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# Towards a fully antisymmetrised dynamics of the neutron-star crust

**Klaas Vantournhout***
*GSI Helmholtzzentrum für Schwerionenforschung GmbH,*
*Planckstrasse 1, 64291 Darmstadt, Germany*
*E-mail:* k.vantournhout@gsi.de

**Natalie Jachowicz**
*Department of Physics and Astronomy, Ghent University,*
*Proeftuinstraat 86, 9000 Gent, Belgium*
*E-mail:* Natalie.Jachowicz@UGent.be

**Jan Ryckebusch**
*Department of Physics and Astronomy, Ghent University,*
*Proeftuinstraat 86, 9000 Gent, Belgium*
*E-mail:* Jan.Ryckebusch@UGent.be

**Hans Feldmeier**
*GSI Helmholtzzentrum für Schwerionenforschung GmbH,*
*Planckstrasse 1, 64291 Darmstadt, Germany*
*E-mail:* h.feldmeier@gsi.de

We present a novel method to study the dynamics of bulk fermion systems such as the neutron-star crust. By introducing periodic boundary conditions into Fermionic Molecular Dynamics, it becomes possible to examine the long-range many-body correlations induced by antisymmetrisation in bulk fermion system. The presented technique treats the spins and the fermionic nature of the nucleons explicitly and permits investigating the dynamics of the system. Despite the increased complexity related to the periodic boundary conditions, the formalism remains computationally feasible.

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*Speaker.

 

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Among the myriad of phenomena in the universe, a neutron star is one of the extremely interesting objects. As an "oversized nucleus", it is one of the most dense and compact objects known. The densities of the inner part of a neutron star are expected to be as large as five to ten times the normal nuclear saturation density $n_0$. This leads to intriguing speculations about the composition of the neutron-star core [1]. The densities of the outer layers of a neutron star are on the average below $n_0$. At these densities, the neutron-star crust consists of protons, neutrons and electrons, organising themselves in nuclear clusters as a result of the short-range nuclear attraction and the long-range Coulomb repulsion. In the crust-core interface of the neutron star at higher densities ($n_0/3$ to $n_0/2$ [1]), the system balances on a subtle interplay between the nuclear surface energies and the Coulomb energy of the neutron-proton-electron system. This results in a multitude of competing quasi-ground states, having sometimes quite different matter distributions, where the system can cool down to. These complex-shaped structures are dubbed "nuclear pastas" [2, 3]. The crust-core interface of a neutron star may represent a sizable fraction of the crustal mass. Furthermore, such matter at sub-saturation densities can contribute 10–20% of the mass in the later stages of a collapsing stellar core. As such, a sound description of the neutron-star crust, or nuclear matter at sub-saturation densities in general, is needed to understand various astrophysical observations [3].

The nuclear pasta phases have been investigated with a broad spectrum of computational techniques [2, 4, 5, 6, 7]. From all these techniques, molecular dynamics is one of the few that is not biased with regard to the geometry of the nuclear clusters. Moreover, thanks to the dynamical aspect, one can go beyond the study of ground-state structures. Classical Molecular Dynamics (CMD) provided a way to study the effect of large density fluctuations on neutrino opacities and to evaluate the breaking strain of the crust [8]. A more advanced model, named Quantum Molecular Dynamics (QMD), was used to study the pasta structures themselves as well as their transitions [5].

When studying phenomena at length scales smaller than the de Broglie wavelength of the system's constituents, CMD breaks down. Under those conditions, quantum effects stemming from the wave character of the nucleons predominate, and statistical many-body correlations related to the system's fermionic content play a fundamental role. In QMD, the effect of fermionic correlations is mimicked by means of a phenomenological Pauli potential. Although this method is quite successful in calculating energies, it fails at reproducing the single-particle occupations in momentum space for the free Fermi gas. Furthermore, in QMD, the spin and the width of the localised states are assumed to be time independent.

The shortcomings of QMD for fermion systems are remedied in Antisymmetric and Fermionic Molecular Dynamics (AMD, FMD) [9, 10]. In these techniques, the many-body state is introduced as a Slater determinant of localised parametrised single-particle states $|\phi_p(\vec{z}_p)\rangle$, and accounts in this way for proper fermion statistics. The time-evolution of the time-dependent parameters $\vec{z}_p$ is then determined by the time-dependent variational principle leading to generalised Hamilton equations of motion [10].

Both AMD and FMD enjoy successes in the study of heavy-ion collisions, ground states of nuclei and astrophysical reaction calculations [9, 11, 12]. However, due to the long-range character of the Pauli correlations, evaluating bulk fermion matter becomes a tedious task. When investigating the properties of bulk matter by means of large simulation volumes, the evaluation of expectation values becomes cumbersome. Moreover, surface effects may influence the results when a large

fraction of the constituents lies on the surface of the simulation volume. A time-honoured method is to introduce a periodic structure in the simulation. When studying bulk matter using a periodic structure, it is crucial to make sure that the studied properties of the small, but infinitely repeated periodic system and the macroscopic system which it represents, are the same. As long as the correlation volume of the interactions does not exceed the simulation volume, the imposed periodicity works fine. However, serious problems arise in the presence of long-range correlations as e.g. induced by Coulomb interactions or by the Pauli exclusion principle. It is indispensable to fully antisymmetrise the many-body wave function representing the system. To simulate bulk matter with localised states, we propose to make the spatial positioning of the single-particle states periodic. A number of particles are placed in unit cells on a lattice $\mathfrak{B}$, that is tessellating space perfectly. Each cell, containing $A$ particles, can be identified by a lattice vector $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ with integer $n_j$. The trial state of the system is thus, with $\hat{T}(\vec{R})$ the translation operator over $\vec{R}$,

$$|\Phi_\infty\rangle = \hat{A} \bigotimes_{\vec{R}\in\mathfrak{B}} \hat{T}(\vec{R}) \left\{ |\phi_1\rangle \otimes \cdots \otimes |\phi_A\rangle \right\}. \tag{1}$$

Using this trial state in the FMD formalism, all expressions become infinite dimensional. However, the introduced spacial periodicity in the trial state leads to a peculiar nested block-Toeplitz structure in the FMD expressions. This is a feature that can be exploited to reduce the numerical cost of the simulation. The structure of the resulting equations resemble those of finite FMD, but integrations are performed in reciprocal lattice space. This way, the one-body operator $\hat{B}_I$ is evaluated as

$$\mathscr{B}_{\rho,I} = \frac{1}{V_{BZ}} \int_{BZ} \sum_{pq=1}^{A} \bar{\bar{\mathscr{B}}}_{I,pq}(\vec{k}) \bar{\bar{\mathscr{O}}}_{qp}(\vec{k})\, d^3\vec{k}, \qquad \bar{\bar{\mathscr{B}}}_{I,pq}(\vec{k}) = \sum_{\vec{R}\in\mathfrak{B}} \langle \phi_p | \hat{B}_I \hat{T}(\vec{R}) | \phi_q \rangle\, e^{i\vec{k}\cdot\vec{R}} \tag{2}$$

$$\bar{\bar{\mathscr{N}}}(\vec{k}) = \sum_{\vec{R}\in\mathfrak{B}} \bar{\bar{n}}_{\vec{R}}\, e^{-i\vec{k}\cdot\vec{R}}, \qquad \bar{\bar{\mathscr{O}}}(\vec{k}) = \bar{\bar{\mathscr{N}}}(\vec{k})^{-1}. \tag{3}$$

Here, $BZ$ represents the first Brillouin zone of the lattice $\mathfrak{B}$ and $\vec{k}$ is a vector in this volume. The overlap matrix $\bar{\bar{n}}_{\vec{R}}$ has the elements $\bar{\bar{n}}_{\vec{R},pq} = \langle \phi_p | \hat{T}(\vec{R}) | \phi_q \rangle$ [13].

In the following, we will show that the proposed technique reproduces the features intrinsic to the fermionic behaviour of the system. The unnormalised single-particle states are Gaussian wave packets of the form $\langle \vec{x} | a\vec{b} \rangle = \exp\{-(\vec{x}-\vec{b})^2/(2a)\}$ where the complex vector $\vec{b}$ represents the mean position in phase space and $a$ is a complex parameter connected with the width of the wave packet. In Fig. 1, we show that our method reproduces the momentum and spatial densities intrinsic to one-dimensional Fermi systems by placing a single particle in a unit cell of size $\ell$. It is clearly visible that with increasing $\sqrt{a}/\ell$ and thus with increasing overlap of neighbouring states, hence increasing influence of the antisymmetrisation, the fermionic behaviour becomes apparent. For $\sqrt{a}/\ell = 1$, the momentum distribution does not show a sharp cutoff near the Fermi momentum because the periodic set of Gaussian wave packets does not constitute a complete set. For $\sqrt{a}/\ell \to \infty$, the antisymmetry operator projects the Gaussian wave packets on plane waves and a sharp cutoff is reached. Even though this one-dimensional example clearly hints at free-fermion behaviour, it can be shown that in more dimensions the momentum distribution evolves towards the first Brillouin zone of the lattice [13]. This effect can be expected as, with increasing overlap,

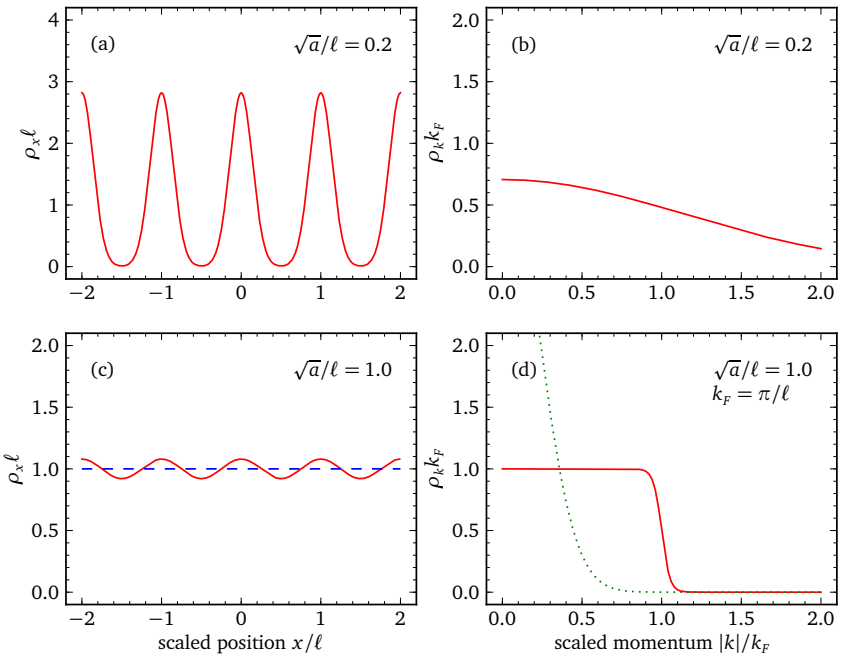


**Figure 1:** Spatial density (panels (a) and (c)) and momentum density (panels (b) and (d)) of equidistant Gaussian wave packets with one-dimensional periodicity. One Gaussian with variance $a$ per unit cell of size $\ell$. For small overlap (top) the system behaves like one of distinguishable particles while for large overlap (bottom) the fermionic behaviour becomes manifest. For comparison, the spatial distribution of a uniform Fermi gas ($\sqrt{a}/\ell \to \infty$) is presented in panel (c) (dashed line) and the momentum distribution of distinguishable particles is presented in panel (d) (dotted line).

the wave packets seem uniform to the unit cell and the system behaves as plane waves in a periodic system. However, as we introduced periodic boundary conditions to eliminate surface effects, a successful investigation of bulk matter obviously requires that influences of the geometry of the chosen boundary conditions can be neglected. In Fig. 2 we show that this is achieved for a situation where 25 single-particle states are randomly distributed in the cell. The figure shows that the spatial and momentum distribution of the system reflects that of a free fermion system. The perturbations on the Fermi-sphere in momentum space, as well as those on the uniform distribution in coordinate space can be understood as a result of the local clustering. Hence, a simulation with the proposed periodic structure reproduces the intrinsic bulk fermion behaviour, independent of the imposed periodic structure. This result was hard to reach using QMD. For comparison, the bottom panels of Fig. 2 display the densities for distinguishable particles occupying the same wave packets. Both the spatial an momentum distribution are quite different from the indistinguishable fermion case. It clearly shows that antisymmetry induces Fermi motion and redistributes density in coordinate and momentum space. This long-range many-body correlation should not be ignored.

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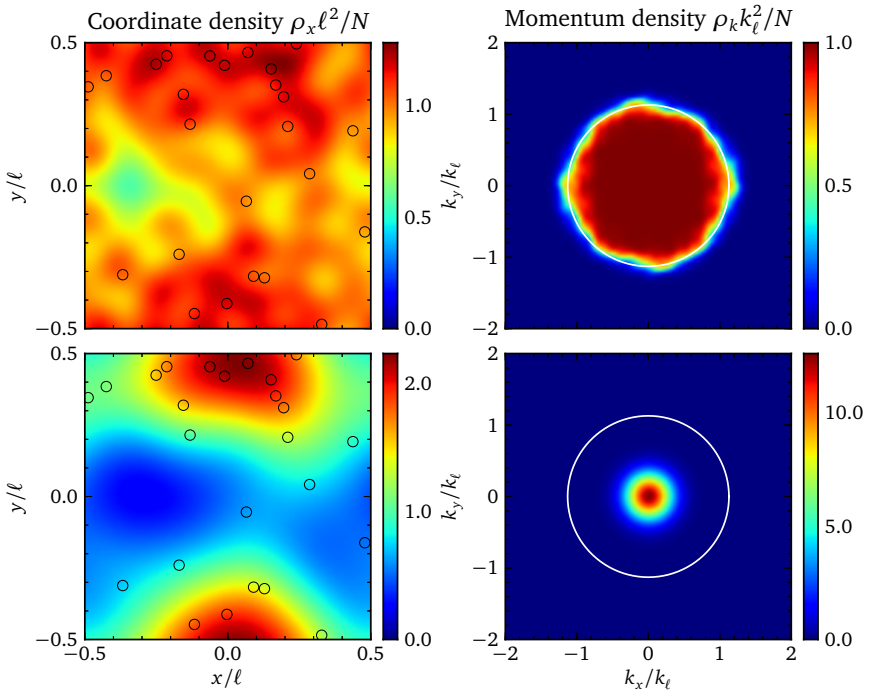


**Figure 2:** Spatial and momentum distribution of $N = 25$ Gaussian wave packets with periodic boundary conditions. The wave packets are randomly placed in the unit cell of a square lattice with unit length $\ell$ and have a variance given by $\sqrt{a} = 0.2\ell$. The mean momentum of the individual wave packets is set to zero. The densities are normalised and coordinates are expressed in units of $\ell$ or $k_\ell = \sqrt{N}\pi/\ell$. The upper two panels depict the antisymmetrised case. The lower two panels represent distinguishable particles. The black circles show the positions of the centroids of the wave packets. The white circle represents the Fermi "sphere" of a system of free particles with the same mean density, $k_F = \sqrt{4\pi N}/\ell$.

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