$ Bloch waves

$$\phi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}} u_{\mathbf{k}}(\mathbf{r}) \Leftrightarrow |\phi_{\mathbf{k}}\rangle = \sum_{\mathbf{q}} a_{\mathbf{k},\mathbf{q}} |\mathbf{k}+\mathbf{q}\rangle$$

The number of parameters in Ψ_N is greatly reduced. So :

- great system size : up to 10^6 electrons
- good precision on energy (< 0.01 mHa)

Wigner Crystal

Electron density in real space is symmetric.
For example : 2D square lattice.

Bloch waves :

$$\phi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) \Leftrightarrow |\phi_{\mathbf{k}}\rangle = \sum_{\mathbf{q}} a_{\mathbf{k},\mathbf{q}} |\mathbf{k}+\mathbf{q}\rangle$$

where **k** belongs to B, the first Brillouin zone of the lattice.

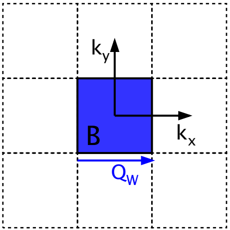
Constraint :

Number of states in B = Number of electrons

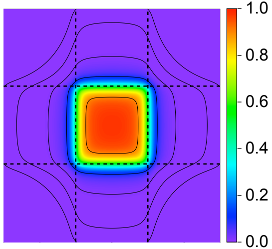
$$Q_W = \alpha_{\text{square}} k_F$$

$$\alpha_{\text{square}} = \sqrt{\pi} \approx 1.77$$

Brillouin zones :



$n(\mathbf{k})$



Incommensurate Crystal

Same as Wigner crystal, but :

Incommensurate crysal :

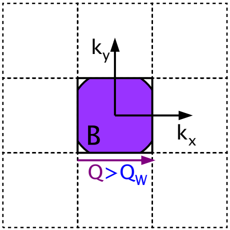
Number of states in $B >$ Number of electrons

$$Q > Q_W$$

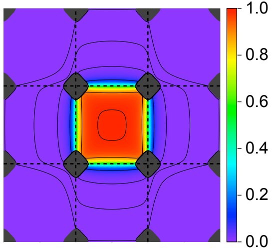
In real space, the electron gas form a crystal with less than one electron per cell.

Note : In the figure on the right, we considered $256^2 \approx 65500$ states in B, so $N \approx 60000$.

Brillouin zones :

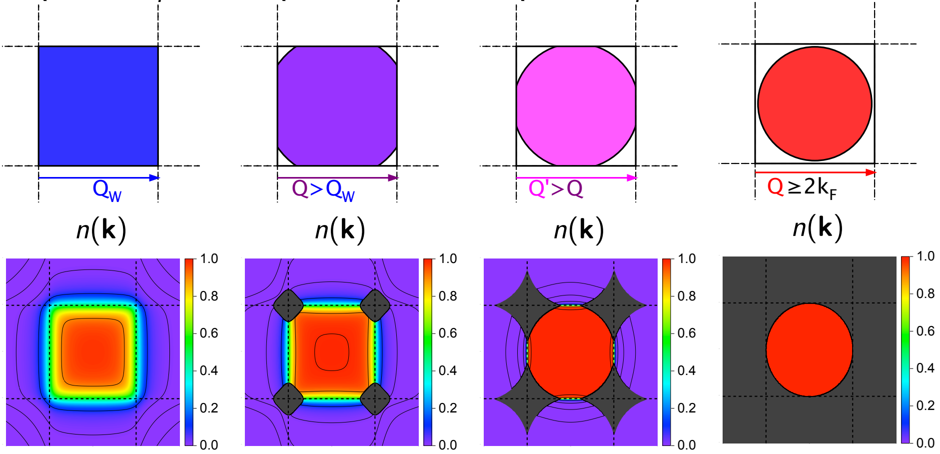


$n(\mathbf{k})$



Interpolation between W and FG

Wigner :	Incommensurate :	Incommensurate :	Fermi Gas :
$Q = Q_W$	$Q > Q_W$	$Q > Q_W$	$Q \geq 2k_F$
$Q \approx 1.77k_F$	$Q \approx 1.84k_F$	$Q \approx 1.98k_F$	



What happens in real space

Wigner :	Incommensurate :	Incommensurate :	Fermi Gas :
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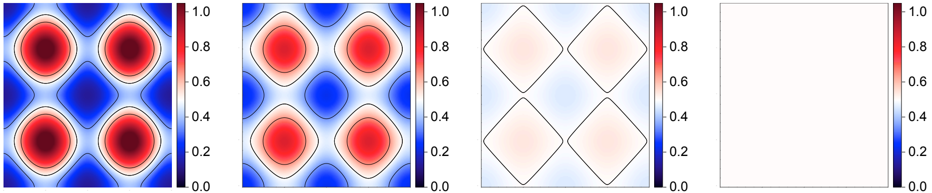
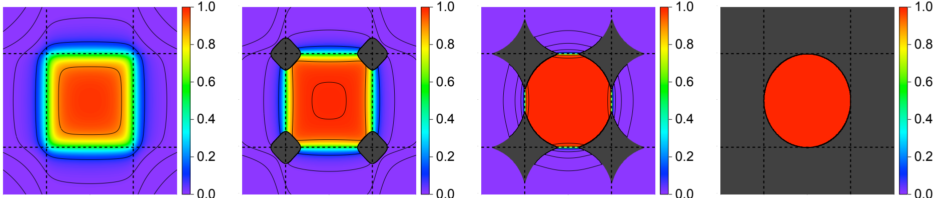
$n(\mathbf{r})$	$n(\mathbf{r})$	$n(\mathbf{r})$	$n(\mathbf{r})$

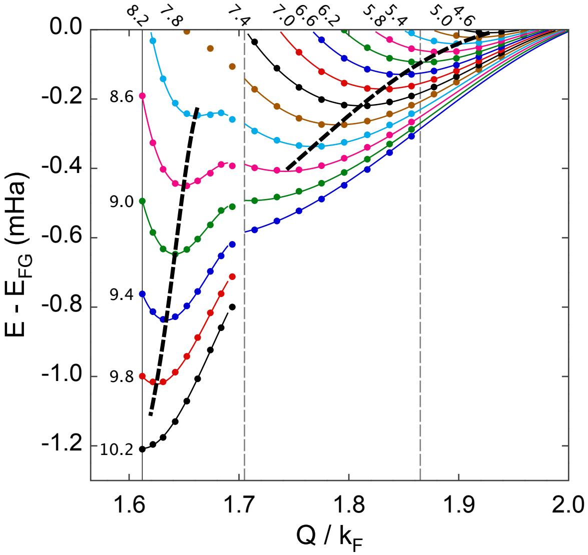


$n(\mathbf{k})$	$n(\mathbf{k})$	$n(\mathbf{k})$	$n(\mathbf{k})$



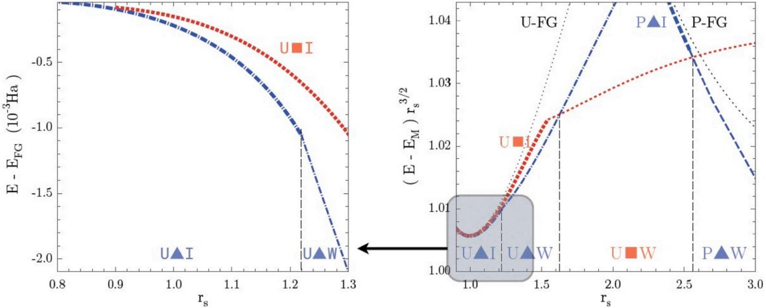
Numerical results at fixed geometry

Example : polarized gas with cubic geometry (3D)



2D phase diagram

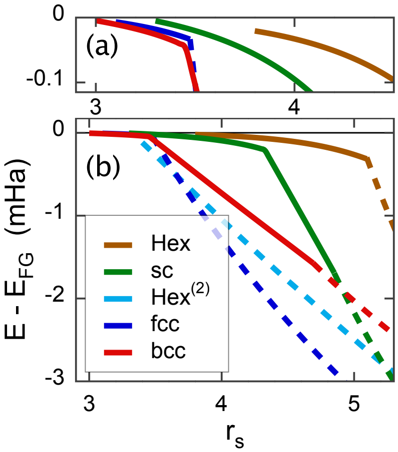
Bernu, Delyon, Holzmann, and Baguet, Phys. Rev. B 84, 115115, 2011

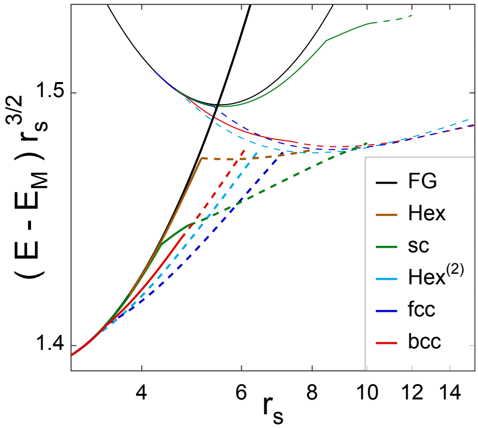


$2.55 < r_s$	▲ «Wigner»	↑↑
$1.55 < r_s < 2.55$	■ «Wigner»	↑↓
$1.225 < r_s < 1.55$	▲ «Wigner»	↑↓
$r_s < 1.225$	▲ «Incommensurate»	↑↓

3D phase diagram

Baguet, Delyon, Bernu, and Holzmann, Phys. Rev. Lett. 111, 166402, 2013



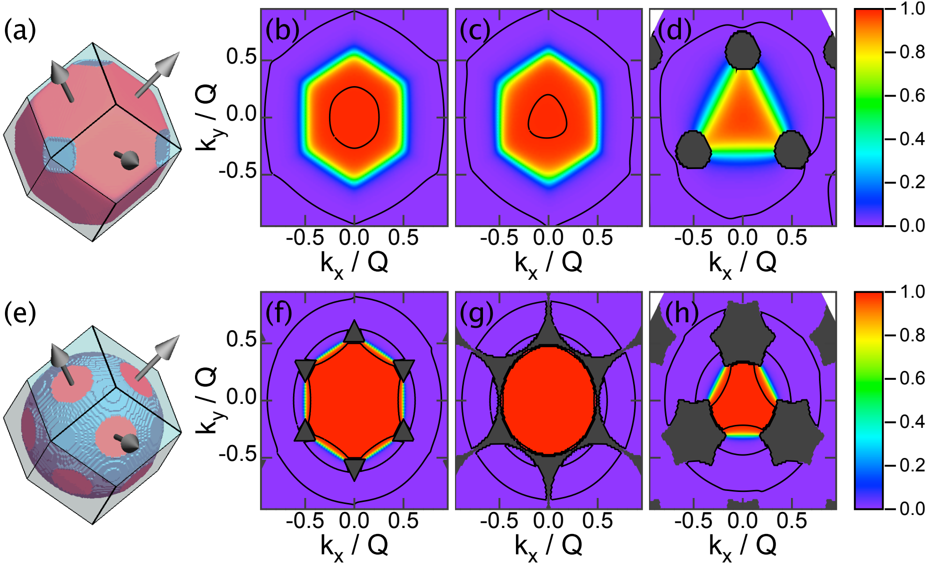


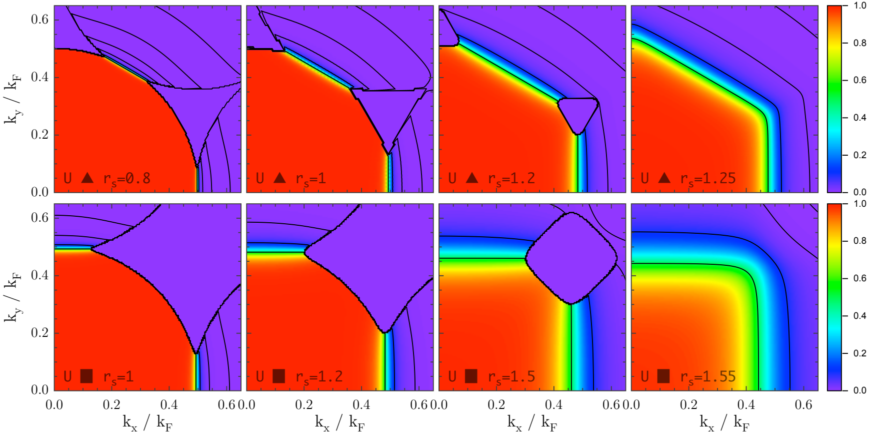
Conclusions

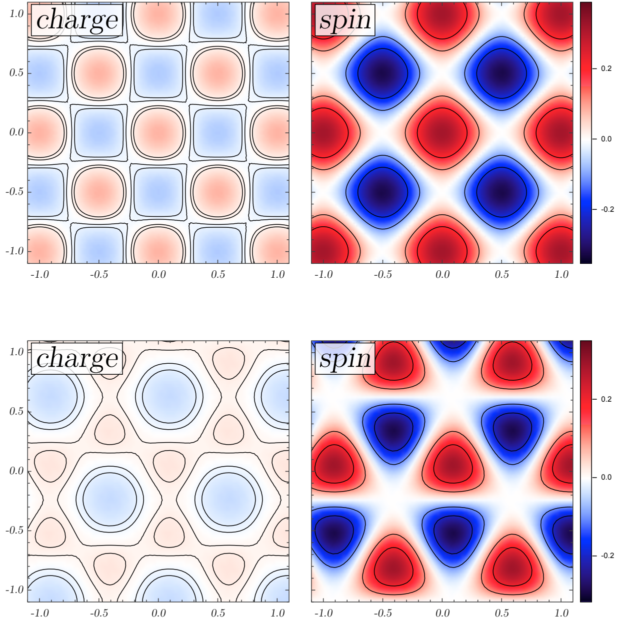
- Transition from the Wigner crystal (large r_s) to the Fermi gas via incommensurate states

- At the thermodynamical limit, the Fermi gas is reached at $r_s = 0$.

- Incommensurate states : crystalline order with a larger modulation than the Wigner crystal ($Q_W < Q(r_s) < 2k_F$).
  At small r_s, these states are well described as Spin Density Waves (SDW).


(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
k_y / Q
k_x / Q
0.5
0.0
-0.5
1.0
0.8
0.6
0.4
0.2
0.0


U ▲ r_s=0.8
U ▲ r_s=1
U ▲ r_s=1.2
U ▲ r_s=1.25
U ■ r_s=1
U ■ r_s=1.2
U ■ r_s=1.5
U ■ r_s=1.55
k_y / k_F
k_x / k_F
0.0
0.2
0.4
0.6
1.0
0.8


charge
spin
charge
spin
1.0
0.5
0.0
-0.5
-1.0
-1.0
-0.5
0.0
0.5
1.0
0.2
0.0
-0.2