Nuclear pasta with a touch of quantum

Towards fully antisymmetrised dynamics for bulk fermion systems

K. Vantournhout N. Jachowicz J. Ryckebusch H. Feldmeier

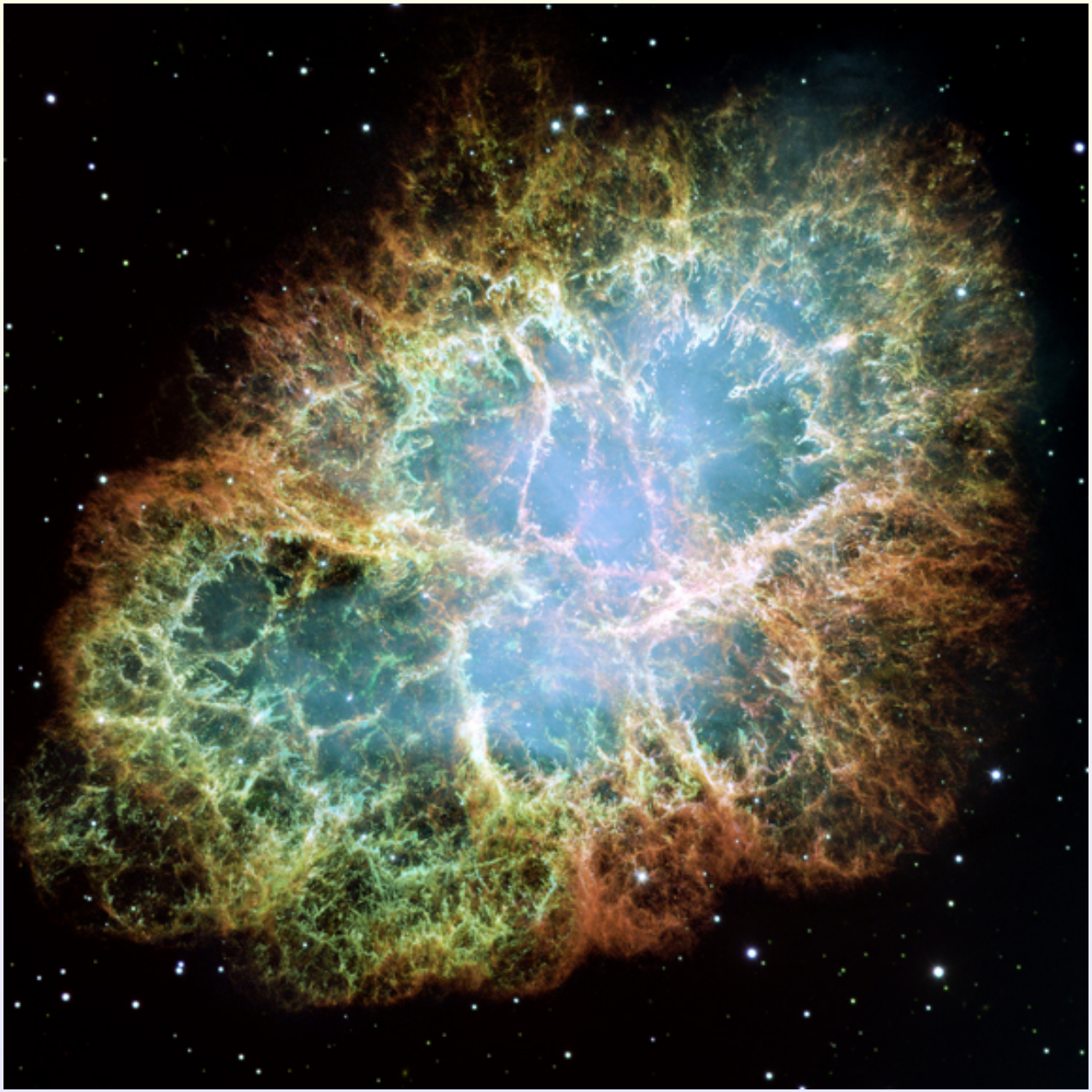
GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, Germany

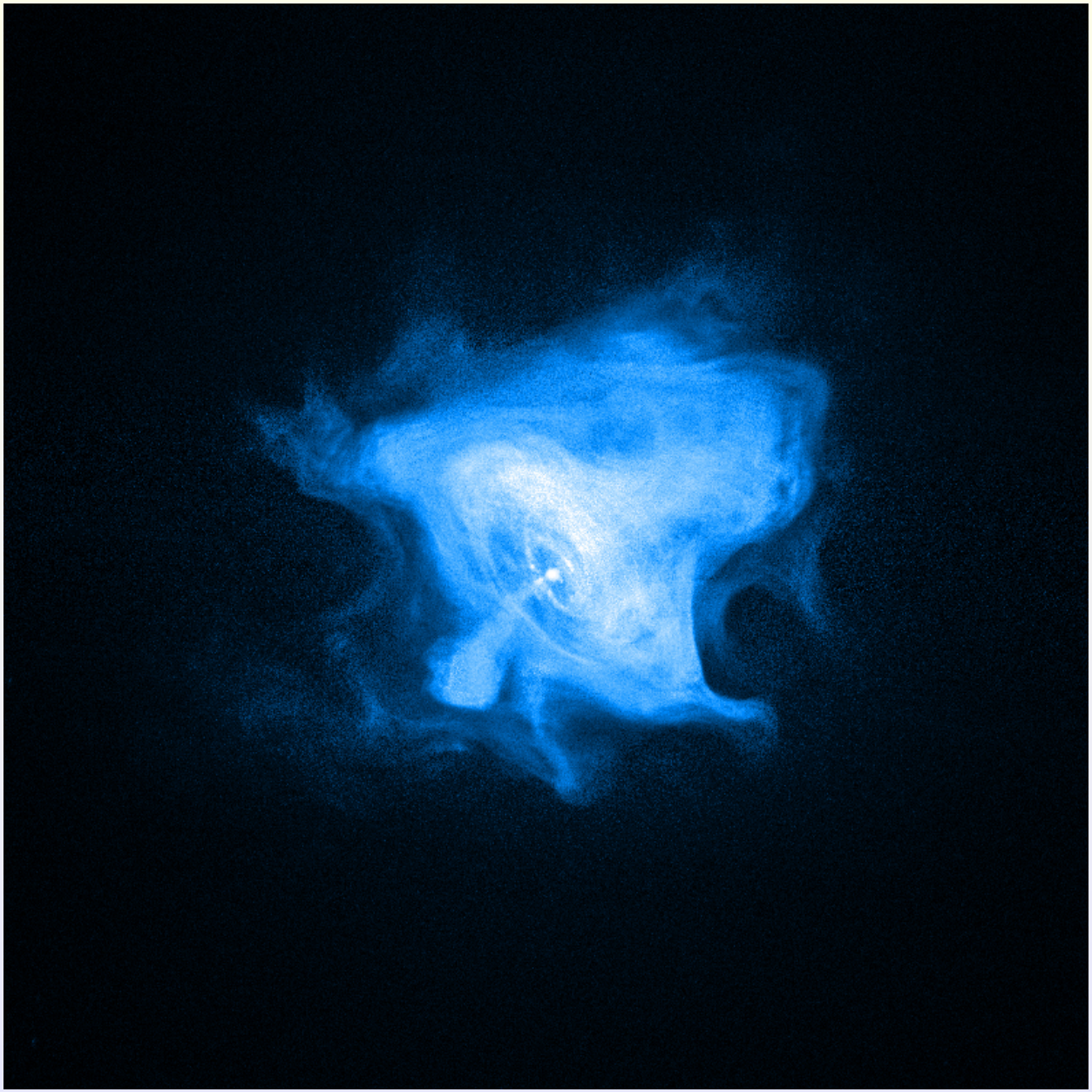
Ghent University, department of physics and Astronomy, Gent, Belgium

11th Symposium on Nuclei in the Cosmos, Heidelberg
July 19 – 23, 2010

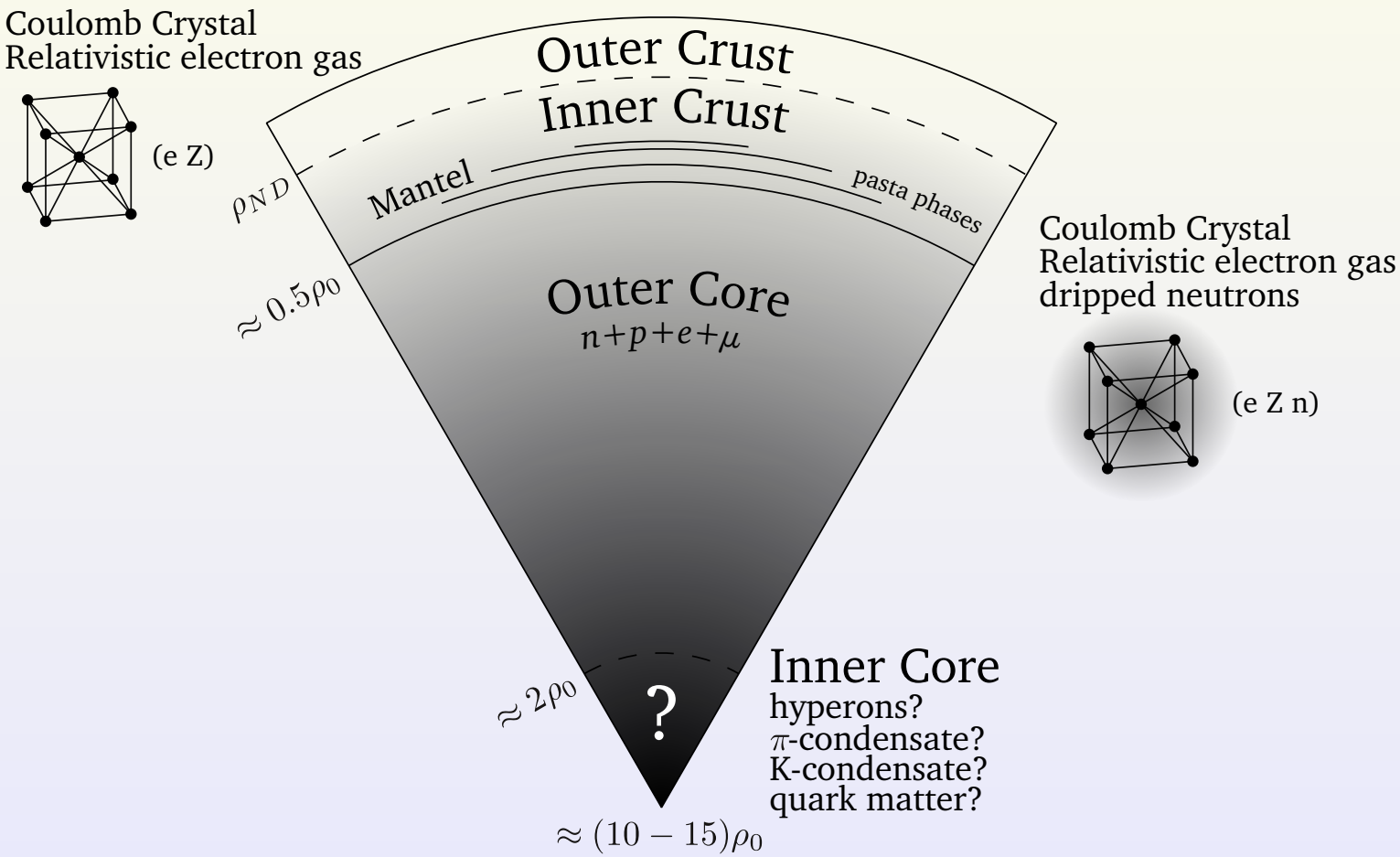
Outline

Outline

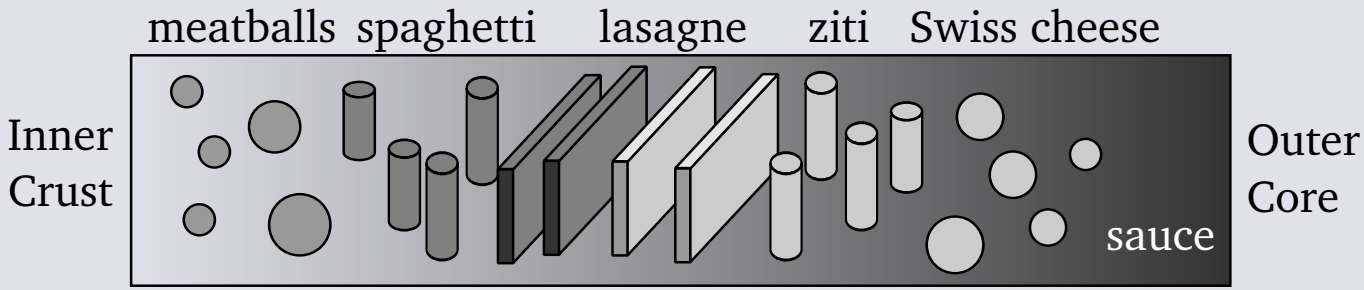




Neutron stars: composition



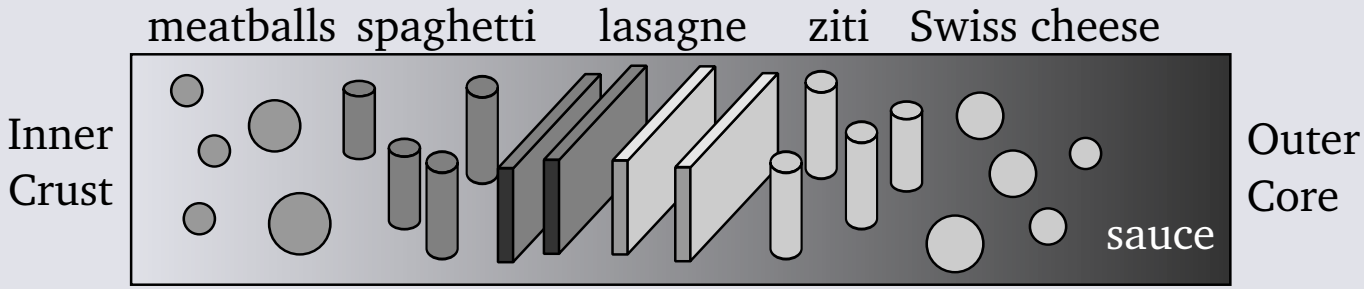
Neutron stars: crustal matter and nuclear pastas



Starting from the inner crust, with increasing density

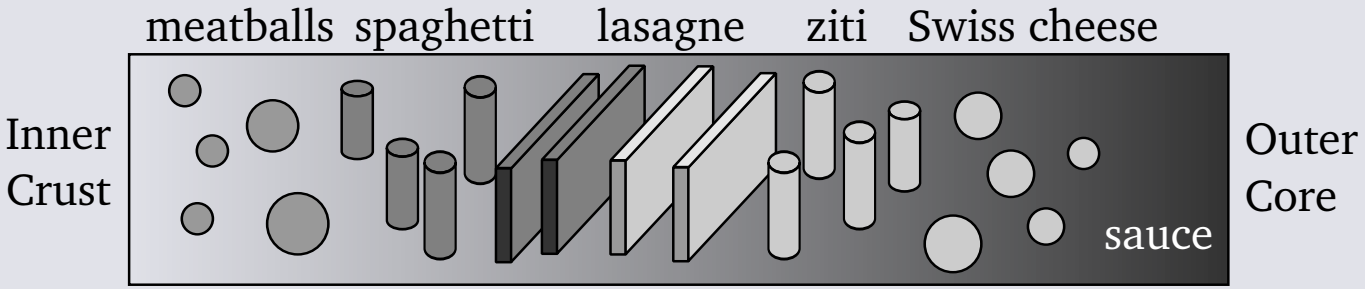
- three-dimensional spherical nuclear clusters (meatballs)
- two-dimensional cylindrical tubes of dense matter (spaghetti)
- one-dimensional slabs interlaid with planar voids (lasagne)
- two-dimensional cylindrical neutron liquids within the nuclear matter (ziti)
- three-dimensional spherical neutron-liquid-bubbles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

Neutron stars: 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.

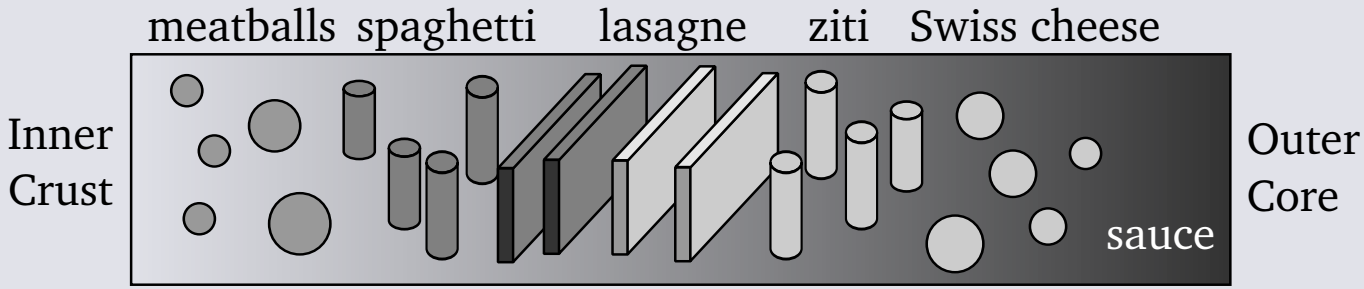
Neutron stars: crustal matter and nuclear pastas



Why is it important?

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

Neutron stars: crustal matter and nuclear pastas



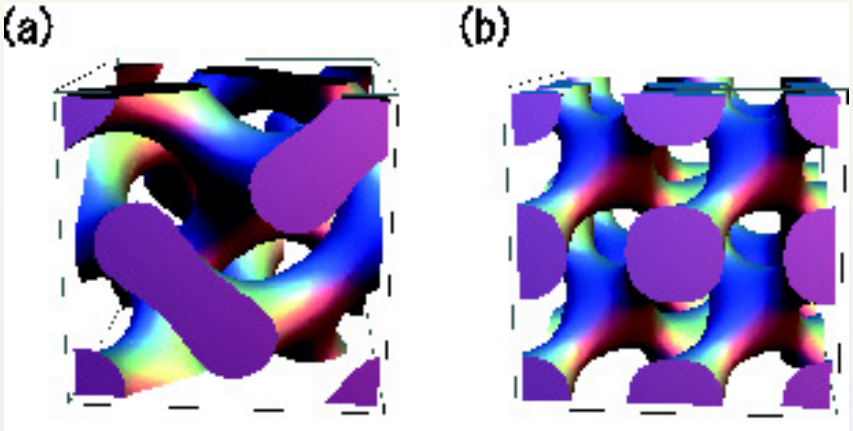
Why is it important?

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

How to study it?

- Liquid drop models
- semi-classical models (Thomas-Fermi)
- Hartree-Fock
- Molecular Dynamics

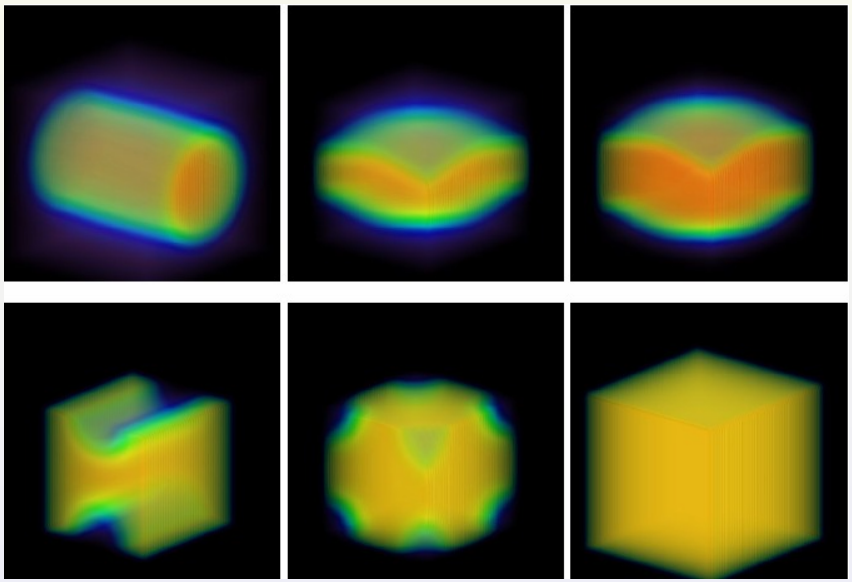
Nuclear pasta's: The liquid drop model



- The geometry you investigate is the geometry you implement
- Semi-empirical method
- generally the canonical pasta phases
- static

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

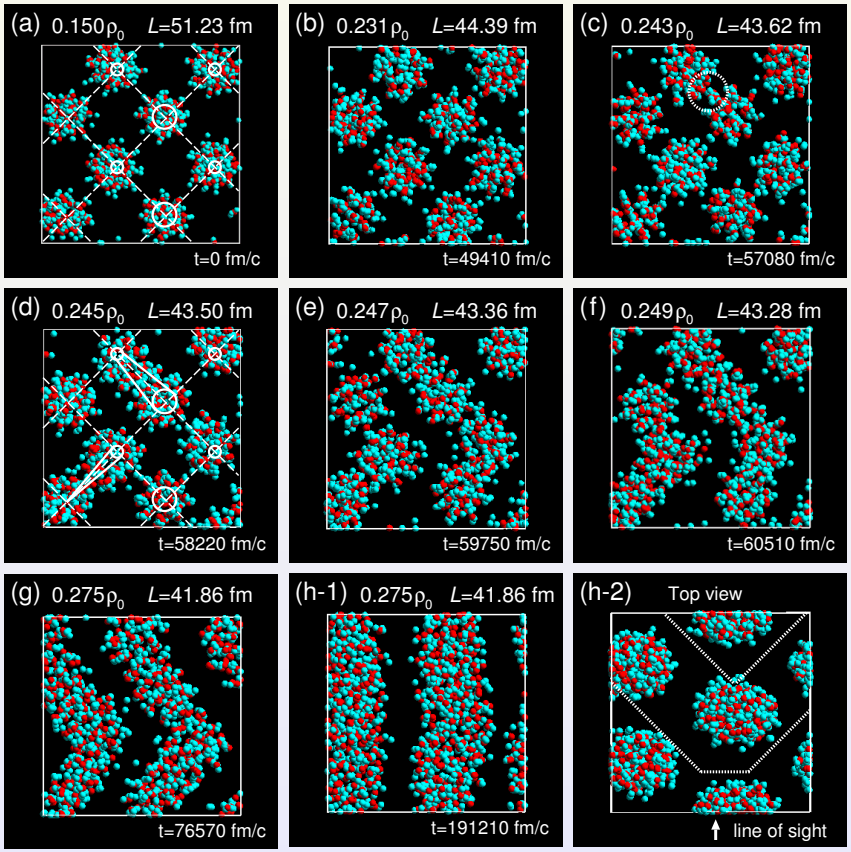
Nuclear pasta's: The Hartree-Fock method



- The geometry you investigate relates to the geometry you implement for the boundry conditions
- mean-field method
- canonical pasta phases
- static

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

Nuclear pasta's: The Quantum molecular dynamics technique



- The geometry you investigate is the geometry you get
- many-body
- canonical and intermediate pasta phases
- time dependence
- Lacks quantum mechanical features

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

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
- ...

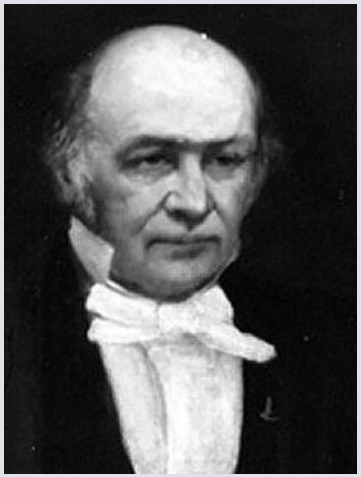
What to study with it

- Nuclear physics
- Condensed matter
- Liquids
- ...

Outline

Molecular dynamics: Classical vs. Quantum mechanical

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

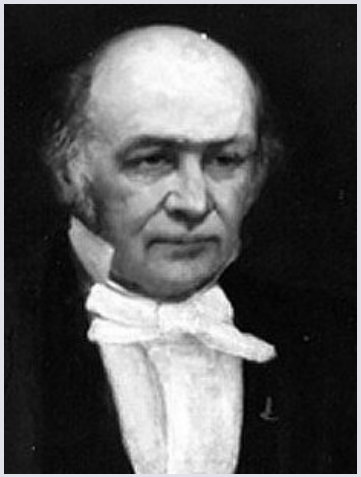
E. Schrödinger

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:
  $|\Psi(t)\rangle = f(t)|\Phi(\boldsymbol{z}(t))\rangle$

Molecular dynamics: Classical vs. Quantum mechanical

W.R. Hamilton



Hamilton's least action principle:

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

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

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 trial state

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.

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

J. C. Slater

Fermionic molecular dynamics: expectation values of operators

- 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 $\mathbf{C}$

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

with $\mathbf{n}_{pq} = \langle q_p|q_q\rangle$ and $\mathbf{o} = \mathbf{n}^{-1}$.

Fermionic molecular dynamics: expectation values of operators

- 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 $\mathbf{C}$

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

Expectation values require the overlap matrix $\mathbf{n}$ and its inverse $\mathbf{o}$.

FMD vs CMD

Advantages of FMD over CMD

FMD handles the evolution of a quantum mechanical Gaussian structured fermion wave function.

- probability distribution are implemented
- Antisymmetry is incorporated leading to Pauli repulsion
- Spin and isospin are variational variables

CMD handles the evolution of classical point particles

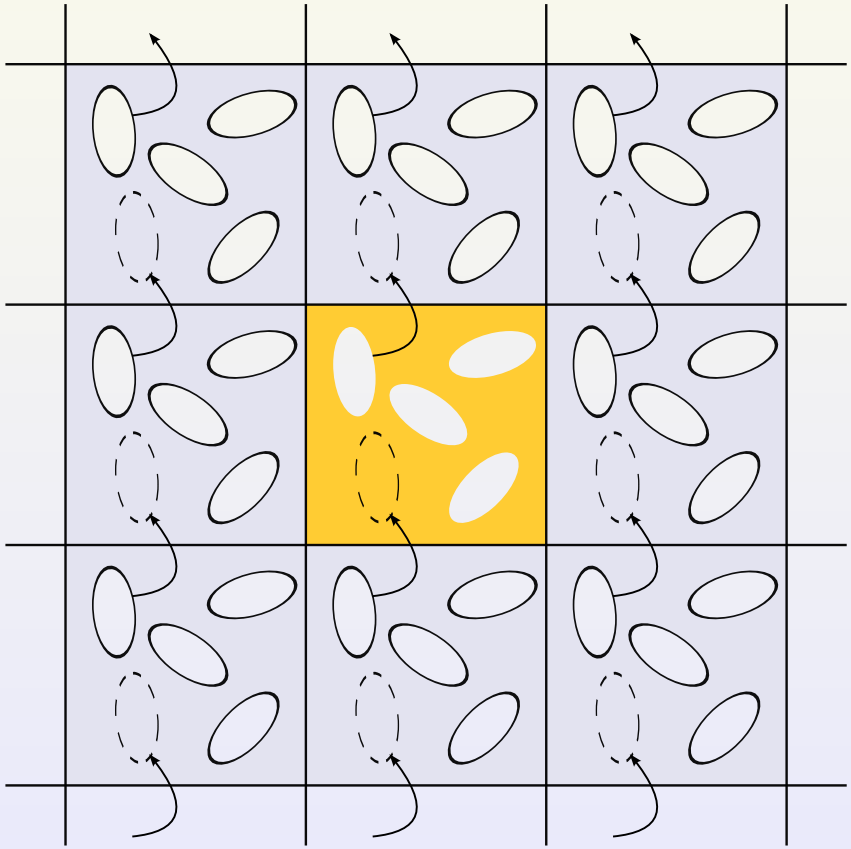
- Pauli potentials could simulate Pauli repulsion

Advantages of CMD over FMD

CMD is an N^2 process while FMD leads to N^4, however we should not be afraid of this!

Outline

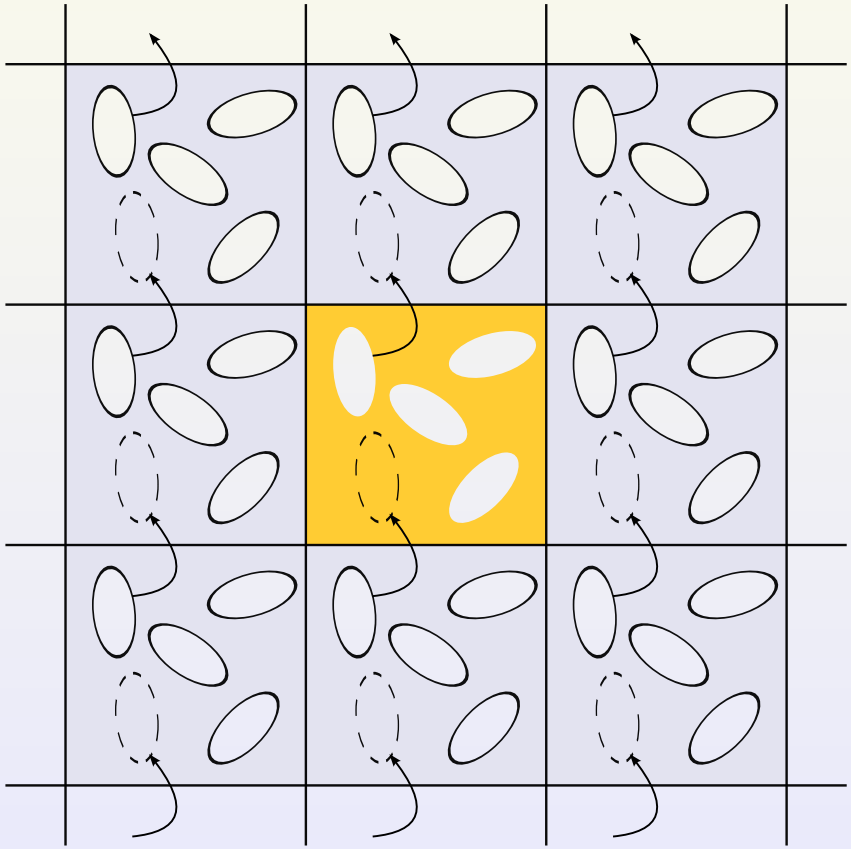
Periodic boundary conditions



Periodic boundary conditions

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

Periodic boundary conditions



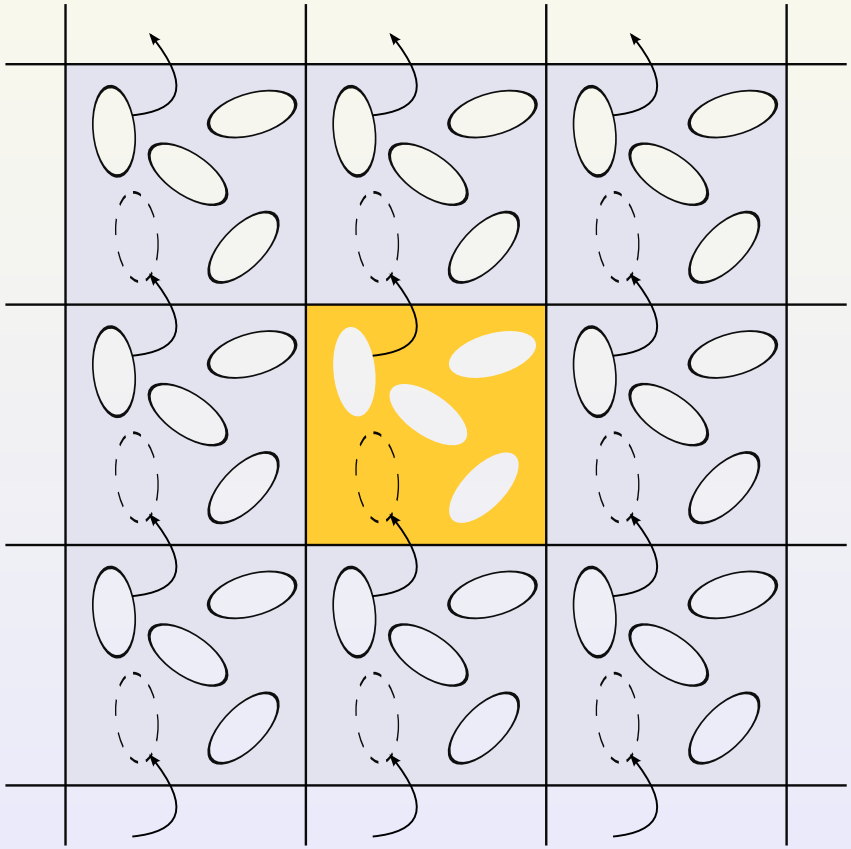
Periodic boundary conditions

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

What about FMD with PBC?

- Fermions require antisymmetrisation

Periodic boundary conditions



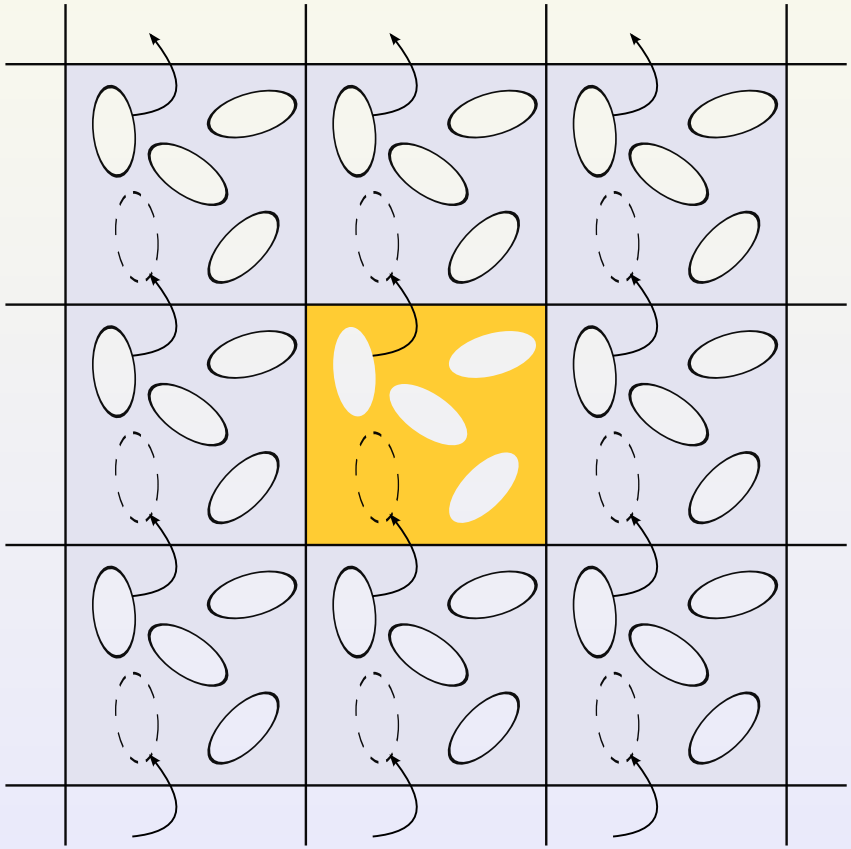
Periodic boundary conditions

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

What about FMD with PBC?

- Fermions require antisymmetrisation
- Antisymmetry does not stop at the border of the unit cell

Periodic boundary conditions



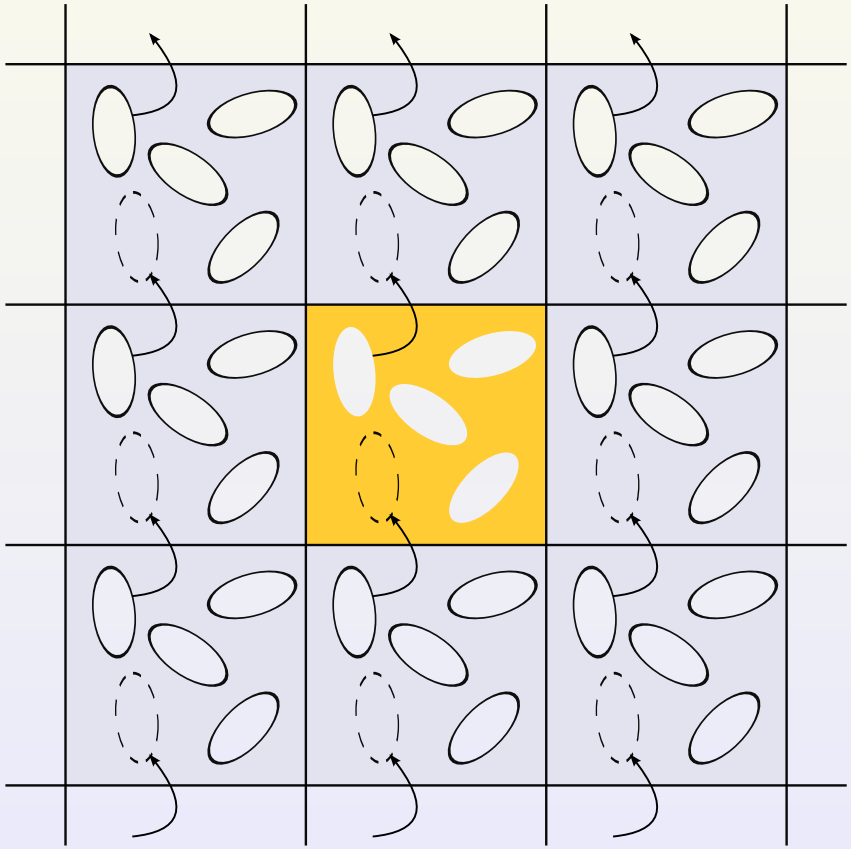
Periodic boundary conditions

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

What about FMD with PBC?

- Fermions require antisymmetrisation
- Antisymmetry does not stop at the border of the unit cell
- FMD must be applied to the infinite periodic system

Periodic boundary conditions



Periodic boundary conditions

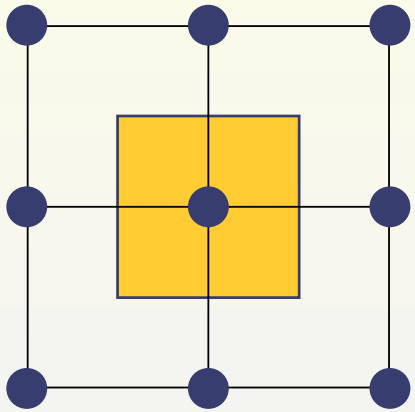
- One unit cell contains N single particle states
- The unit cell is periodically replicated in all directions

What about FMD with PBC?

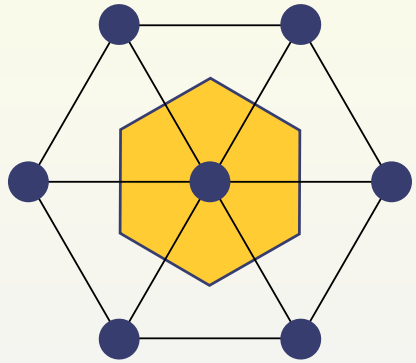
- Fermions require antisymmetrisation
- Antisymmetry does not stop at the border of the unit cell
- FMD must be applied to the infinite periodic system

HOW?

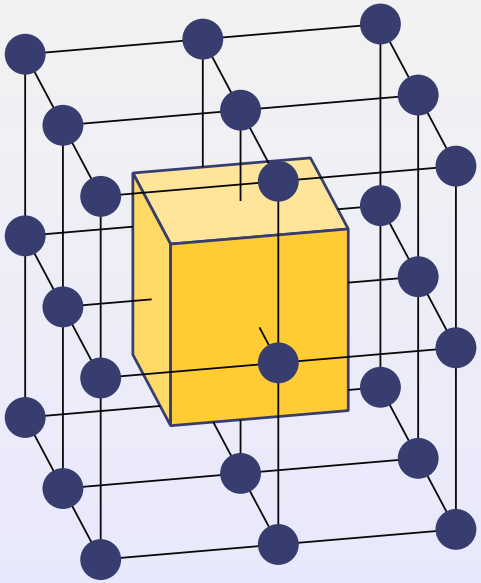
Periodic Boundary Conditions: Common unit cells



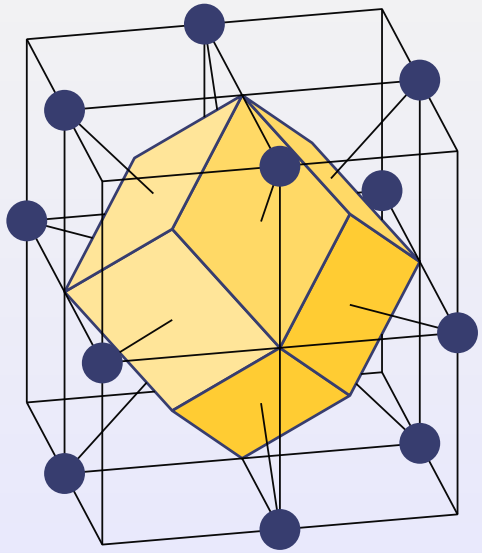
Square lattice



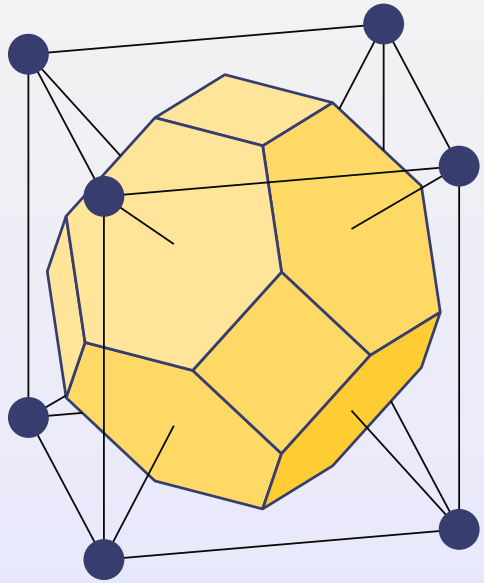
Hexagonal lattice



Simple cubic



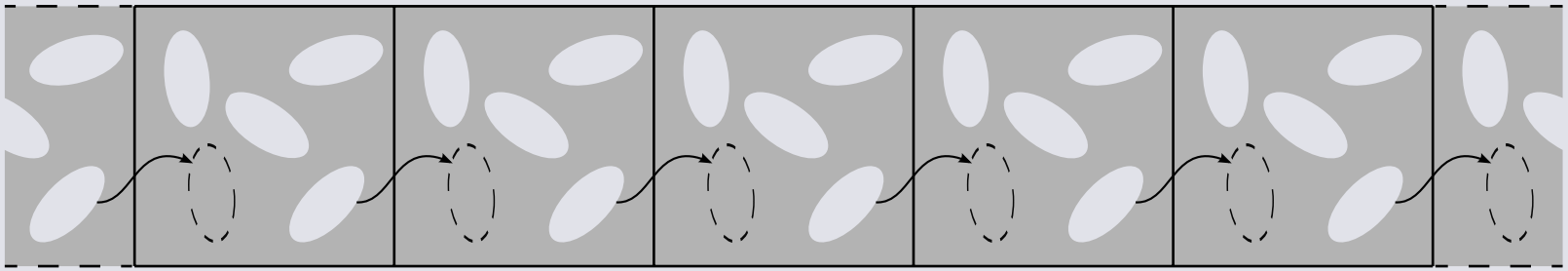
Face-centred cubic



Body-centred cubic

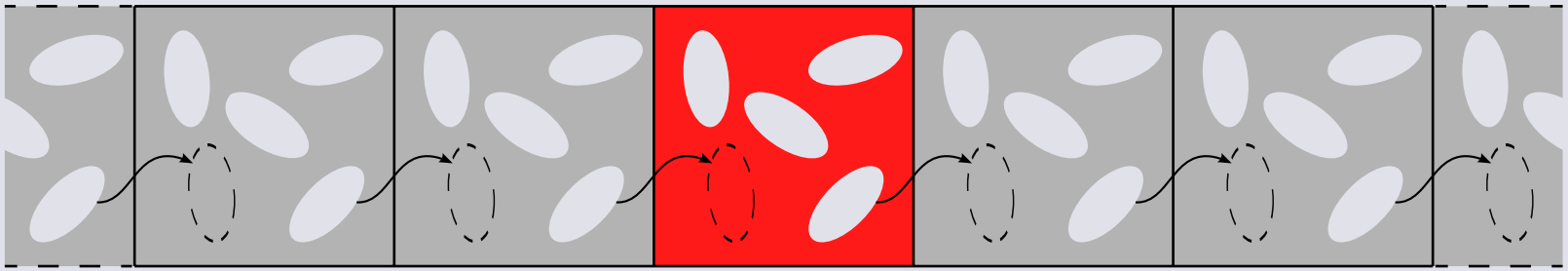
Toeplitz structures reflect the periodicity

The PBC create an infinitely large system, leading to an overlap matrix **N** that is bidirectional-infinite dimensional. What is its structure?



Toeplitz structures reflect the periodicity

The PBC create an infinitely large system, leading to an overlap matrix $\mathbf{N}$ that is bidirectional-infinite dimensional. What is its structure?



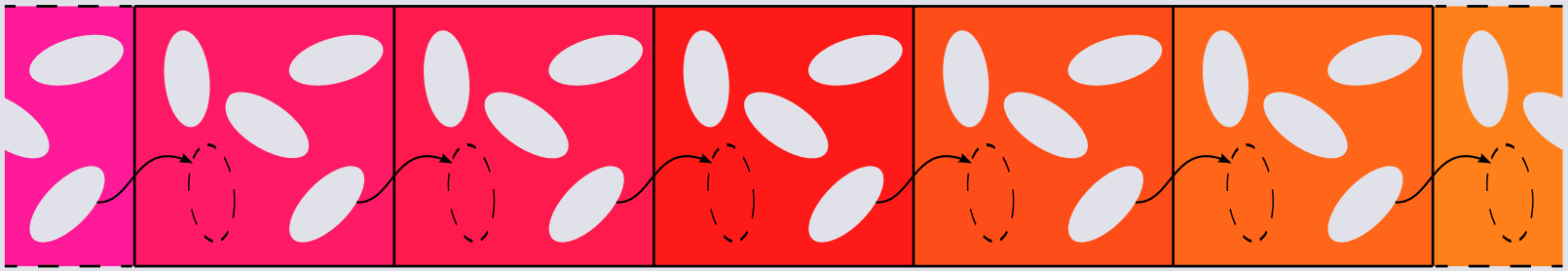
- Overlap of two unit cells shifted over $\boldsymbol{P} = P\boldsymbol{a}_1$ and $\boldsymbol{Q} = Q\boldsymbol{a}_1$:

$$\begin{aligned}\mathbf{N}_{PQ,pq} &= \langle q_p | \mathcal{T}^\dagger(P\boldsymbol{a}_1)\mathcal{T}(Q\boldsymbol{a}_1)|q_q\rangle \\ &= \langle q_p | \mathcal{T}\left((Q-P)\boldsymbol{a}_1\right)|q_q\rangle\end{aligned}$$

$$\mathbf{N} = \begin{pmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{pmatrix}$$

Toeplitz structures reflect the periodicity

The PBC create an infinitely large system, leading to an overlap matrix $\mathbf{N}$ that is bidirectional-infinite dimensional. What is its structure?



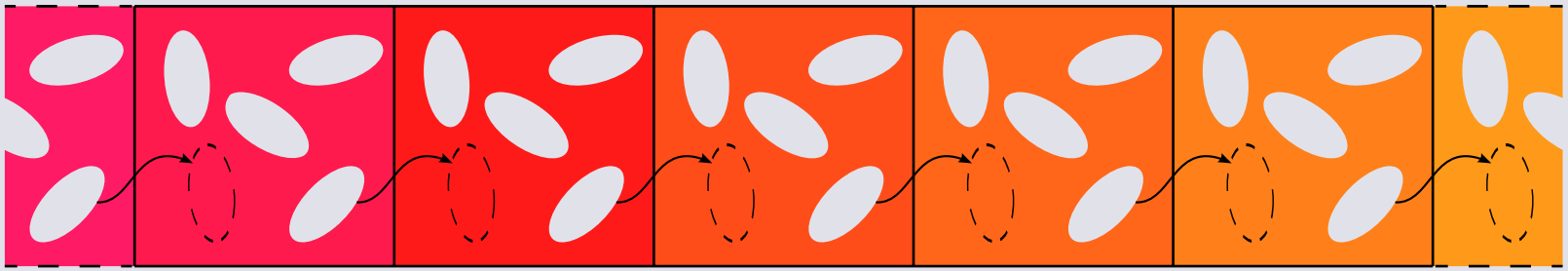
- Only the relative displacement plays a role

$$\mathbf{N}_{PQ,pq} = \langle q_p | \mathcal{T}\left((Q-P)\boldsymbol{a}_1\right) | q_q \rangle$$
$$= \mathbf{n}_{P-Q,pq} =$$

$$\mathbf{N} = \left(\right.$$  $$\left. \right)$$

Toeplitz structures reflect the periodicity

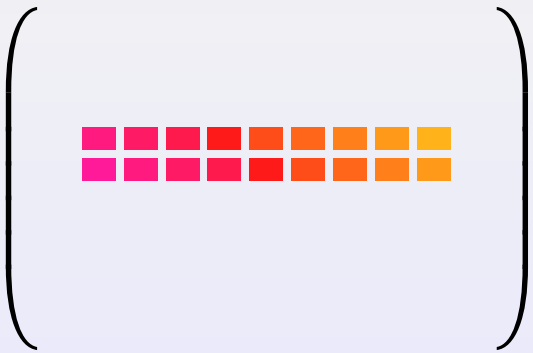
The PBC create an infinitely large system, leading to an overlap matrix $\mathbf{N}$ that is bidirectional-infinite dimensional. What is its structure?



- Only the relative displacement plays a role

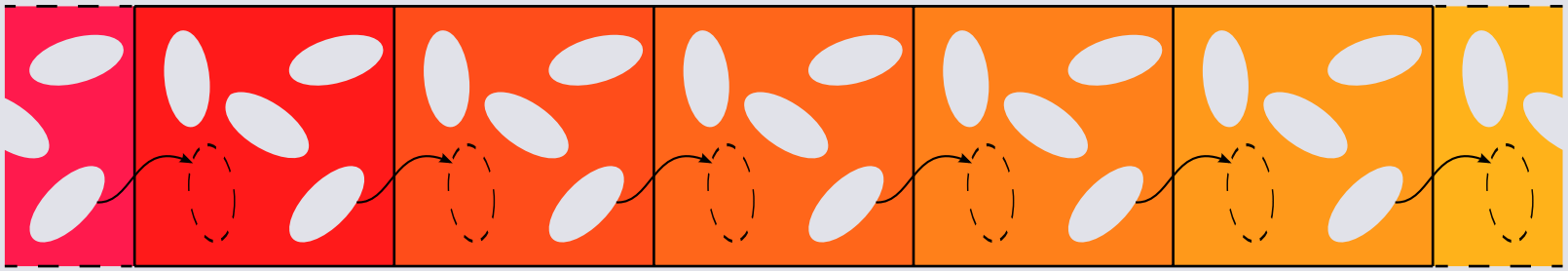
$$\mathbf{N}_{PQ,pq} = \langle q_p | \mathcal{T}\left((Q-P)\boldsymbol{a}_1\right) | q_q \rangle$$
$$= \mathbf{n}_{P-Q,pq} =$$

$$\mathbf{N} =$$



Toeplitz structures reflect the periodicity

The PBC create an infinitely large system, leading to an overlap matrix $\mathbf{N}$ that is bidirectional-infinite dimensional. What is its structure?



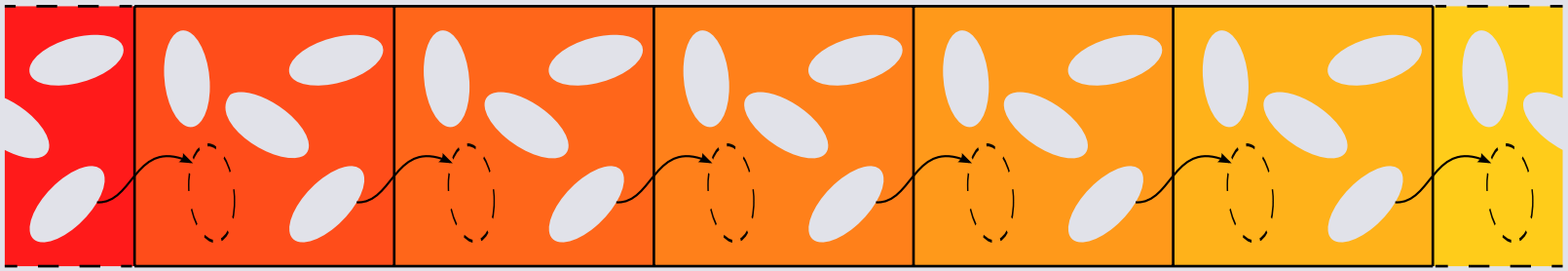
- Only the relative displacement plays a role

$$\mathbf{N}_{PQ,pq} = \langle q_p | \mathcal{T}\left((Q-P)\boldsymbol{a}_1\right) | q_q \rangle$$
$$= \mathbf{n}_{P-Q,pq} =$$

$$\mathbf{N} = \left(\right.$$  $$\left. \right)$$

Toeplitz structures reflect the periodicity

The PBC create an infinitely large system, leading to an overlap matrix $\mathbf{N}$ that is bidirectional-infinite dimensional. What is its structure?



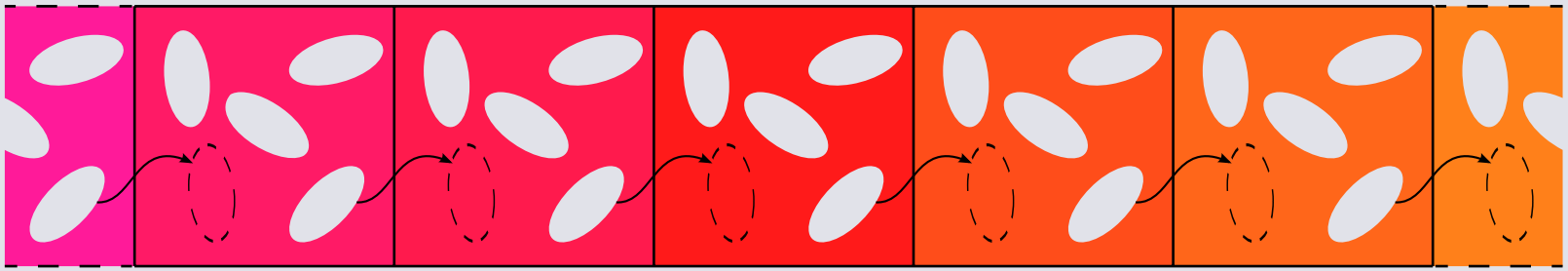
- Only the relative displacement plays a role

$$\mathbf{N}_{PQ,pq} = \langle q_p | \mathcal{T}\left((Q-P)\boldsymbol{a}_1\right) | q_q \rangle$$
$$= \mathbf{n}_{P-Q,pq} =$$

$$\mathbf{N} = \left(\right.$$  $$\left. \right)$$

Toeplitz structures reflect the periodicity

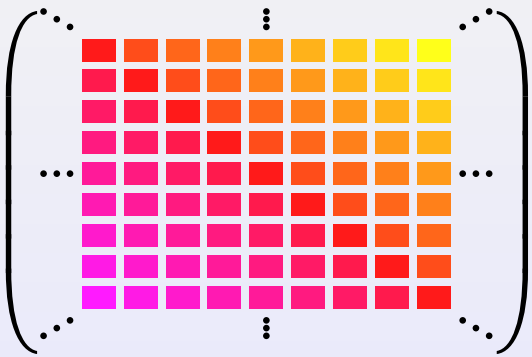
The PBC create an infinitely large system, leading to an overlap matrix $\mathbf{N}$ that is bidirectional-infinite dimensional. What is its structure?



- Only the relative displacement plays a role

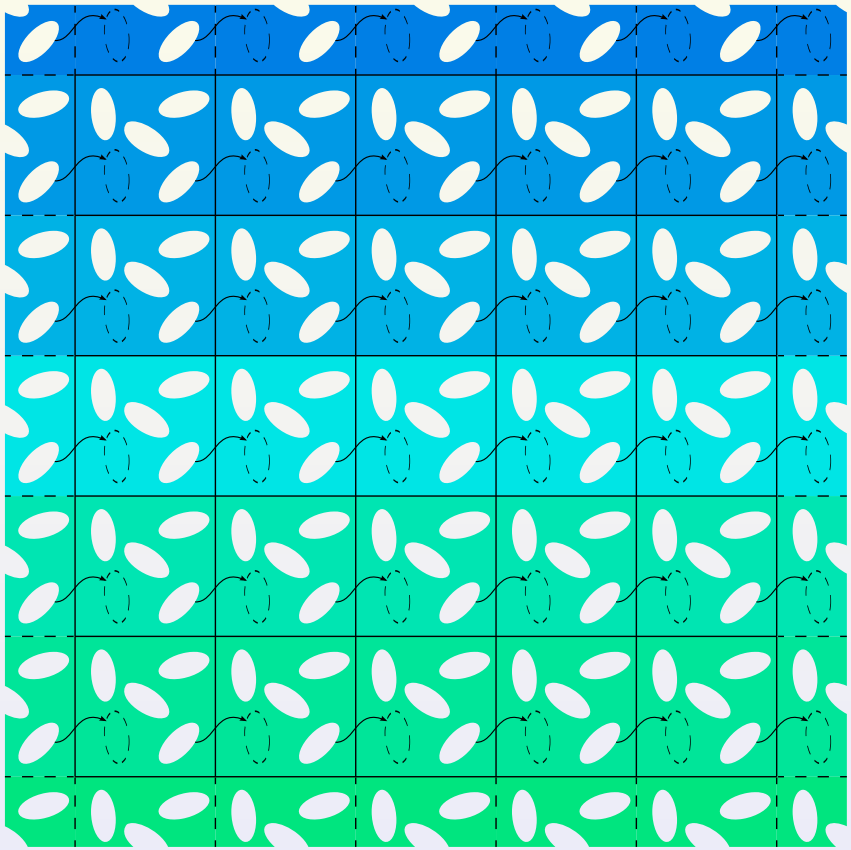
$$\mathbf{N}_{PQ,pq} = \langle q_p | \mathcal{T}\left((Q-P)\boldsymbol{a}_1\right) | q_q \rangle$$
$$= \mathbf{n}_{P-Q,pq} =$$

$$\mathbf{N} =$$



A Toeplitz structure reveals itself in the overlap matrix.

Toeplitz structures reflect the periodicity

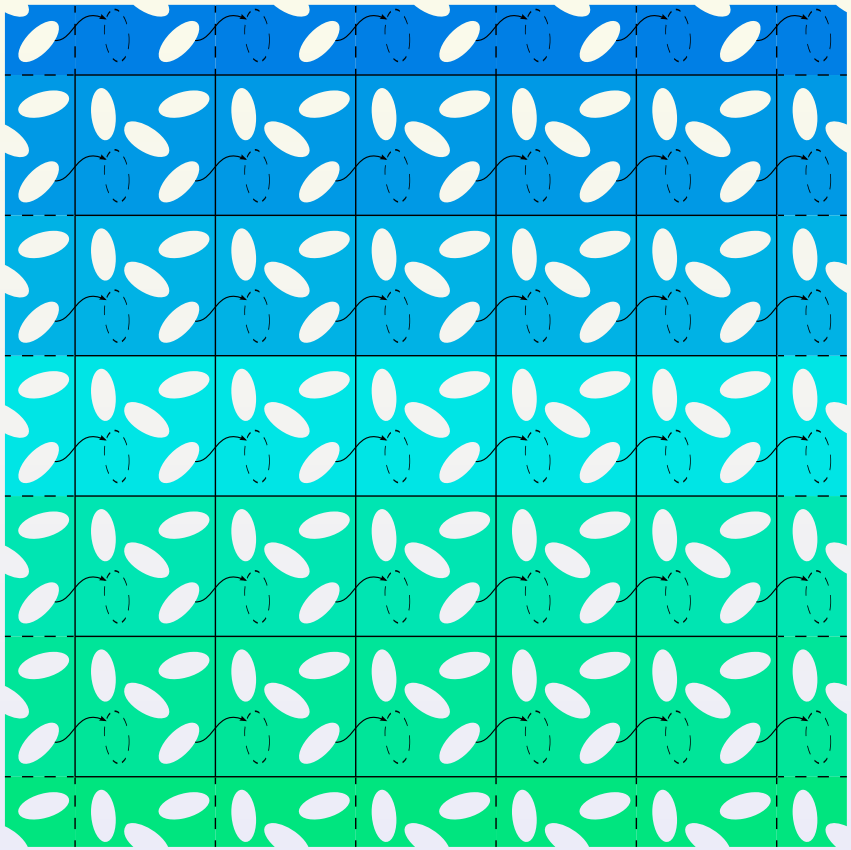


$$\mathbf{N} = \left(\begin{array}{c} \vdots \\ \cdots \\ \vdots \\ \cdots \\ \vdots \end{array} \right)$$

$$\blacksquare = \left(\begin{array}{c} \vdots \\ \cdots \\ \vdots \\ \cdots \\ \vdots \end{array} \right)$$

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

Toeplitz structures reflect the periodicity



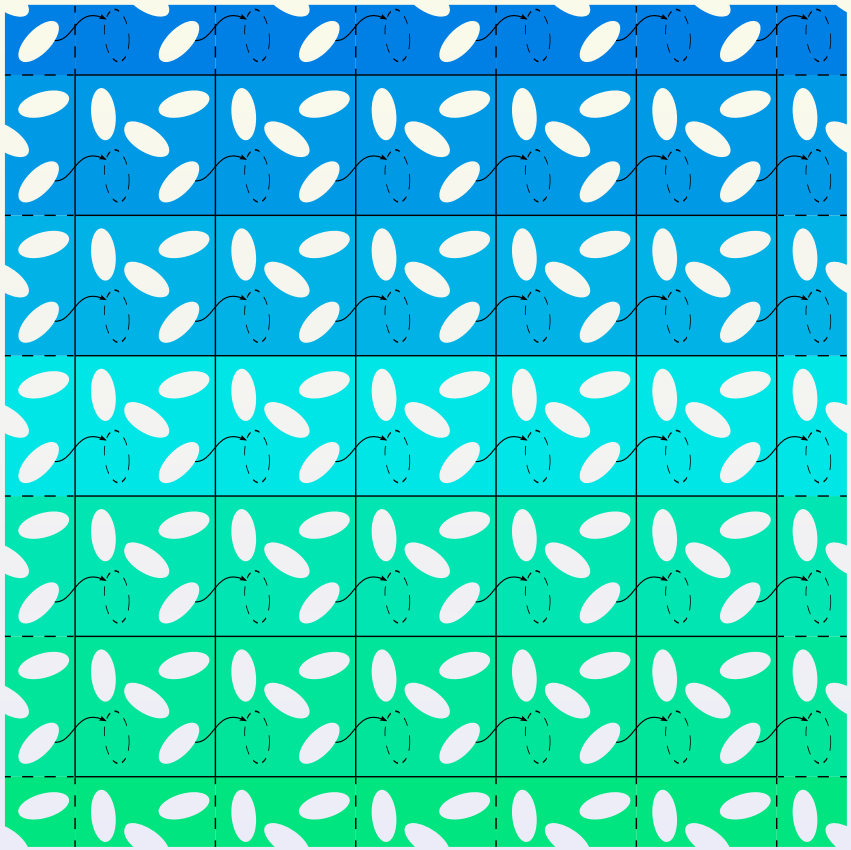
$$\mathbf{N} = \left(\begin{array}{ccc} \ddots & \vdots & \ddots \\ \cdots & & \cdots \\ \ddots & \vdots & \ddots \end{array} \right)$$

$$\blacksquare = \left(\begin{array}{ccc} \ddots & \vdots & \ddots \\ \cdots & & \cdots \\ \ddots & \vdots & \ddots \end{array} \right)$$

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

The overlap matrix has a nested block Toeplitz structure where each block is referred to by a unique displacement vector.

Toeplitz structures reflect the periodicity



$$\mathbf{N} = \left(\begin{array}{c} \vdots \\ \cdots \\ \vdots \end{array} \right)$$

$$\blacksquare = \left(\begin{array}{c} \vdots \\ \cdots \\ \vdots \end{array} \right)$$

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

This structure wanders into the FMD formalism.

expectation values in BFMD

After some exciting math, one finds

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

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

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

Here we have $\mathscr{N}_{pq}(\boldsymbol{k}) = \sum_{\boldsymbol{R}\in\mathfrak{B}} \mathbf{n}_{\boldsymbol{R},pq} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}$ and $\mathscr{O}(\boldsymbol{k}) = \mathscr{N}(\boldsymbol{k})^{-1}$.

expectation values in BFMD

After some exciting math, one finds

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

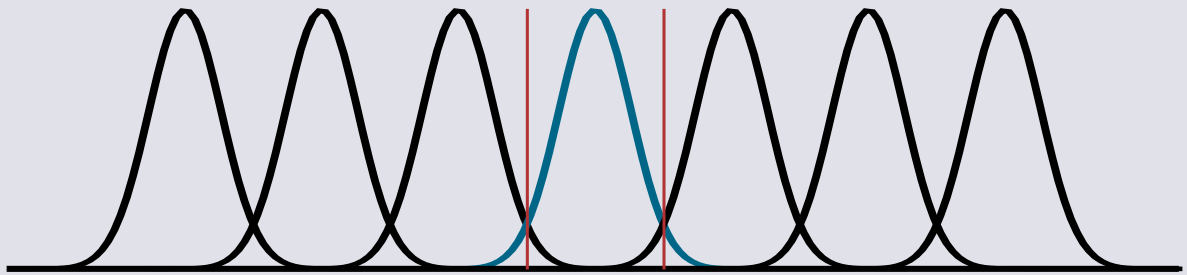
$$\mathscr{B}_{\rho,II} = \frac{1}{2V_{BZ}^2} \iint_{BZ \otimes BZ} \sum_{\boldsymbol{R} \in \mathfrak{B}} \sum_{pqrs=1}^{A} \mathscr{B}_{II,\boldsymbol{R},pqrs}(\boldsymbol{k}_1, \boldsymbol{k}_2) \times \left[\mathscr{O}_{qp}(\boldsymbol{k}_1) \mathscr{O}_{sr}(\boldsymbol{k}_2) - \mathscr{O}_{qr}(\boldsymbol{k}_1)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

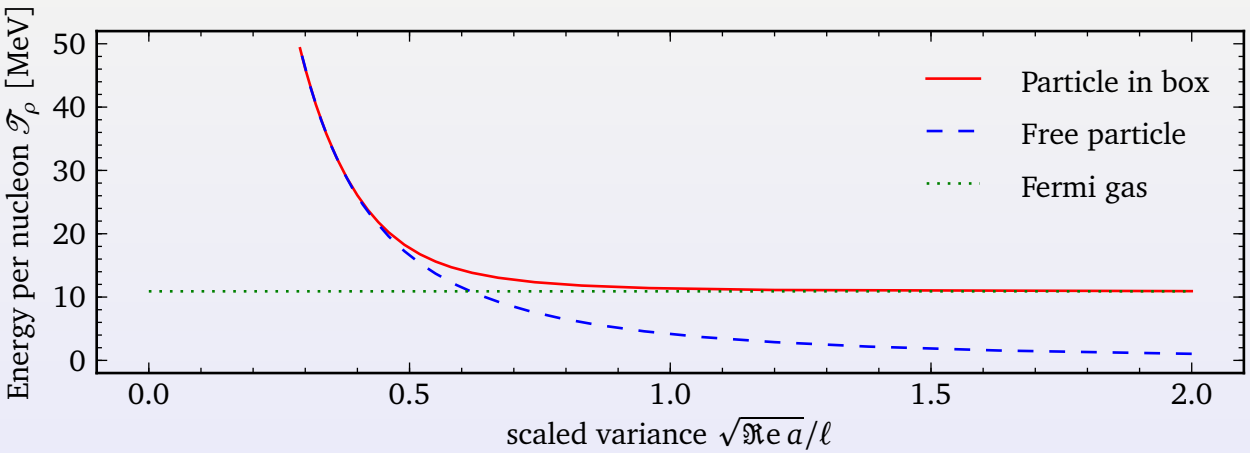
$$\mathbf{C}_{\rho,ab} = \frac{1}{V_{BZ}} \int_{BZ} \left(\frac{\partial^2 \mathscr{N}_{ab}(\boldsymbol{k})}{\partial \boldsymbol{z}_a^\star \partial \boldsymbol{z}_b} - \sum_{pq=1}^{A} \frac{\partial \mathscr{N}_{ap}(\boldsymbol{k})}{\partial \boldsymbol{z}_a^\star} \cdot \mathscr{O}_{pq}(\boldsymbol{k})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

Expectation values become mere integrals over the first Brillouin zone of the lattice.

Outline

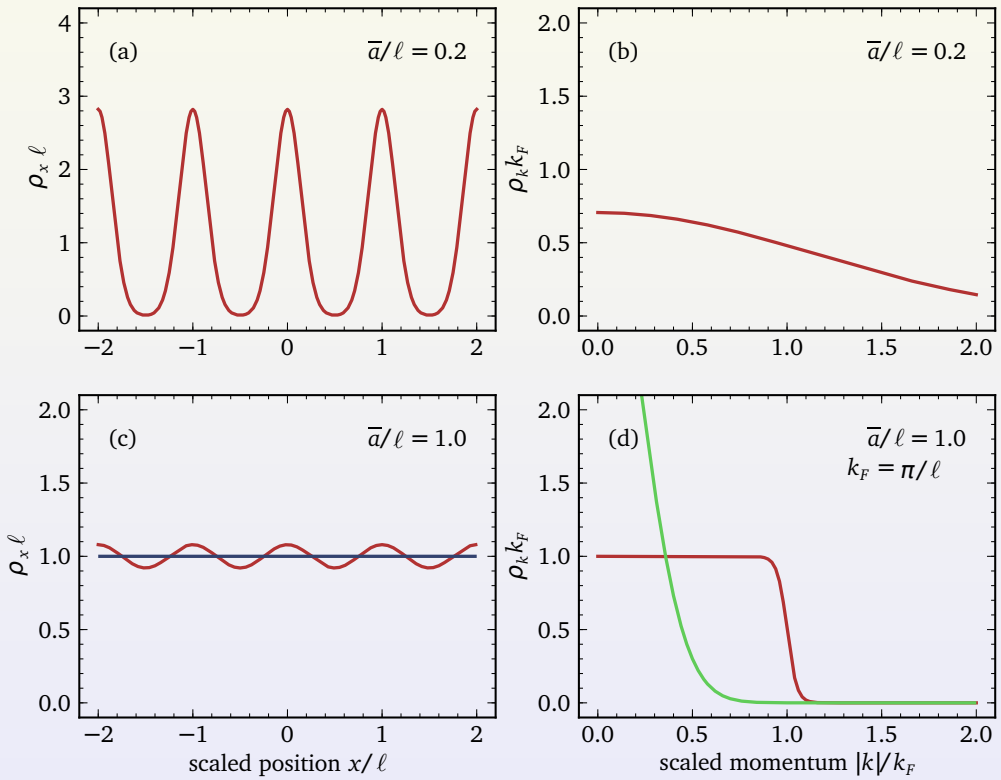
Kinetic energy of a one dimensional fermion system





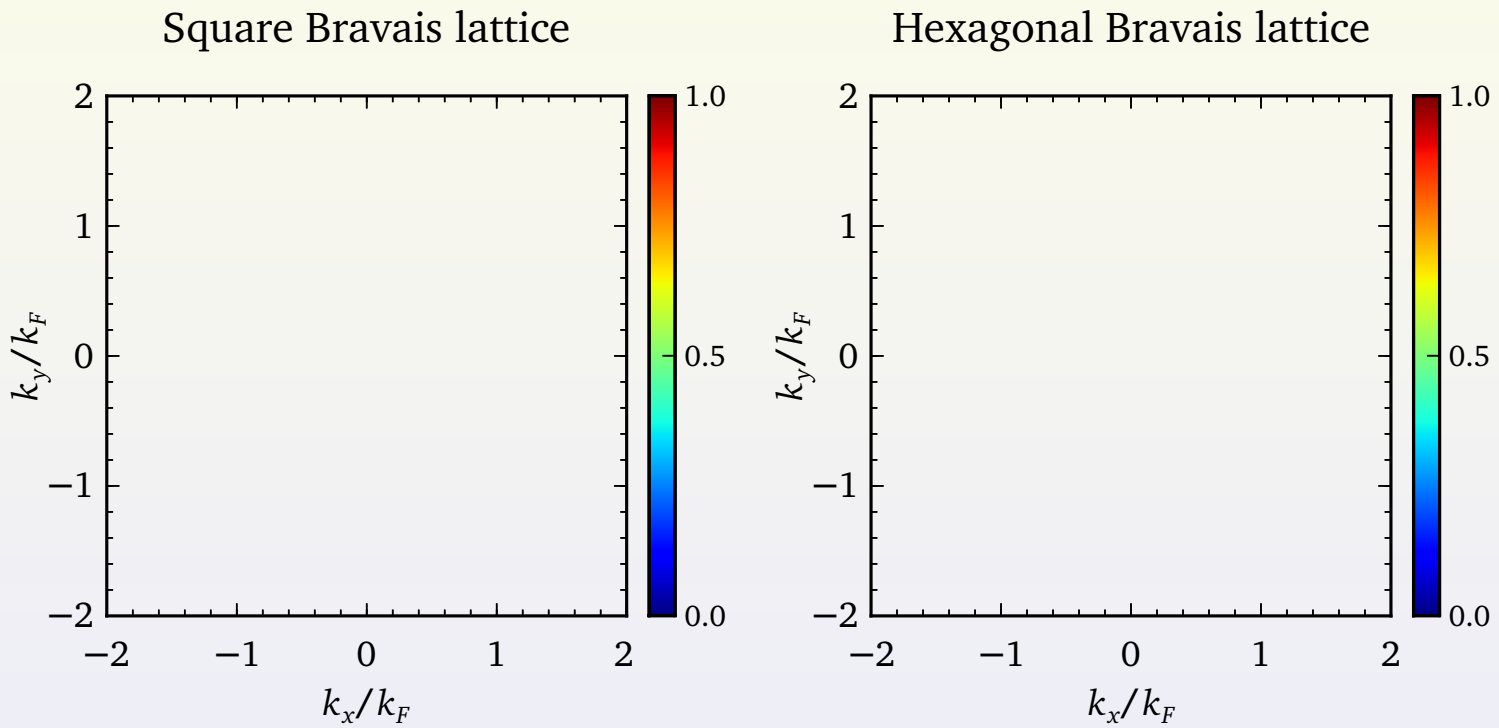
The larger the overlap, the more the particles behave as free fermions

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

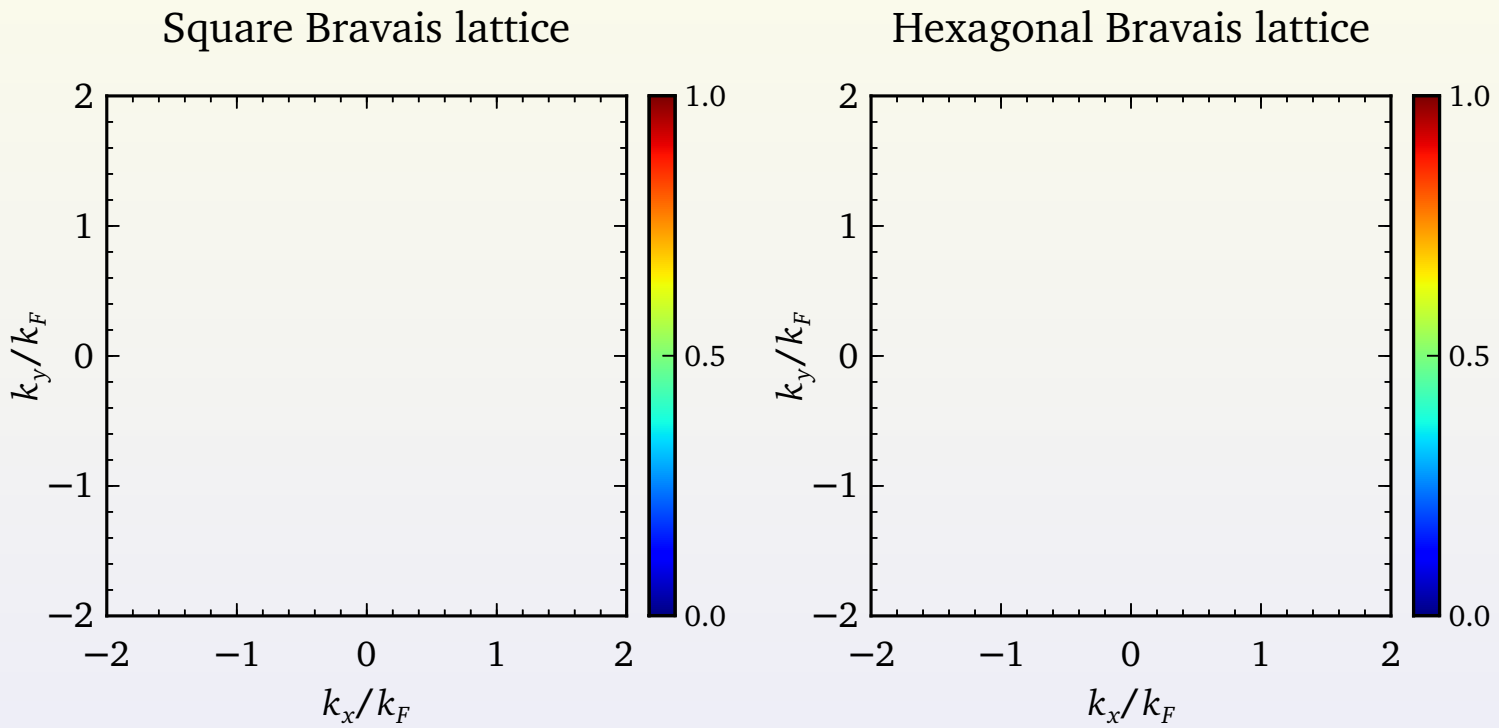
Momentum density in two dimensions



One Gaussian per cell

- $\sqrt{a}/\ell = 0.2$

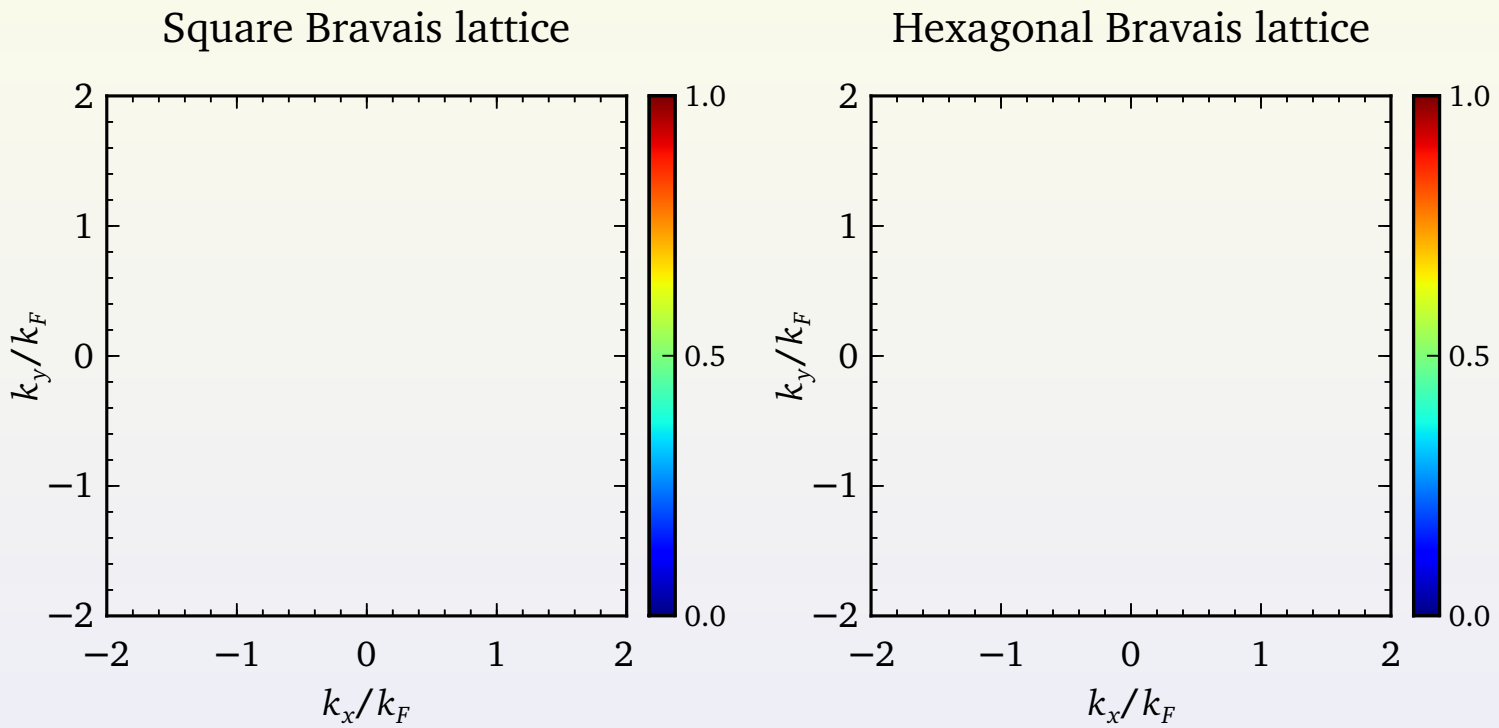
Momentum density in two dimensions



One Gaussian per cell

- $\sqrt{a}/\ell = 0.3$

Momentum density in two dimensions

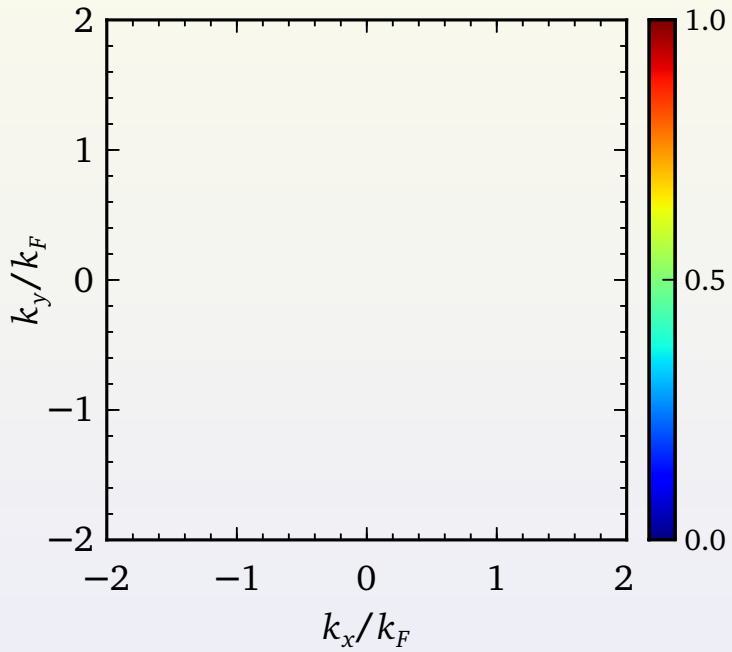


One Gaussian per cell

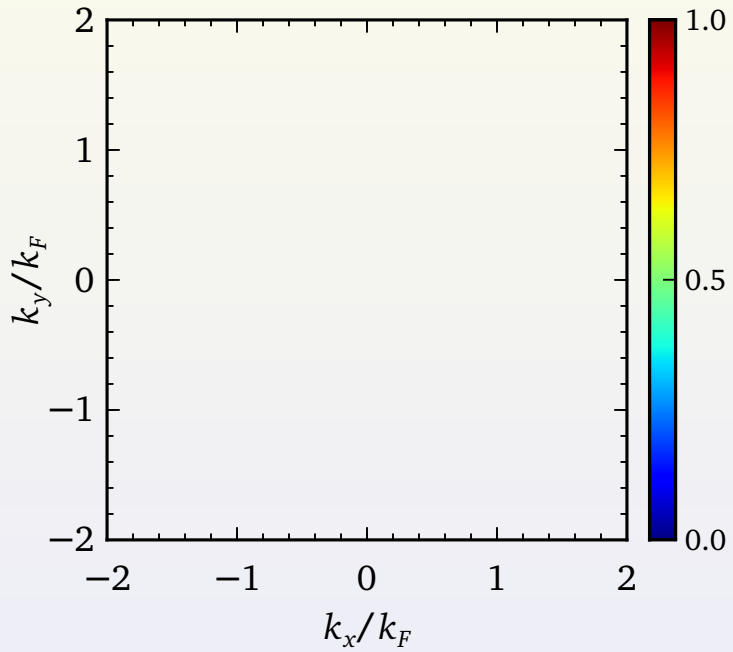
- $\sqrt{a}/\ell = 0.6$

Momentum density in two dimensions

Square Bravais lattice



Hexagonal Bravais lattice

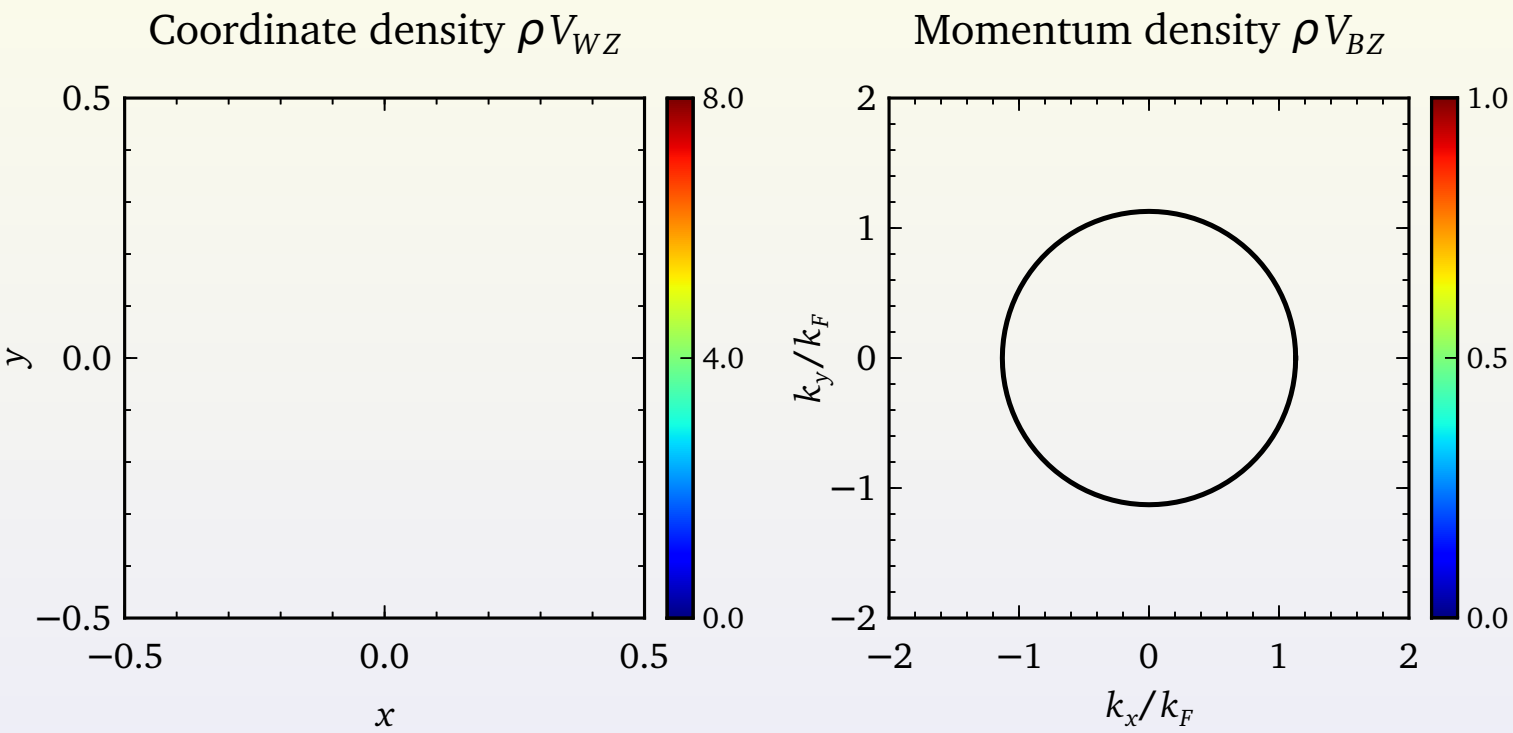


One Gaussian per cell

- $\sqrt{a}/\ell = 1.0$

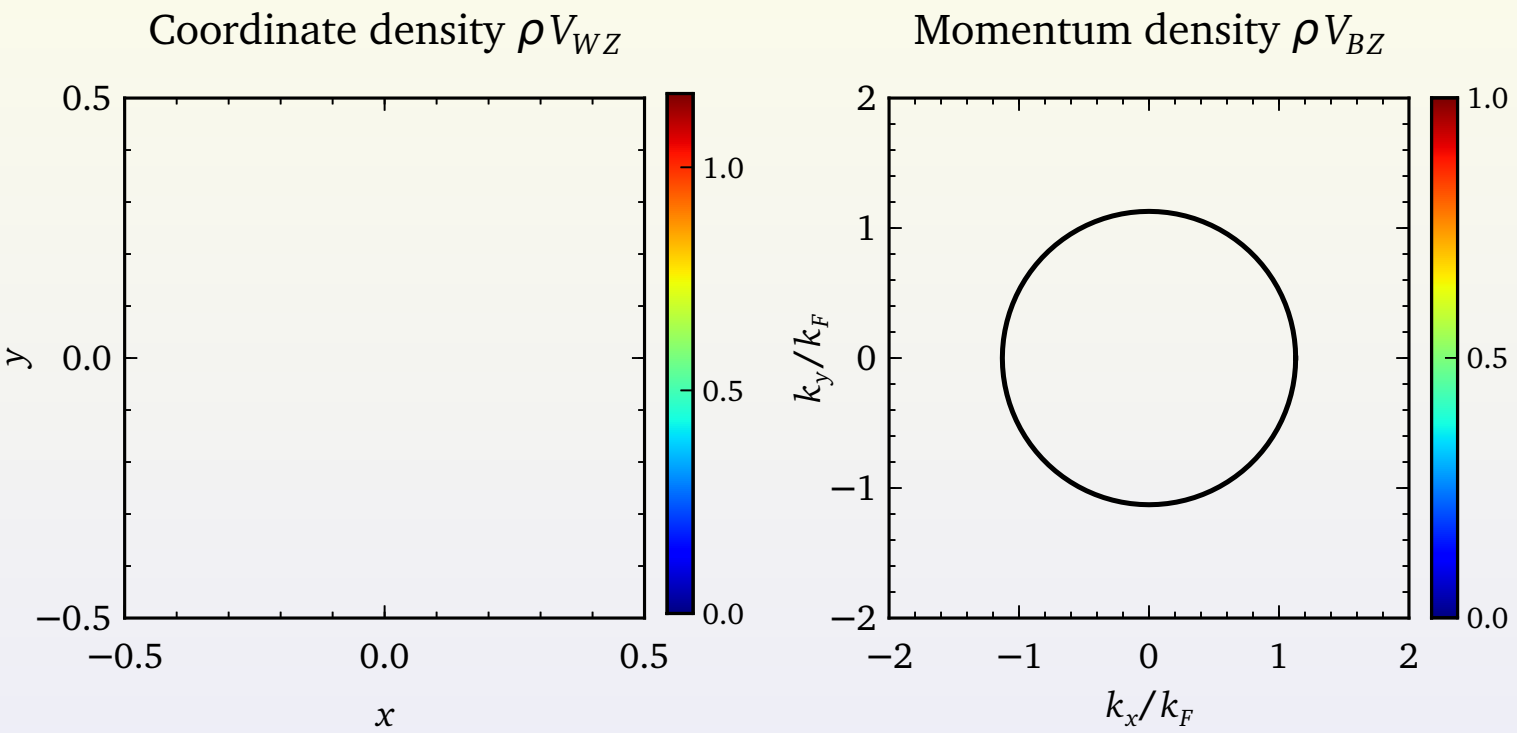
With increasing overlap, the momentum distribution evolves towards the first Brillouin zone.

Lattice versus random



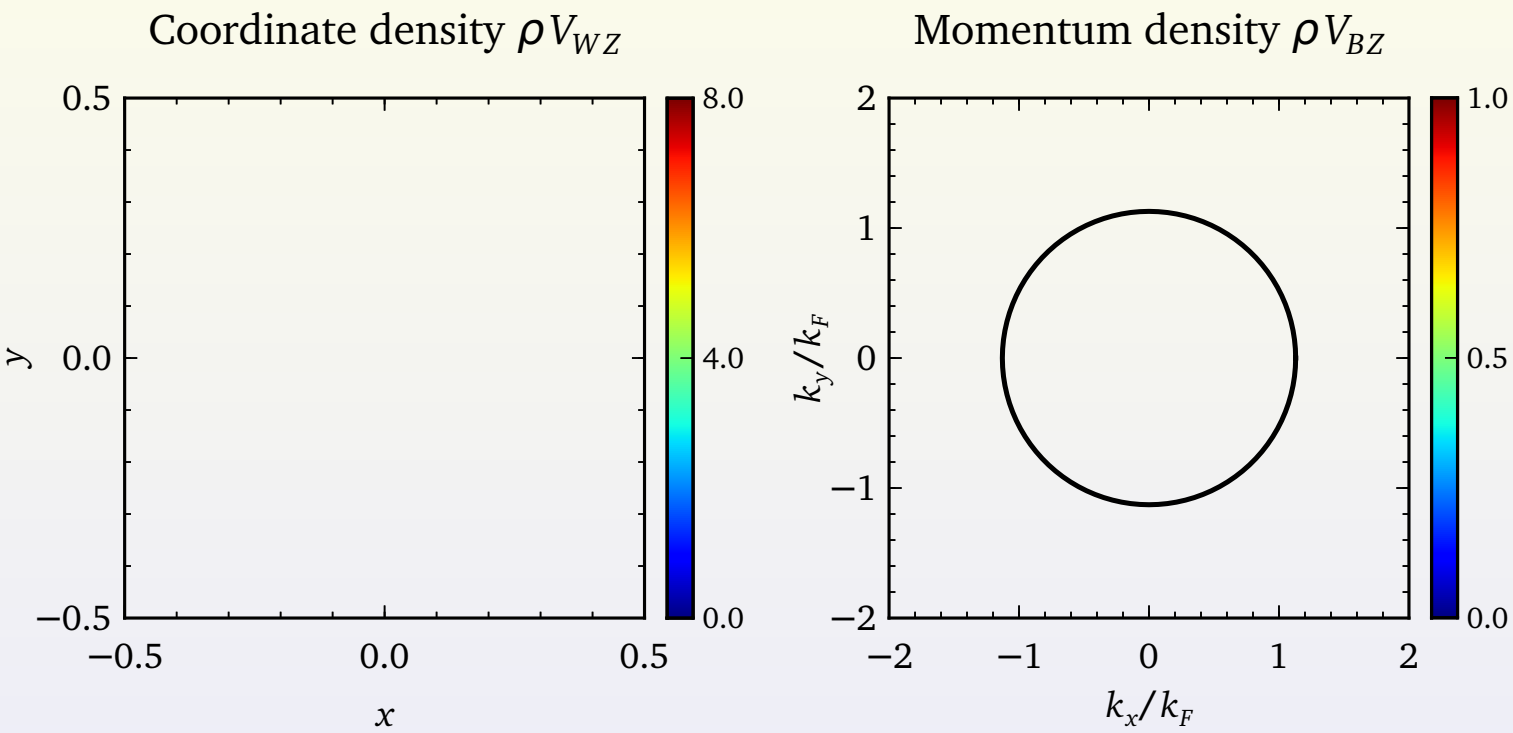
Gaussian width: $\sqrt{a} = 0.2\ell/5$

Lattice versus random



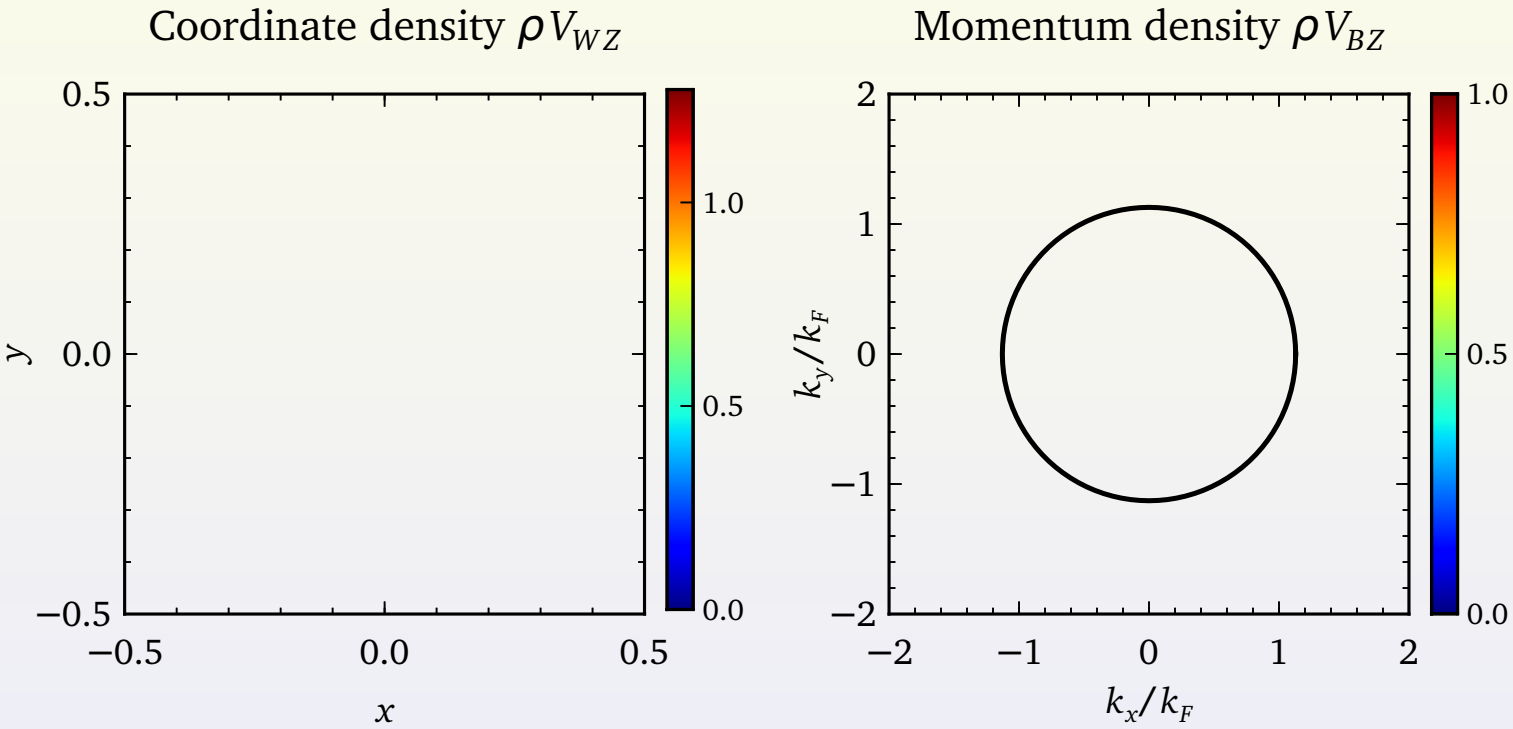
Gaussian width: $\sqrt{a} = \ell/5$

Lattice versus random



Gaussian width: $\sqrt{a} = 0.2\ell/5$

Lattice versus random



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

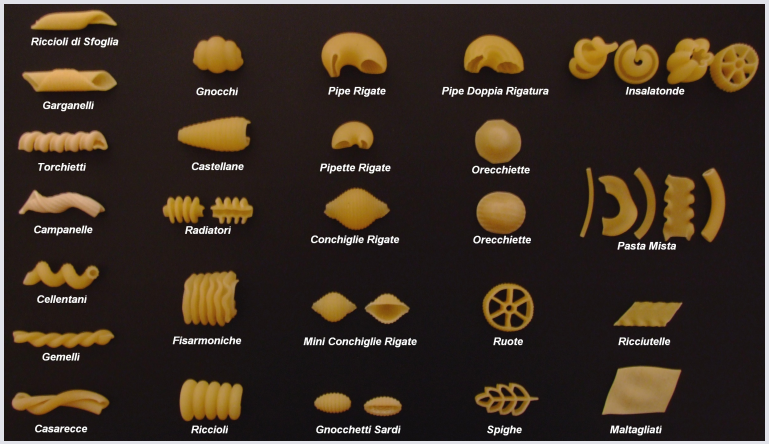
A random distribution of fermions with large overlap clearly shows a uniform coordinate density and a spherical momentum density.

Outline

Conclusion . . .

- We introduced a molecular dynamics technique to study fermion behaviour.
- The overlap matrix of a fermion system, and its inverse, are the key elements of FMD.
- We introduced periodic boundary conditions to study bulk matter and showed that the problem becomes tractable and computational friendly.
- We showed that fermionic 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.

Solving computational issues

- A good numerical time-reversable energy-conserving integrator for the equations of motion
- Introducing a thermometer for the system
- Adapting the Ewald-summation for long-range interactions as the Coulomb interaction

The study of nuclear matter

- Its ground state by means of proper nuclear potentials
- Structure functions through dynamics
- and more . . .

This slide intentionally left blank