A quantum approach towards a dynamical simulation of the neutron-star crust

Adding Quantum to the Pasta

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Particle and Nuclear Astrophysics, Erice - Sicily
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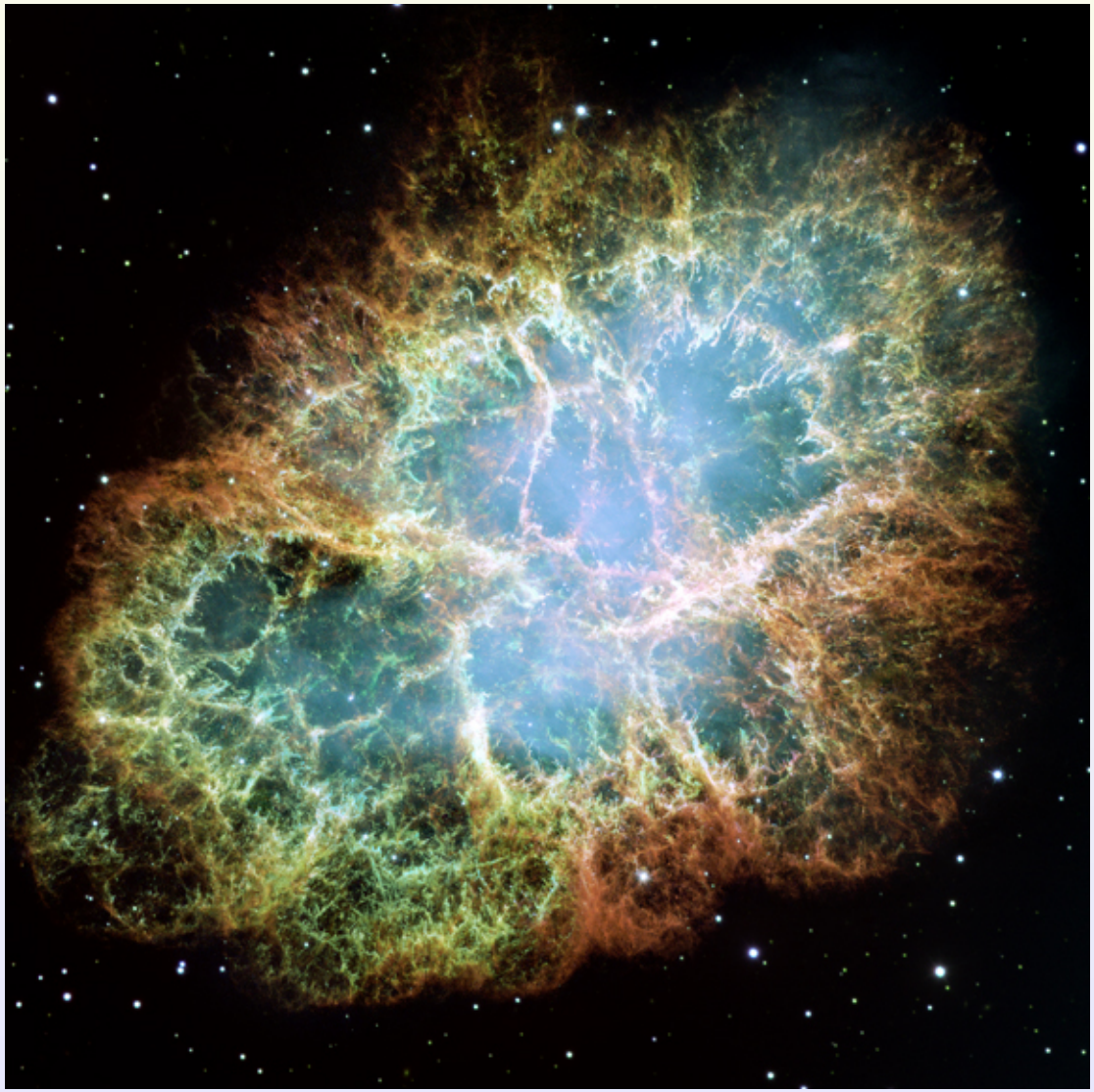
Outline

Introduction: preface

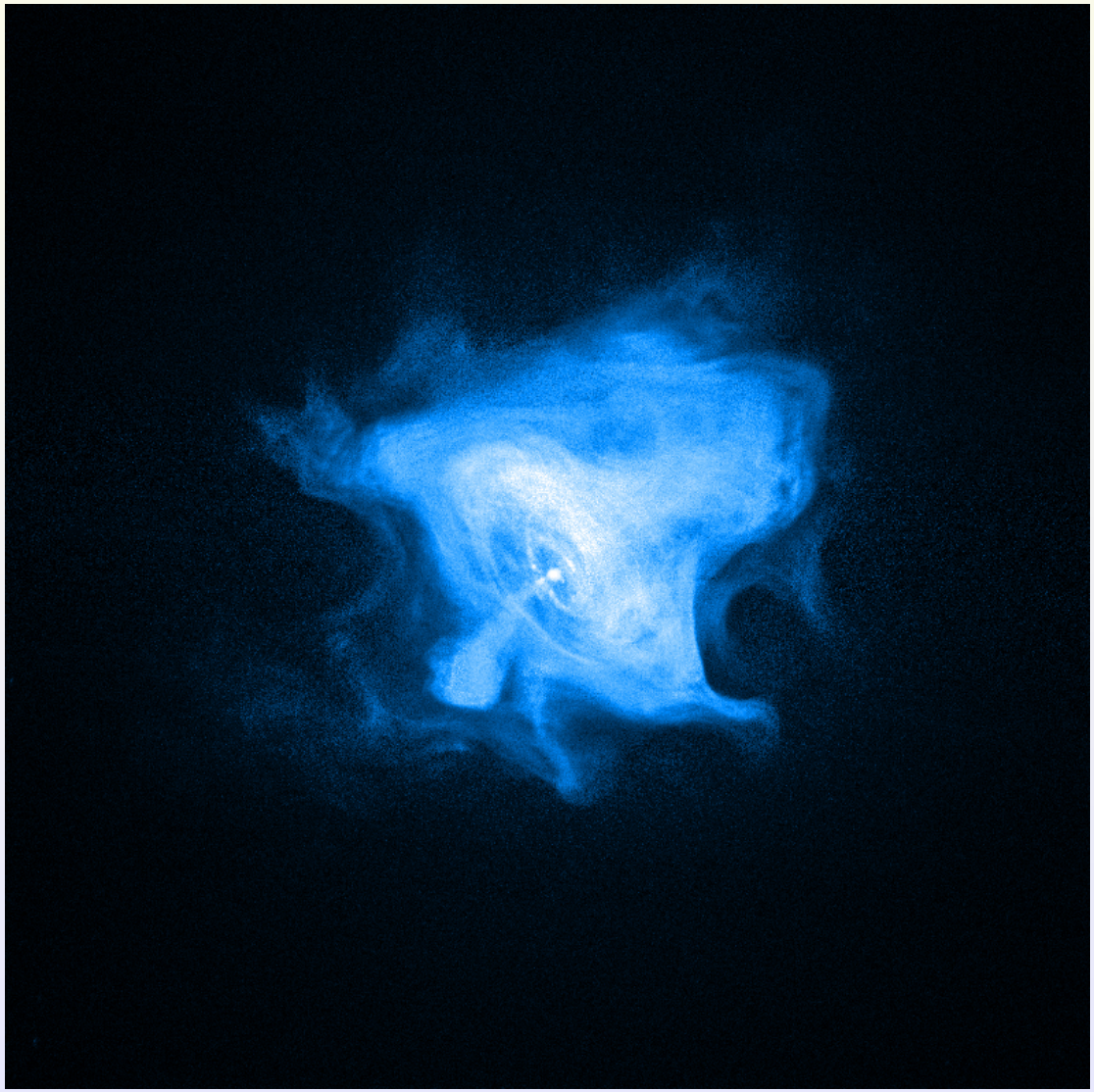
Eta Carinae and the bipolar Homunculus Nebula which surrounds the star.

Introduction: preface



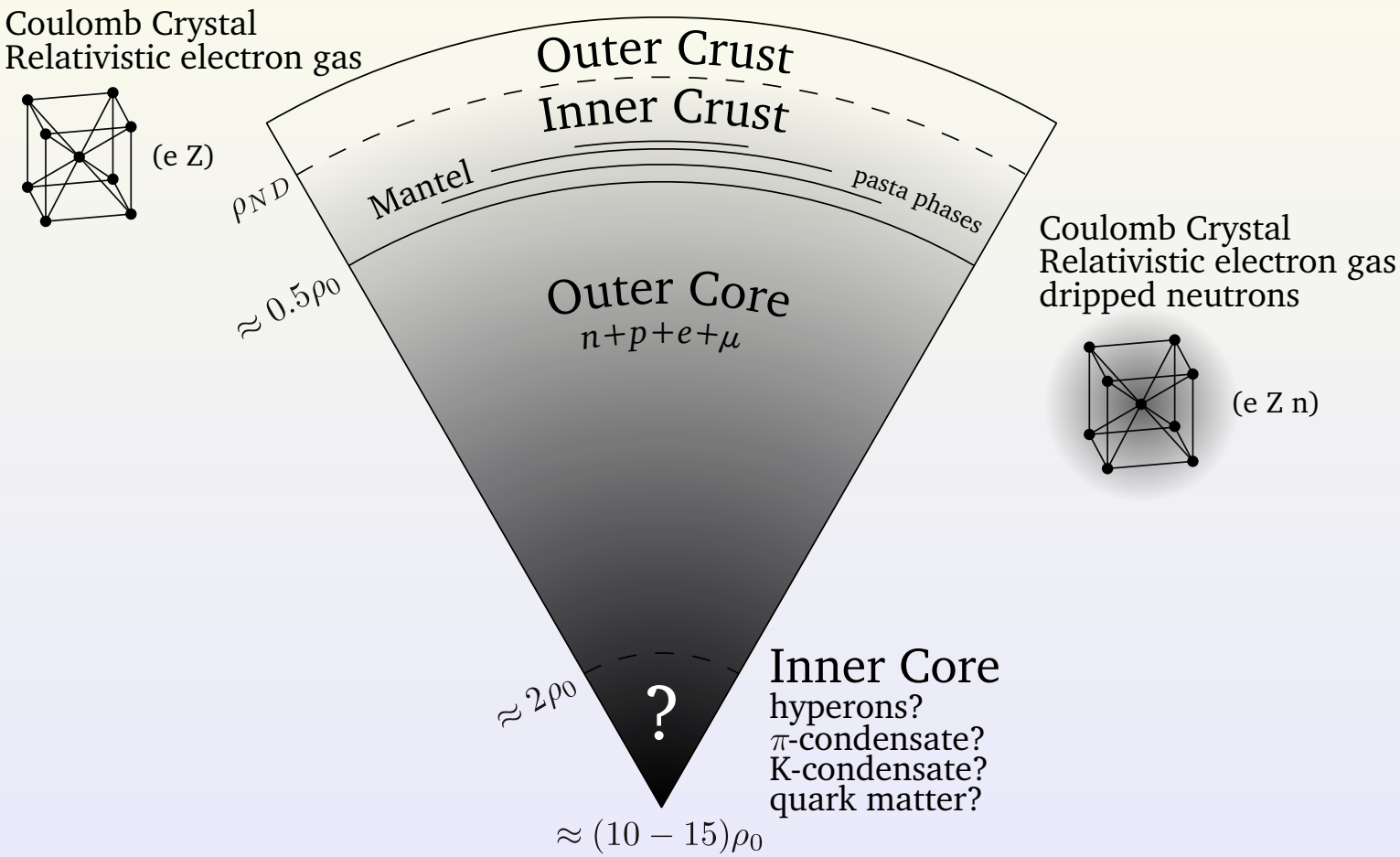
Crab nebulae

Introduction: preface

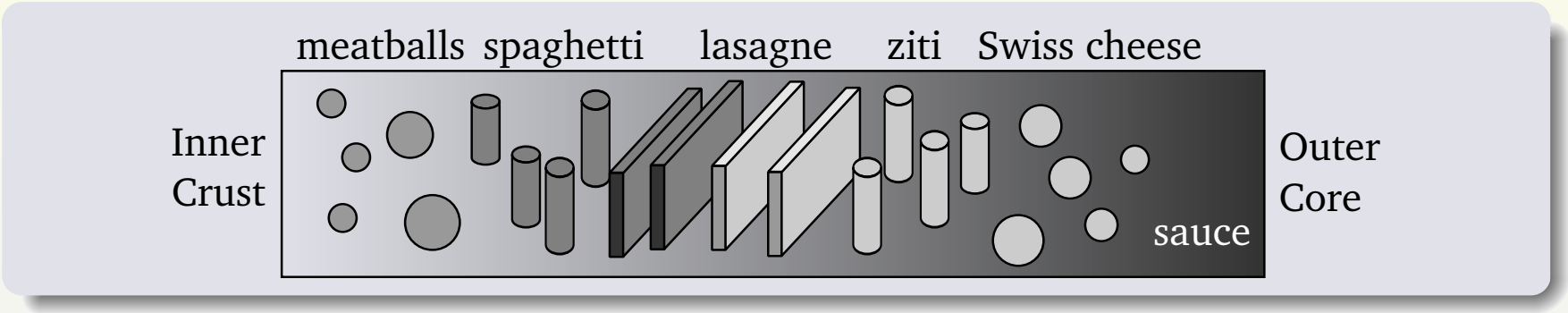


Crab pulsar

Introduction: composition of a neutron star



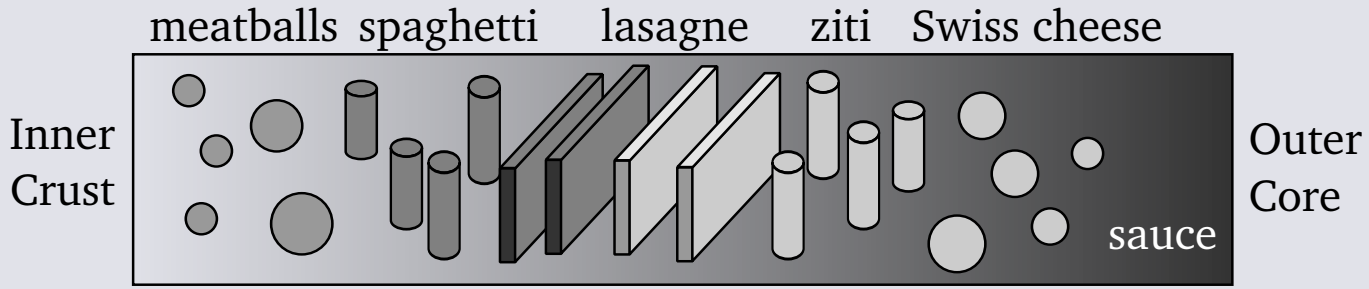
Introduction: crustal matter and nuclear pastas



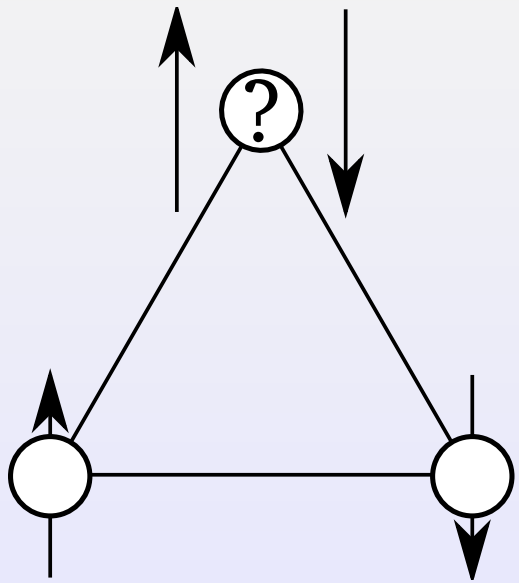
Starting from the inner crust, with increasing density

- three-dimensional spherical nuclear clusters (meatballs)
- two-dimensional cylindrical tubes of dense matter (spaghetti)
- one-dimensional slabs interlaid with planar voids (lasagne)
- two-dimensional cylindrical neutron liquids within the nuclear matter (ziti)
- three-dimensional spherical neutron-liquid-bubbles embedded in the nuclear matter (Swiss cheese)
- transition to the neutron star core, uniform neutron matter (sauce)

Introduction: crustal matter and nuclear pastas



The matter is frustrated. The system finds itself in a dynamical competition between the short-range nuclear attraction and the long-ranged Coulomb repulsion, making it, for the system, impossible to minimise all its elementary interactions. This results in a multitude of competing quasi-ground states from which the system has to choose and leads to complex-shaped nuclei.



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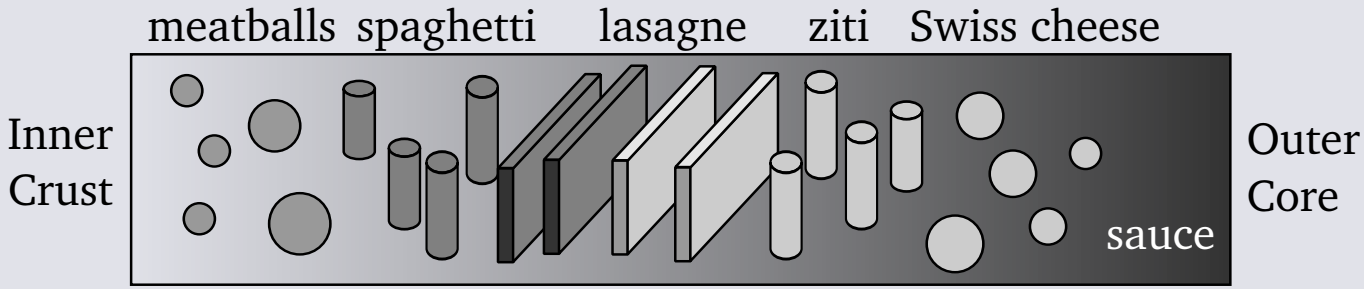
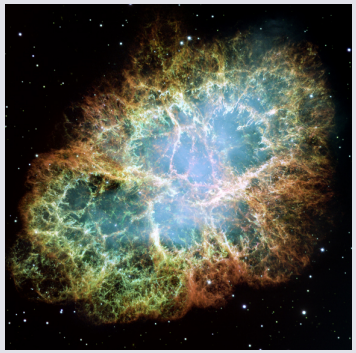


Where does the crust play a role?

- Supernova physics



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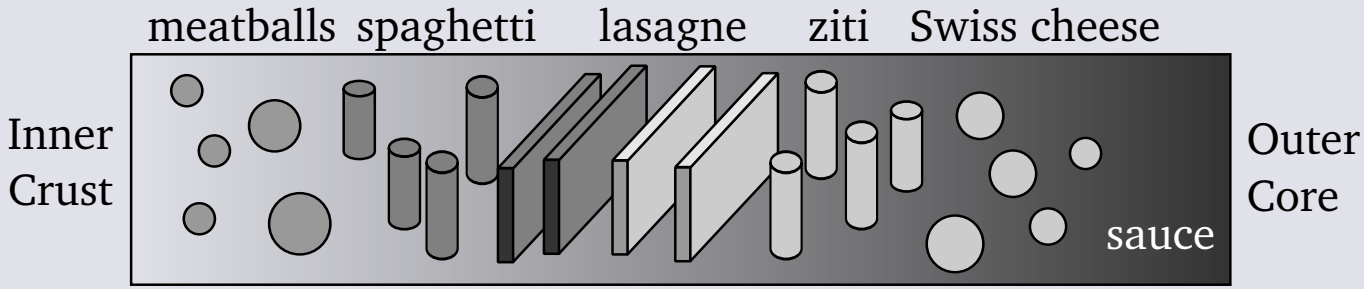
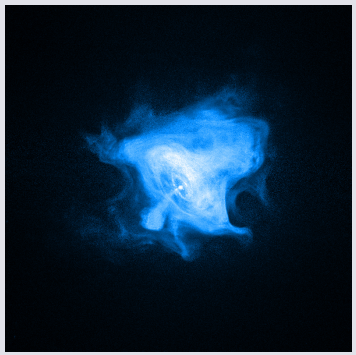


Where does the crust play a role?

- Supernova physics
- Neutron star cooling



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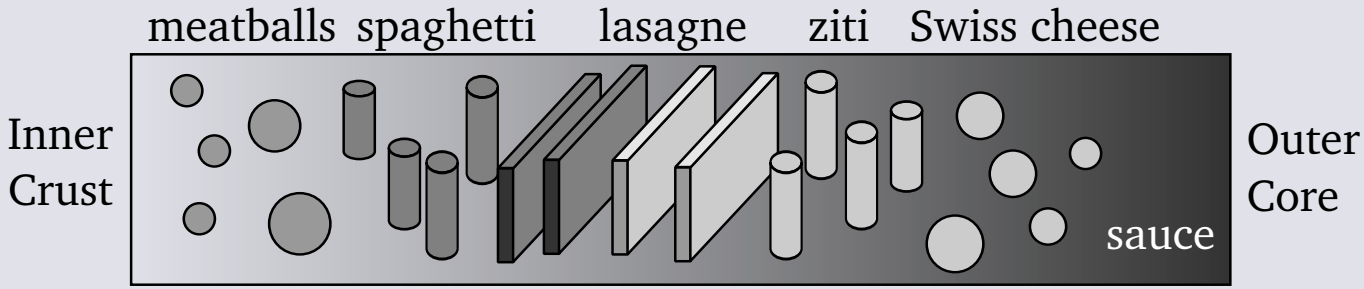
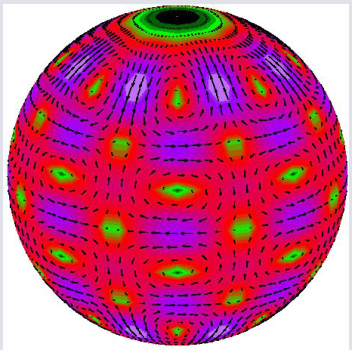


Where does the crust play a role?

- Supernova physics
- Neutron star cooling
- The r-process
- Neutron star glitches



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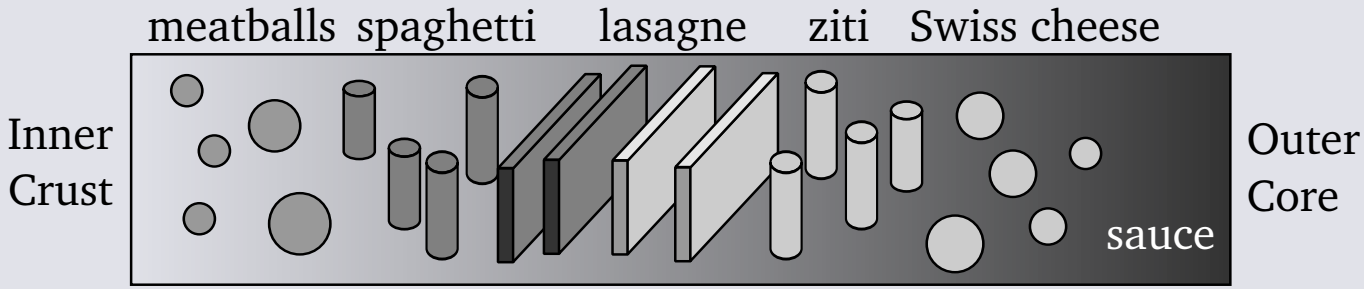
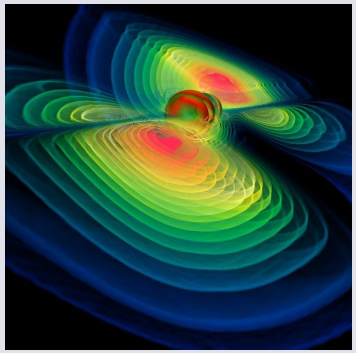


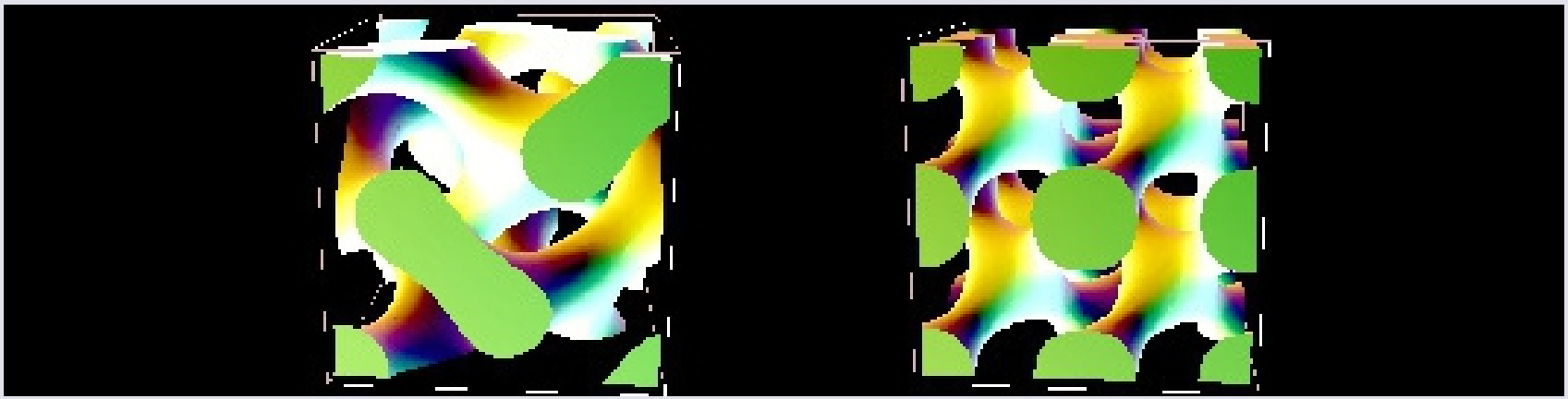
Where does the crust play a role?

- Supernova physics
- Neutron star cooling
- The r-process
- Neutron star glitches
- Gravitational waves



pasta recipe: pasta alla liquid drop

The liquid-drop model

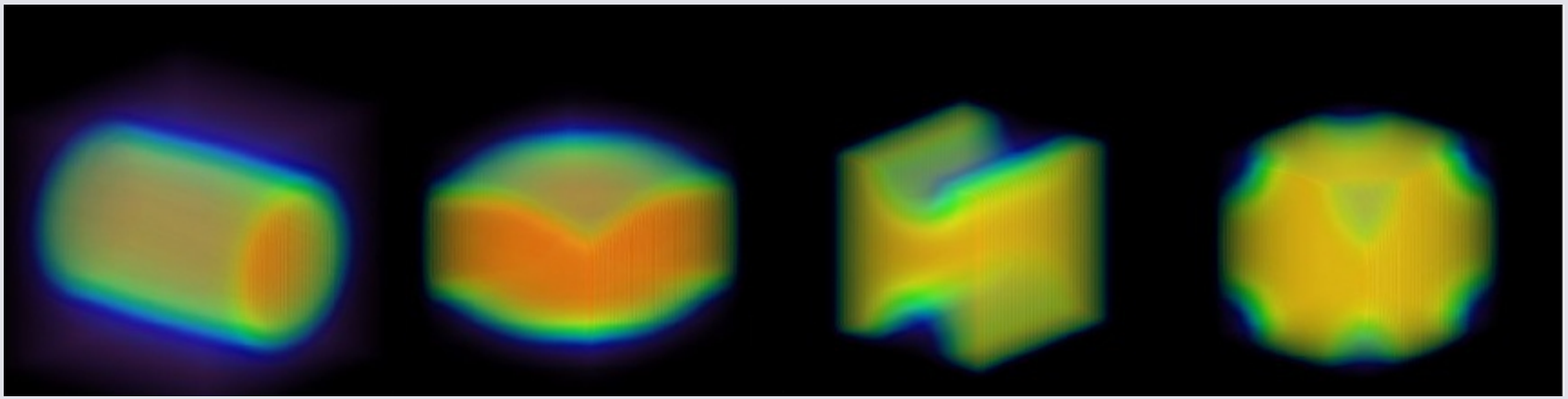


K. Nakazato et al., *Phys. Rev. Lett.* **103**, 132501 (2009)

- Semi-empirical model
- mainly studies the canonical pasta phases
- does not allow dynamics
- the hardcoded geometry is studied
- computationally fairly simple

pasta recipe: pasta in scatola alla Hartree-Fock

The Hartree-Fock model

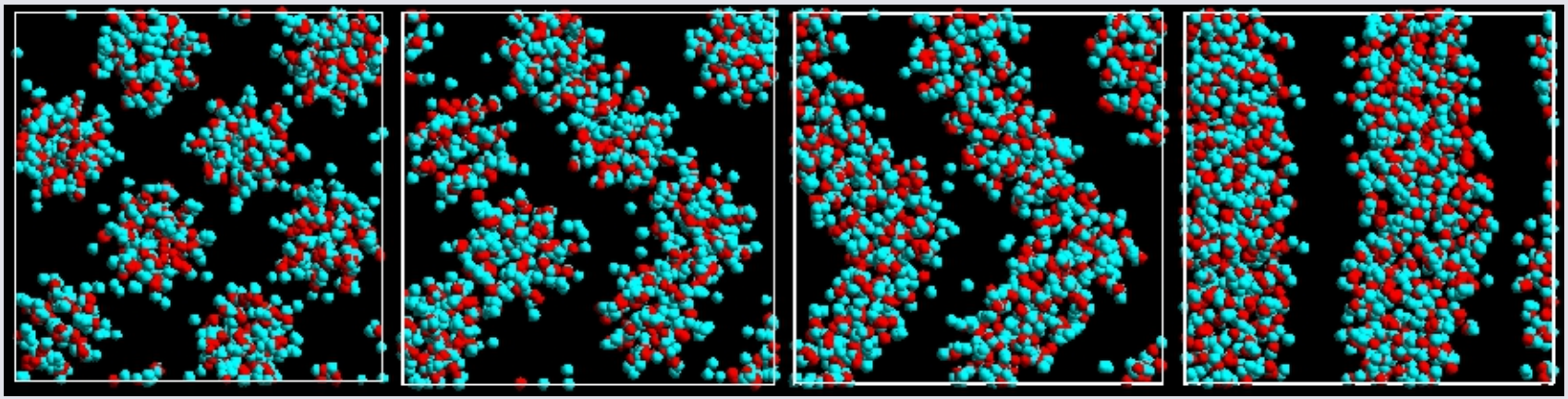


W.G. Newton et al., *Phys. Rev. C* **79**, 055801 (2009)

- mean-field model
- studies the canonical pasta phases
- does not allow dynamics
- the studied geometry strongly depends on the box-geometry
- computationally very intensive (large configuration space)

pasta recipe: pasta classica con dinamica molecolare

The molecular-dynamics technique



G. Watanabe et al., *Phys. Rev. Lett.* **103**, 121101 (2009)

- a quantum-dressed classical many-body technique
- studies the canonical and intermediate pasta phases
- allows dynamics
- the studied geometry is independent of the box-geometry
- computationally intensive

Why molecular dynamics?

- The study of time-dependent effects
- Matter out-of-equilibrium
- Unbiased with regard to the geometry of the nuclear clusters
- Thermodynamical properties through ergodic principle
- Phase transitions of matter
- ...

Pro

- N^2 process
- complete set of mathematical tools are available

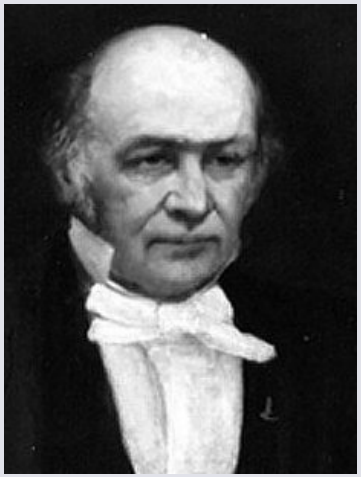
Contra

- lacks quantum features
- mimics fermion behaviour by a Pauli potential

How can we include those quantum properties?

Fermionic molecular dynamics: the equations of motion

W.R. Hamilton



Hamilton's least action principle:

- $S = \int \mathscr{L} dt = \int \sum_i \boldsymbol{P}_i \cdot \dot{\mathbf{Q}}_i - H dt$
- point particles

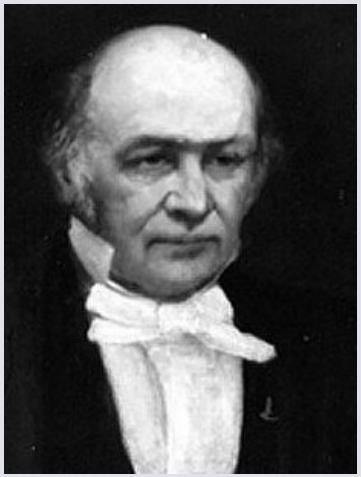
E. Schrödinger

The time-dependent variational principle:

- $S = \int \mathscr{L} dt = \int \left\langle \Psi \left| i\frac{\partial}{\partial t} - \mathcal{H} \right| \Psi \right\rangle dt$
- parametrised trial state:
  $|\Psi(t)\rangle = f(t)|\Phi(\boldsymbol{z}(t))\rangle$

Fermionic molecular dynamics: the equations of motion

W.R. Hamilton



Hamilton's least action principle:

$$\dot{\mathbf{Q}}_i = \frac{\partial H}{\partial \boldsymbol{P}_i}$$

$$\dot{\boldsymbol{P}}_i = -\frac{\partial H}{\partial \mathbf{Q}_i}$$

The time-dependent variational principle:

$$i\mathbf{C}\cdot\dot{\boldsymbol{z}} = \frac{\partial \mathscr{H}}{\partial \boldsymbol{z}^\star}$$

$$\mathbf{C} = \frac{\partial^2 \ln\langle\Phi|\Phi\rangle}{\partial \boldsymbol{z}^\star \partial \boldsymbol{z}}$$

E. Schrödinger

Fermionic molecular dynamics: the wave function

J. C. F. Gauß

The fermion wave function, a quantum-dressed Gaussian wave packet

$$|q_p\rangle = \sum_k c_{kp} |\mathbf{A}_{kp} \boldsymbol{b}_{kp}\rangle \otimes |\chi_{kp}\rangle \otimes |\zeta_{kp}\rangle,$$

$$\langle \boldsymbol{x} | \mathbf{A} \boldsymbol{b} \rangle = \exp\left\{ -\frac{1}{2} (\boldsymbol{x} - \boldsymbol{b}) \cdot \mathbf{A}^{-1} \cdot (\boldsymbol{x} - \boldsymbol{b}) \right\}$$

An antisymmetric A-body system is a Slater determinant of fermion wave functions.

$$\langle x_1, \ldots, x_A | \Phi \rangle = \frac{1}{\sqrt{A!}} \det \begin{pmatrix} \langle x_1 | q_1 \rangle & \cdots & \langle x_1 | q_A \rangle \\ \vdots & \ddots & \vdots \\ \langle x_A | q_1 \rangle & \cdots & \langle x_A | q_A \rangle \end{pmatrix}$$

J. C. Slater

Fermionic molecular dynamics: the expectation values

- One-body operator

$$\mathscr{B}_I = \frac{\langle Q|\mathcal{B}_I|Q\rangle}{\langle Q|Q\rangle} = \sum_{pq=1}^{A} \langle q_p|\mathcal{B}_I|q_q\rangle \mathbf{o}_{qp}$$

- Two-body operator

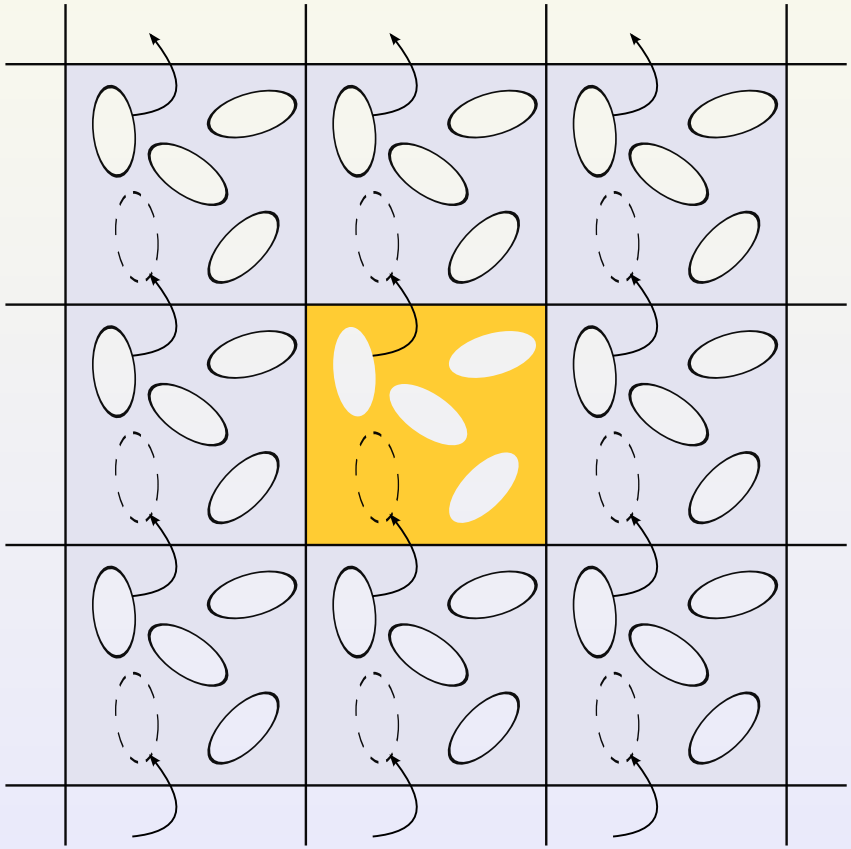
$$\mathscr{B}_{II} = \frac{\langle Q|\mathcal{B}_{II}|Q\rangle}{\langle Q|Q\rangle} = \frac{1}{2}\sum_{pqrs=1}^{A} \langle q_p q_r|\mathcal{B}_{II}|q_q q_s\rangle(\mathbf{o}_{qp}\mathbf{o}_{sr} - \mathbf{o}_{qr}\mathbf{o}_{sp})$$

- The metric $\mathbf{C}$

$$\mathbf{C}_{ab} = \left(\frac{\partial^2 \mathbf{n}_{ab}}{\partial \boldsymbol{z}^\star_a \partial \boldsymbol{z}_b} - \sum_{pq=1}^{A} \frac{\partial \mathbf{n}_{ap}}{\partial \boldsymbol{z}^\star_a} \cdot \mathbf{o}_{pq} \cdot \frac{\partial \mathbf{n}_{qb}}{\partial \boldsymbol{z}_b}\right) \cdot \mathbf{o}_{ba}$$

FMD has matrix formalism with $\mathbf{n}_{pq} = \langle q_p|q_q\rangle$ and $\mathbf{o} = \mathbf{n}^{-1}$ containing all relevant fermion physics

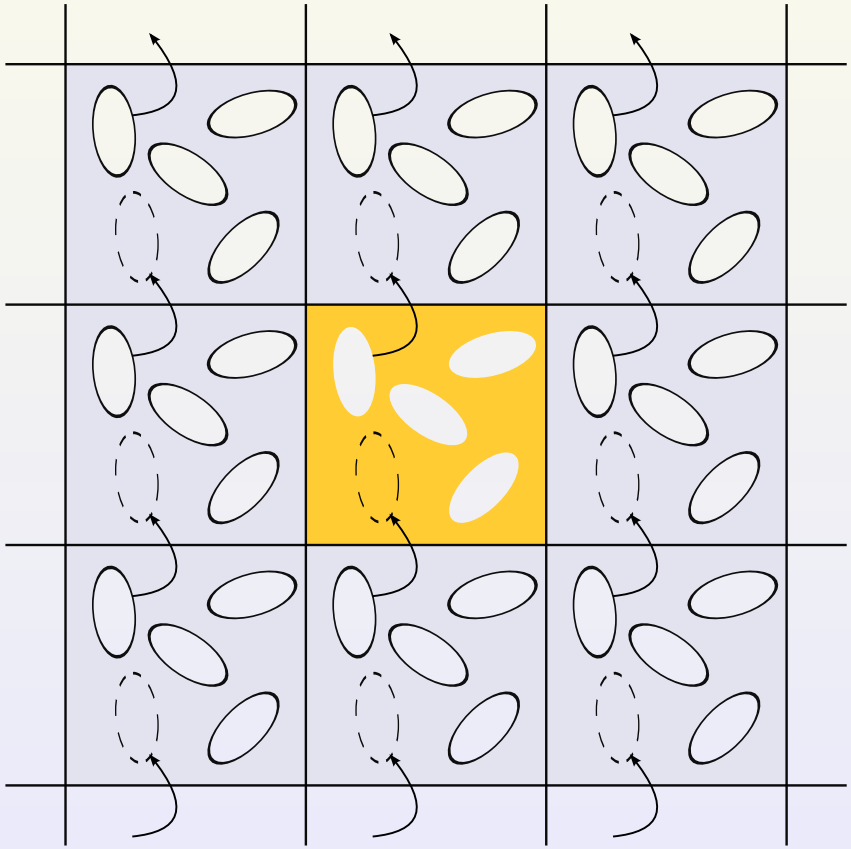
Fermionic molecular dynamics: bulk systems



Periodic boundary conditions

- One unit cell contains N single particle states
- The unit cell is periodically replicated in all directions

Fermionic molecular dynamics: bulk systems



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What about FMD with PBC?

- Fermions require antisymmetrisation

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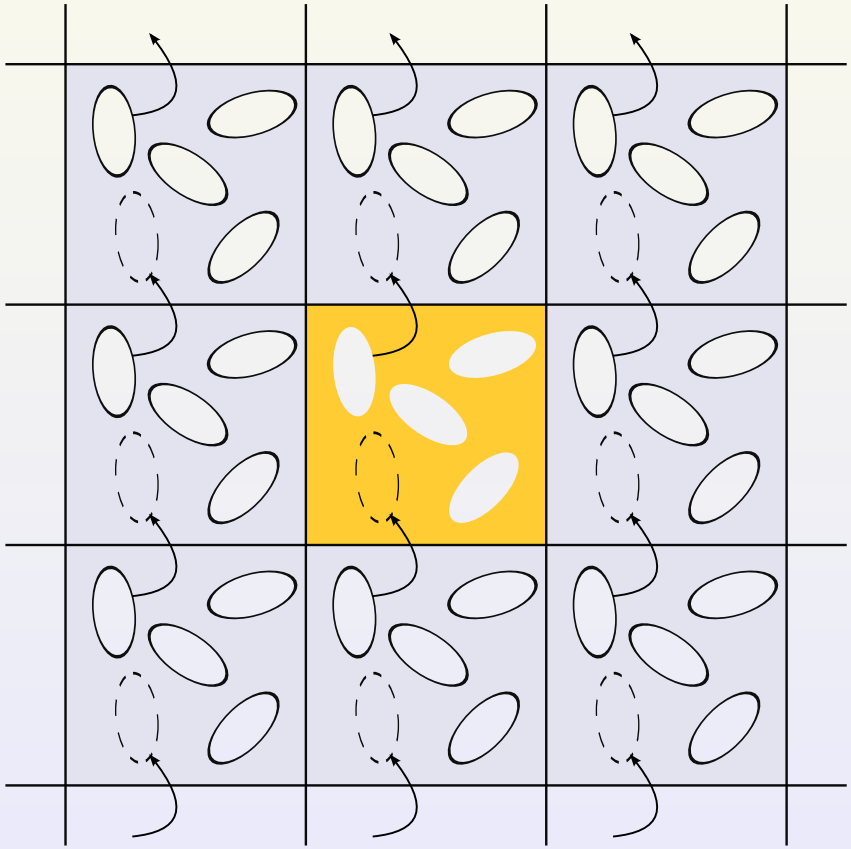

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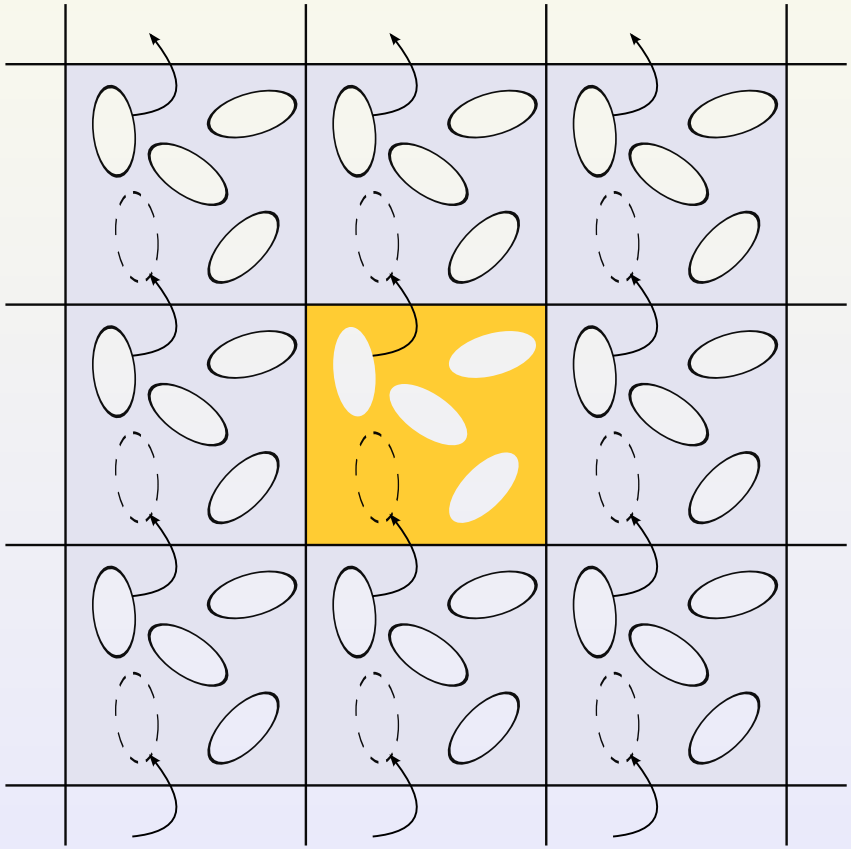

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- FMD must be applied to the infinite periodic system

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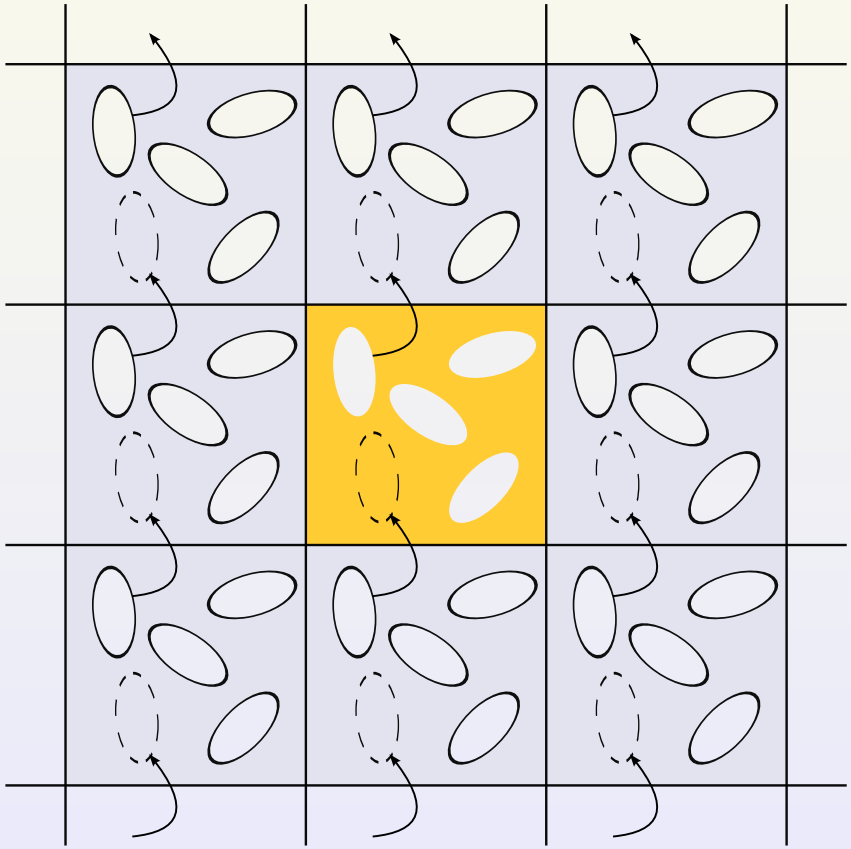

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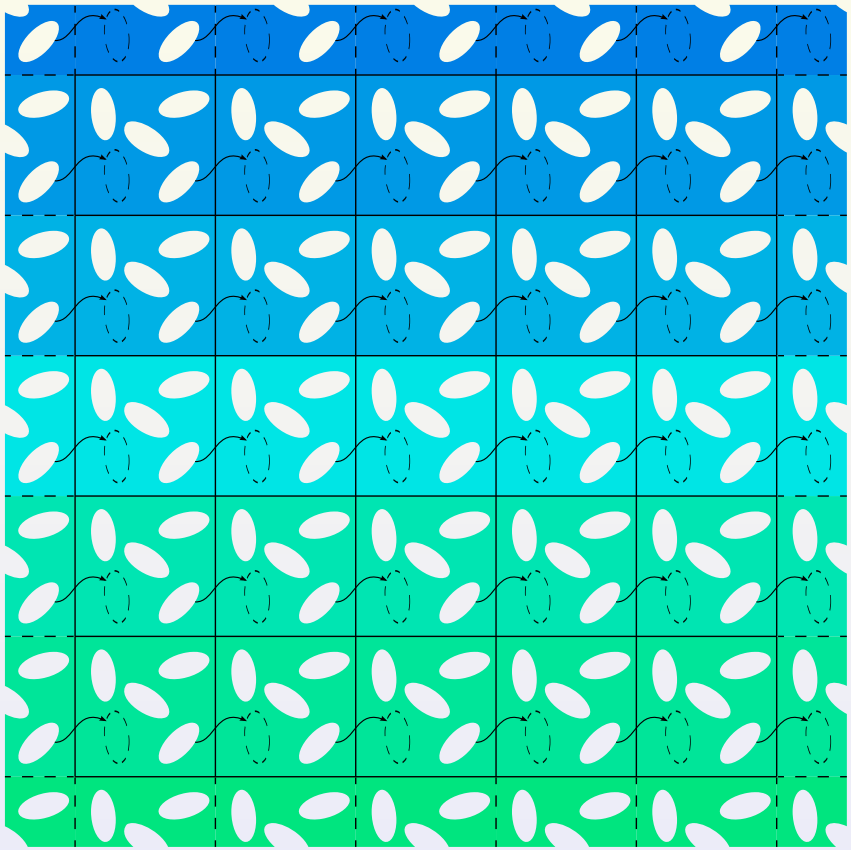
infinite matrices? HOW??

Fermionic molecular dynamics: the bulk overlap matrix



$$\mathbf{N} = \begin{pmatrix} \ddots & \vdots & \ddots \\ \cdots & & \cdots \\ \ddots & \vdots & \ddots \end{pmatrix}$$

$$\blacksquare = \begin{pmatrix} \ddots & \vdots & \ddots \\ \cdots & & \cdots \\ \ddots & \vdots & \ddots \end{pmatrix}$$

$$\blacksquare = \mathbf{n}_{\boldsymbol{P}-\boldsymbol{Q},pq} = \langle q_p | \mathcal{T}(\boldsymbol{Q}-\boldsymbol{P}) | q_q \rangle$$

The overlap matrix has a nested block Toeplitz structure which is analytically invertible!

Fermionic molecular dynamics: bulk expectation values

After some exciting math, one finds

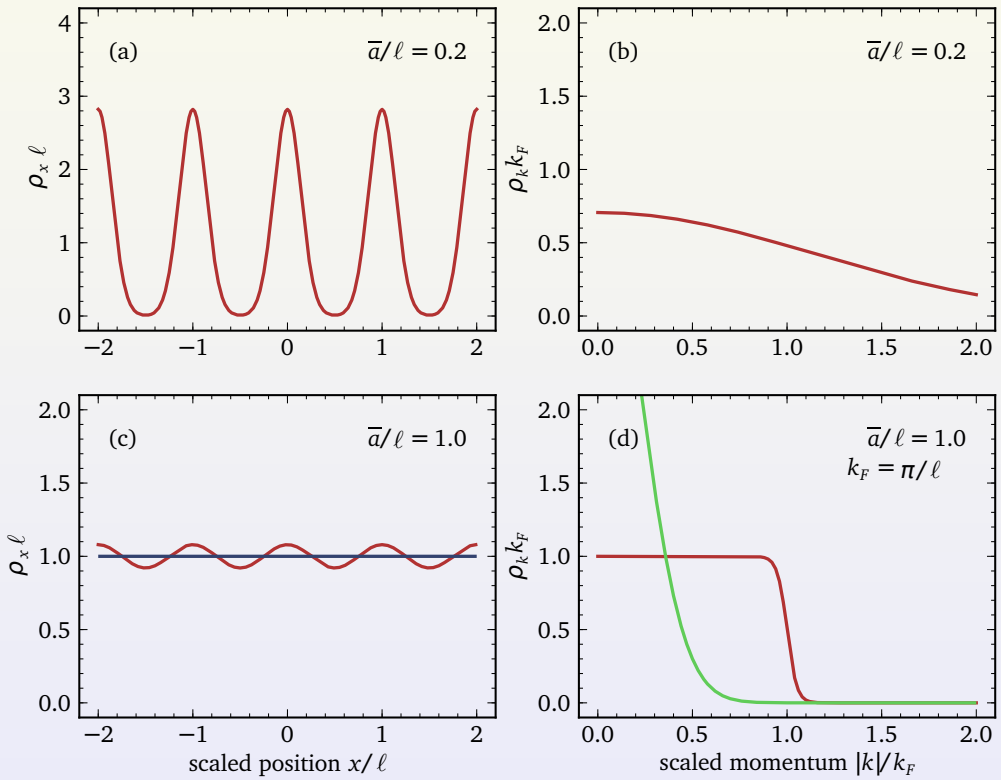
$$\mathscr{B}_{\rho,I} = \frac{1}{V_{BZ}} \int_{BZ} \sum_{pq=1}^{A} \mathscr{B}_{I,pq}(\boldsymbol{k}) \mathscr{O}_{qp}(\boldsymbol{k}) d\boldsymbol{k},$$

$$\mathscr{B}_{\rho,II} = \frac{1}{2V_{BZ}^2} \iint_{BZ \otimes BZ} \sum_{\boldsymbol{R} \in \mathfrak{B}} \sum_{pqrs=1}^{A} \mathscr{B}_{II,\boldsymbol{R},pqrs}(\boldsymbol{k}_1, \boldsymbol{k}_2) \times \left[\mathscr{O}_{qp}(\boldsymbol{k}_1) \mathscr{O}_{sr}(\boldsymbol{k}_2) - \mathscr{O}_{qr}(\boldsymbol{k}_1) \mathscr{O}_{sp}(\boldsymbol{k}_2) e^{i\boldsymbol{R}\cdot(\boldsymbol{k}_2 - \boldsymbol{k}_1)} \right] d\boldsymbol{k}_1 d\boldsymbol{k}_2$$

$$\mathbf{C}_{\rho,ab} = \frac{1}{V_{BZ}} \int_{BZ} \left(\frac{\partial^2 \mathscr{N}_{ab}(\boldsymbol{k})}{\partial \boldsymbol{z}_a^\star \partial \boldsymbol{z}_b} - \sum_{pq=1}^{A} \frac{\partial \mathscr{N}_{ap}(\boldsymbol{k})}{\partial \boldsymbol{z}_a^\star} \cdot \mathscr{O}_{pq}(\boldsymbol{k}) \cdot \frac{\partial \mathscr{N}_{qb}(\boldsymbol{k})}{\partial \boldsymbol{z}_b} \right) \times \mathscr{O}_{ba}(\boldsymbol{k}) d\boldsymbol{k}$$

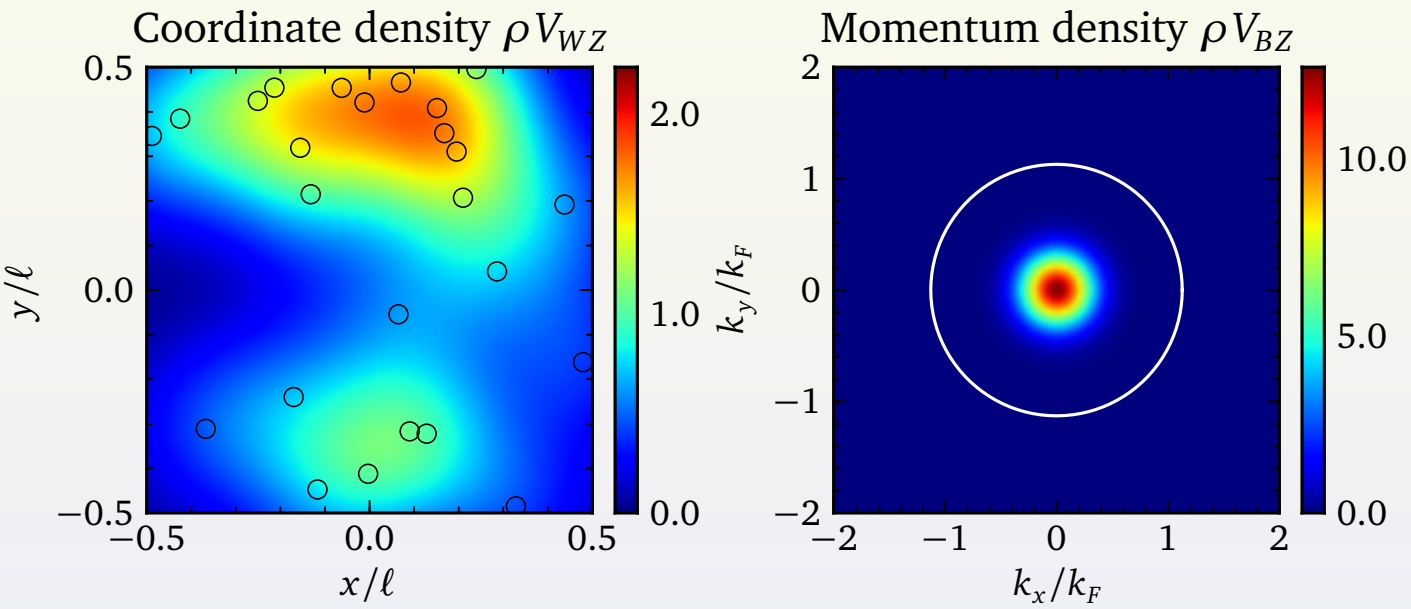
The equations of FMD and BFMD have a similar structure with finite sized matrices. The integration over the first Brillouin zone reflects the infinite structure of the system.

Results: densities of a one-dimensional fermion system



- For small overlap: the particles behave as distinguishable particles
- For large overlap: the particles reproduce free Fermi gas behaviour

Results: densities of a two-dimensional fermion system

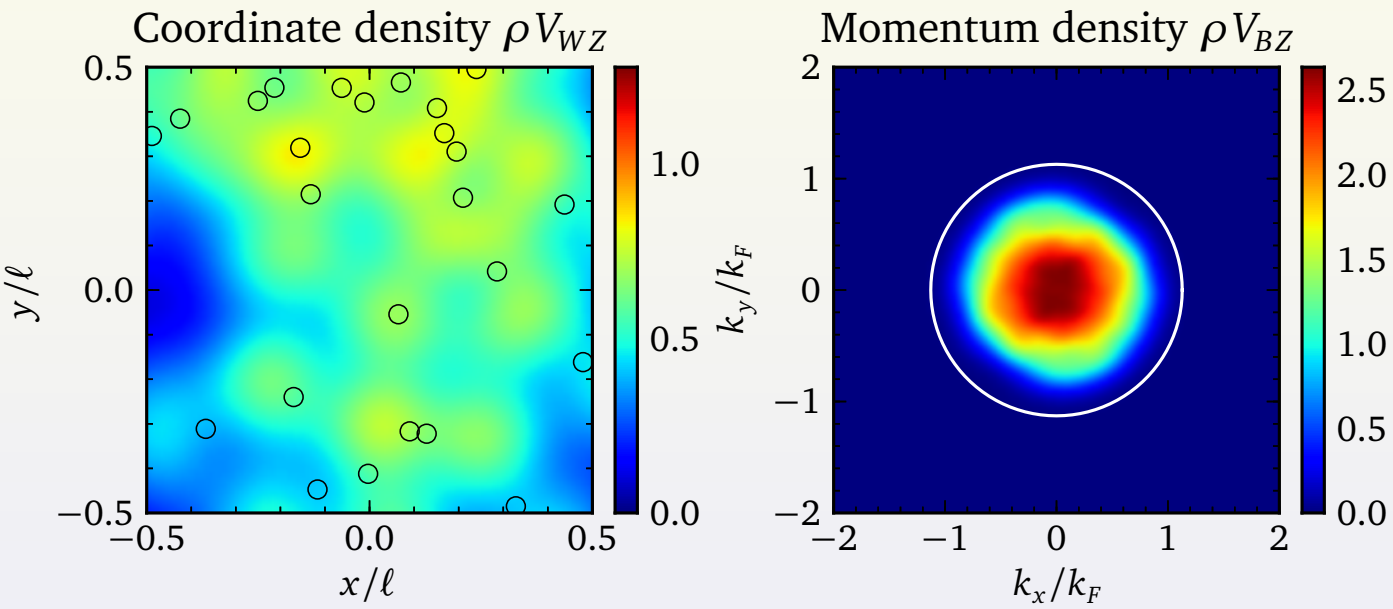


Gaussian width: $\sqrt{a} = \ell/5$

- without periodicity
- without antisymmetry

Densities in momentum and coordinate space are summed.

Results: densities of a two-dimensional fermion system



Gaussian width: $\sqrt{a} = \ell/5$

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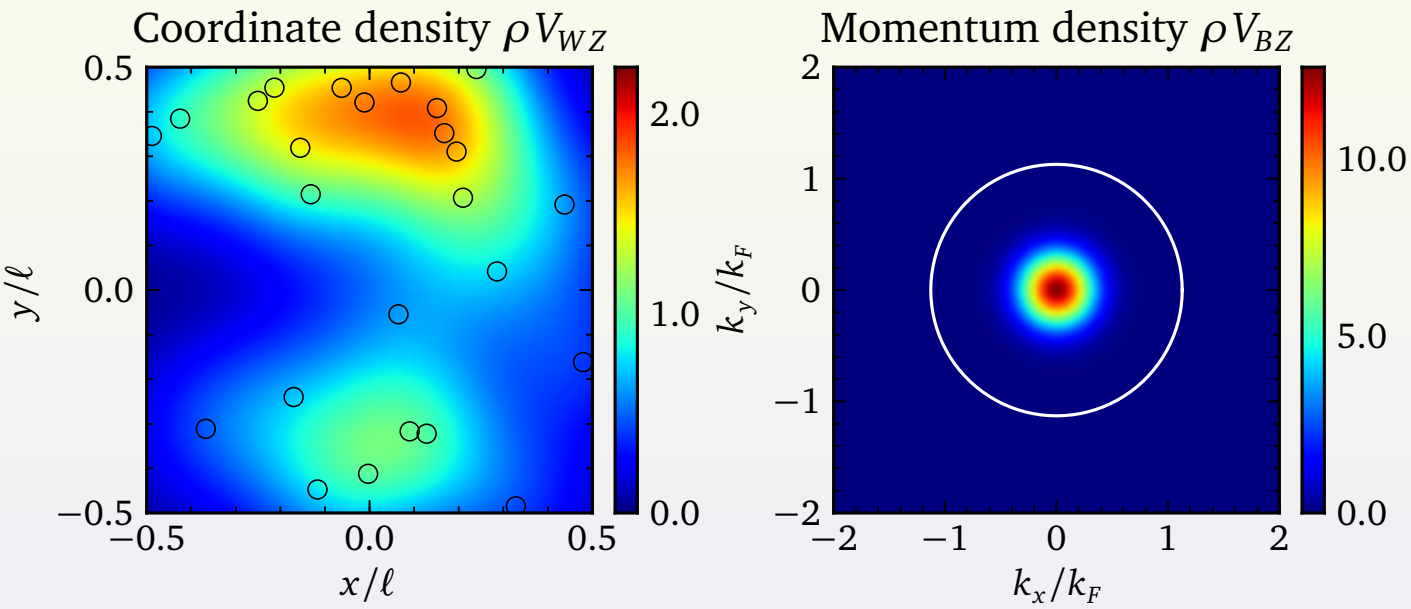
Antisymmetry enables the Pauli-exclusion principle. It seems like particles are pushed away.

Results: densities of a two-dimensional fermion system



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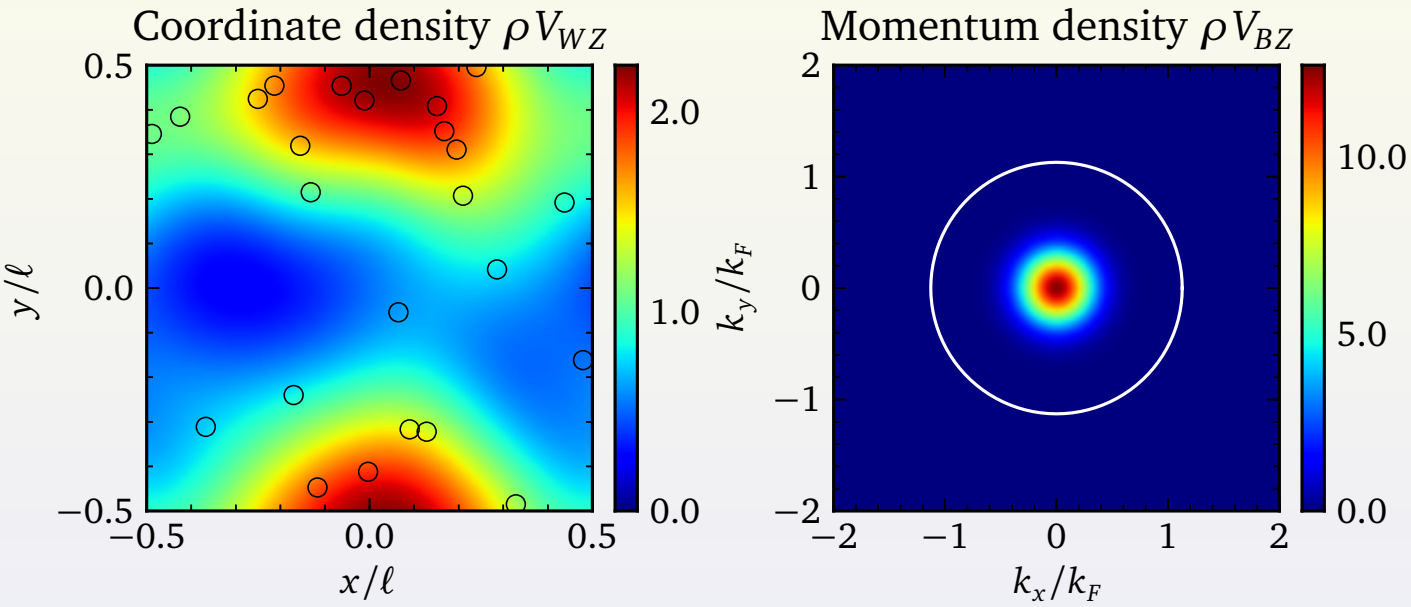

Gaussian width: $\sqrt{a} = \ell/5$

- with periodicity
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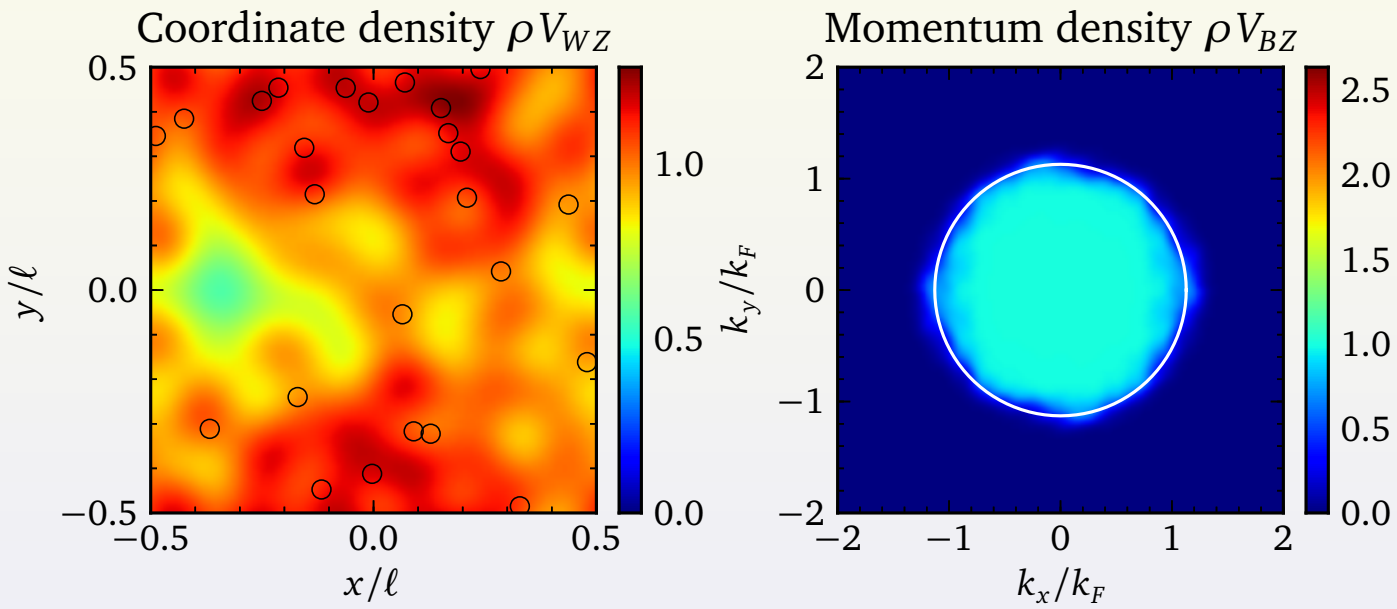
Densities in momentum and coordinate space are summed and periodic corrections added in the spatial density.

Results: densities of a two-dimensional fermion system



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Antisymmetry is a long-range many-body correlation. Both densities tend to that of a free fermion system.

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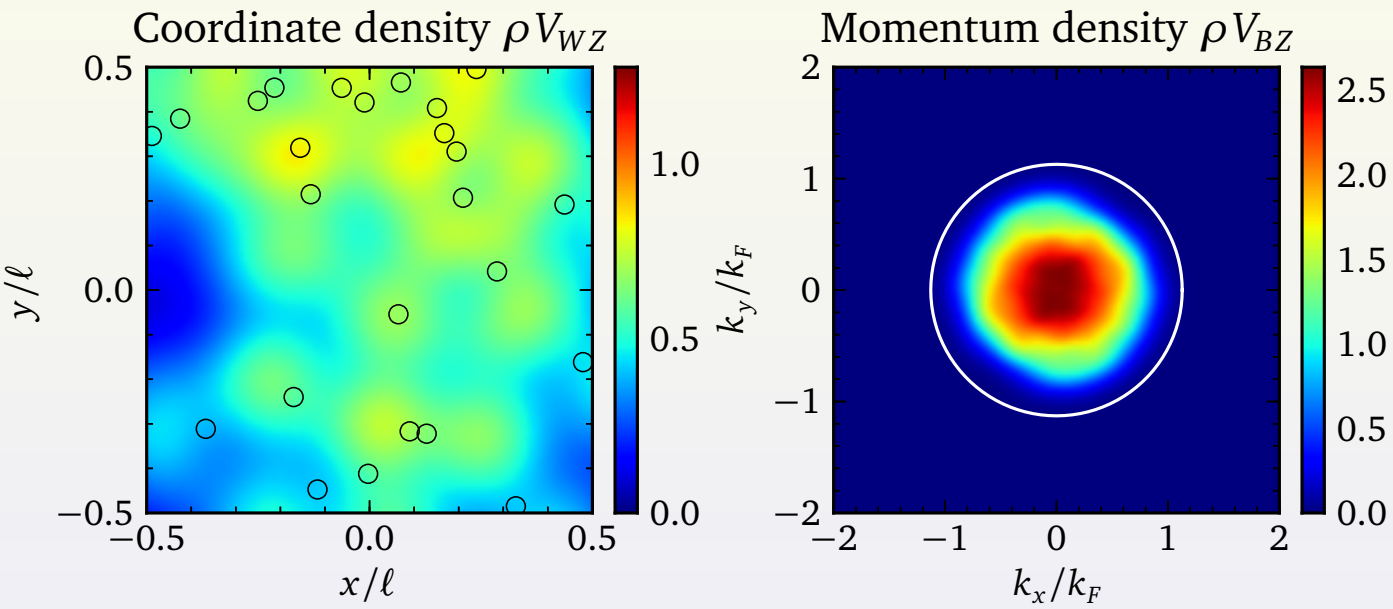

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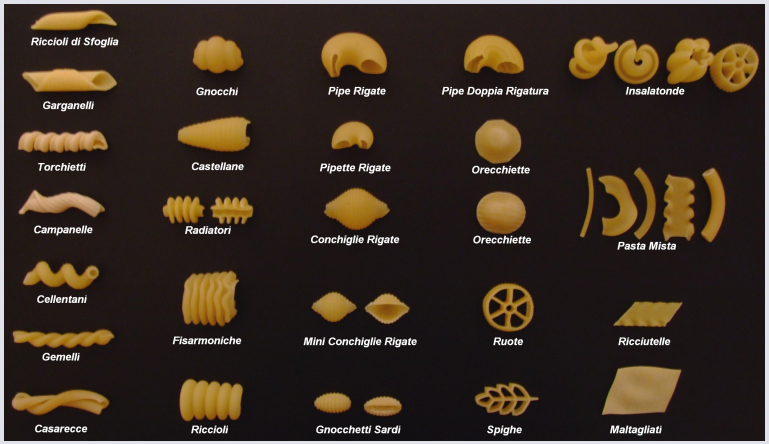
Conclusion . . .

- We introduced fermionic molecular dynamics introducing quantum concepts as uncertainty principle, spin and Pauli-exclusion principle.
- The equations allow a full antisymmetrisation by means of a matrix formalism.
- We introduced periodic boundary conditions to study bulk fermion matter.
- The equation becomes tractable and computational friendly and address fully antisymmetrised bulk matter.
- We showed that antisymmetry influences enormously the density distributions and can not be ignored.
- Fermion behaviour is accounted for.

. . . and outlook



- Boil an 8 to 20 solar-mass star in its own plasma.
- Meanwhile, drain some hydrogen from a nearby star and add a touch of helium to it. Don't take too much, or the hydrogen sauce will ignite itself!
- When the star is well done, a neutrino flash will burst out of the star. At that point, quickly peel the outer layers of the star down to the neutron core. Don't wait too long, or your dish will explode.
- Skim the crust of the neutron core, and place it on a nice uranium plate.
- Poor over the hydrogen sauce and sprinkle some freshly grated planet on.
- Serve the dish to the closest black hole.

The study of nuclear matter

- Adding realistic potentials
- ground state of crustal matter
- Structure functions through dynamics
- and more . . .

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