

METHODOLOGICAL NOTES PACS numbers: **26.60.–c**, 26.60.Gj, 31.15.bt, **64.10.+h**

On variational trial functions in extended Thomas–Fermi method

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DOI: https://doi.org/10.3367/UFNe.2024.11.039804

Contents

Abstract. Parametrized nucleon density distributions are widely employed for the calculation of the properties of atomic nuclei and dense inhomogeneous matter in compact stars within the Thomas–Fermi method and its extensions. We show that the use of insufficiently smooth parametrizations may deteriorate the accuracy of this method. We discuss and clarify the smoothness condition using the example of the so-called 'nuclear pasta' in the neutron star mantle.

Keywords: superdense matter, neutron star crust, Thomas–Fermi model, equation of state and phase equilibrium

1. Introduction

Thomas [1] and Fermi [2] suggested a statistical description of an atom with a large number of electrons. They used the local electron number density to calculate the potential energy and chemical potential of an electron in the self-consistent field of other electrons and the nucleus. Subsequently, the Thomas–Fermi (TF) method was refined by various corrections and applied for studying a large variety of many-body systems and dense matter (see, e.g., Refs [3–6] for reviews). We will focus on the extended Thomas–Fermi (ETF) theory, characterized by the inclusion of so-called gradient corrections, which are functions of density derivatives.

The first extension of the TF model was proposed by von Weizsäcker [7] for the description of heavy atomic nuclei. He introduced a gradient correction to the kinetic energy of a system of nucleons in order to capture the surface effect on the nuclear binding energy. Kompaneets and Pavlovskii [8] showed that the leading-order quantum correction to the TF model actually equals 1/9 of the von Weizsäcker gradient correction. Kirzhnits [9] introduced a regular perturbative method for the derivation of corrections in powers of gradient operator ∇ applied to an effective potential. Note that this approach leads to the appearance of quantum corrections for the energy E as well as for the number density n. Hodges [10] represented the Kirzhnits method in a more straightforward way, derived, for the first time, the correct explicit form of the corrections to power 4 in ∇, and showed that the quantum corrections to the density can be excluded from explicit consideration by writing the final expression for the energy in terms of the operator ∇ applied to the particle number density (see also [11, 12]).

The gradient corrections can be derived from the Wigner–Kirkwood expansion of the Bloch density matrix around its value obtained in the TF approximation in powers of the reduced Planck constant $\hbar$ (see, e.g., Refs [4, 5]). The lowest order terms of the ETF model reproduce the TF expressions, and the remaining expansion includes only even powers of $\hbar$. The lowest-order corrections ($\propto \hbar^2$) involve the terms with $(\nabla n)^2$ and $\nabla^2 n$. Going up to order $\hbar^4$ in the expansion, one obtains the next correction, containing up to the fourth derivatives of n.

Besides the gradient corrections, other refinements of the TF model include shell corrections, exchange and correlation effects [3, 5, 6], and a pairing interaction correction to describe many-nucleon systems [13]. In this context, Brack et al. [12, 14] developed a theory, named TEFT, which generalizes the ETF model to finite temperatures T.

It is worth saying more about the description of many-nucleon systems. Unlike plasma, consisting of electrons and atomic nuclei, which, under laboratory conditions can be considered as point particles interacting according to the Coulomb law, in many-nucleon systems the main role is played by strong interactions between nucleons having finite sizes and consisting of quarks. In a plasma, as a rule, the Born–Oppenheimer approximation is applicable, when the electron dynamics is calculated neglecting the motion of

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Received 27 June 2024, revised 7 November 2024
Uspekhi Fizicheskikh Nauk **195** (7) 738 – 746 (2025)
Translated by the authors

nuclei, whereas, in many-nucleon systems, protons and neutrons act as two equal kinds of particles. Moreover, in order to correctly describe the properties of relatively light nuclei, it is necessary to add a three-particle potential to the two-particle interaction potential determined from nucleon scattering experiments [15–17]. To theoretically describe the properties of heavier atomic nuclei and dense matter, as a rule, self-consistent field methods with phenomenological *effective* potentials of two-particle nucleon–nucleon interactions are used, designed in such a way as to simulate many-particle effects as well (see Ref. [18] for a review). The effective potentials that make it possible to reproduce the properties of atomic nuclei have a complex form. A well-known class of such potentials is the Skyrme potential [19] and its modifications (for example, [20]). Hartree–Fock equations with Skyrme interactions for spherical nuclei were first derived in Ref. [21]. They have the form of Schrödinger equations for single-particle wave functions, which include *effective masses* of nucleons M^* and self-consistent potentials depending on the particle number density, kinetic energy density, and spin-orbital density.

The nucleons in dense matter can form Cooper pairs and become superfluid. The most accurate self-consistent field method for such matter is Hartree–Fock–Bogoliubov (HFB) (see reviews [4, 18] and references therein). It can be used to describe heavy atomic nuclei (including neutron-rich nuclei in the outer crust of neutron stars). However, if nuclei, or rather nucleon clusters, are embedded in highly degenerate neutron matter (for instance, in the inner crust of neutron stars), the HFB method becomes too expensive. In such a case, the HFB method can be fairly accurately approximated using the computationally much faster ETF method with consistent shell and pairing corrections added perturbatively at the end of the ETF calculation [22–25] (see [26] for detailed comparisons with the HFB method).

A semi-phenomenological TF theory of atomic nuclei, which included a second-order gradient correction with an empirically adjusted coefficient, was developed by Bethe [27] (his paper also gives basic references to preceding models). Brack et al. [28] found that the fourth-order ETF theory does not need such empirical adjustment to reproduce the nuclear binding energies to within a few MeV, while the inaccuracy reached tens of MeV if only the second-order corrections were included. The modern ETF theory, which relies on accurately calibrated effective nucleon–nucleon interactions and includes Strutinsky shell corrections [29, 30] and pairing corrections [4, 13], allows one to reproduce all measured masses of heavy nuclei with typical errors of ~ 0.7 MeV (e.g., [31]; see Ref. [18] for a review and references).

In the following, we will consider applications of the ETF model to the exotic states of dense matter, where the nucleon clusters are not necessarily quasi-spherical but may also take the shapes of cylinders (dubbed 'spaghetti') and plates ('lasagna') [32, 33]. In addition to these 'pasta phases' with nucleon clusters immersed in a more dilute background of free nucleons (mainly neutrons) and electrons, 'inverse' pasta phases may exist with localized nucleon depletions in the dense matter [34], called 'anti-spaghetti' or 'bucatini' (inverted cylinders) and 'Swiss cheese' (inverted spheres) [35–37]. The pasta phases may be in thermodynamic equilibrium (the ground state) at mean nucleon number densities $\bar{n} \sim 0.05-0.08\ \mathrm{fm}^{-3}$. The nuclear pasta layers are called the mantle; they are located between the solid crust and the liquid core of a neutron star (see, e.g., [35, 36] and references therein). In terms of its elastic properties, the mantle is close to liquid crystals, as shown in Ref. [38] (see [39–41] for the current state of the theory of mantle elasticity).

The densities in the mantle are only 2–3 times lower than the nuclear saturation density n_{sat}, which corresponds to zero pressure in the model of uniform symmetric nuclear matter and is close to the typical number density of the nucleons in heavy atomic nuclei.[1]

The TF model and its refined versions are often combined with the Wigner–Seitz (WS) approximation [46, 47], which reduces the problem to the consideration of a single WS cell, replaced by an overall neutral sphere of the same volume (see Ref. [48] for a discussion of the limitations of this approximation). Analogously for the phase with cylindrical nuclei, an overall neutral cylinder is considered. In the case of plate-like nuclei, the true WS cell is a slab, so that a further geometrical simplification is unnecessary.

The ground state of dense matter corresponds to the minimum of energy $E = \int_V \mathcal{E}\,\mathrm{d}V$ for a given nucleon number $N \equiv \int_V (n_{\mathrm{p}} + n_{\mathrm{n}})\,\mathrm{d}V$ in volume V under the charge neutrality constraint $\int_V (n_{\mathrm{p}} - n_{\mathrm{e}})\,\mathrm{d}V = 0$, where n_{e}, n_{p}, and n_{n} are the local number densities of electrons, protons, and neutrons, respectively, and $\mathcal{E}$ is the energy density, which can be conventionally decomposed as

$$\mathcal{E} = \mathcal{E}_{\mathrm{nuc}} + \mathcal{E}_{\mathrm{e}} + \mathcal{E}_{\mathrm{Coul}} + \mathcal{E}_{\mathrm{cor}}\,. \tag{1}$$

Here, $\mathcal{E}_{\mathrm{nuc}}$ and $\mathcal{E}_{\mathrm{e}}$ are contributions from the nucleons and electrons, respectively, $\mathcal{E}_{\mathrm{Coul}}$ denotes energy density due to Coulomb interactions (beyond those already accounted for in $\mathcal{E}_{\mathrm{nuc}}$ and $\mathcal{E}_{\mathrm{e}}$), and $\mathcal{E}_{\mathrm{cor}}$ stands for various corrections which may appear in the refined theory, such as shell and pairing corrections. The nuclear energy density $\mathcal{E}_{\mathrm{nuc}}$ can be written in the nonrelativistic approximation as (e.g., Ref. [49])

$$\mathcal{E}_{\mathrm{nuc}} = \sum_q \frac{\hbar^2}{2M_q^*}\,\tau_q + \mathcal{V}\,, \tag{2}$$

where M_q^* is a density-dependent effective mass of a nucleon of type q ($q = \mathrm{n}$ for neutrons and $q = \mathrm{p}$ for protons), τ_q is the normalized kinetic energy of a nucleon generated by the momentum square operator in the Hamiltonian, and $\mathcal{V}$ stands for the sum of potential-energy terms. In the ETF model, both terms in (2) depend on local number densities $n_q(\mathbf{r})$, their gradients $\nabla n_q(\mathbf{r})$, and spin current densities $\mathbf{J}_q(\mathbf{r})$ with coefficients determined by an employed realization of the Skyrme-type potential. The gradient expansion enables one to express $\tau_q(\mathbf{r})$ and $\mathbf{J}_q(\mathbf{r})$ (and therefore $\mathcal{E}_{\mathrm{nuc}}$) as functions entirely of the nucleon densities $n_q(\mathbf{r})$ and their derivatives [49].

The energy minimum can be found by solving the corresponding Euler–Lagrange (EL) equations. For example, Barkat et al. [50] numerically solved the EL equations derived from the semi-phenomenological theory of Bethe [27]. Later, the EL equations were solved by different authors in the TF and ETF models for finite nuclei [51–53] and nuclear matter [51, 54, 55] using the so-called imaginary time-step method [56]. However, the fourth-order ETF theory, when

[1] Estimates of the saturation density vary from $0.14\ \mathrm{fm}^{-3}$ [4] to $0.17\ \mathrm{fm}^{-3}$ [42, 43]. The value $n_{\mathrm{sat}} = 0.16\ \mathrm{fm}^{-3}$ is most often quoted, based on a study by Tondeur et al. [44]. Recent experimental results suggest $n_{\mathrm{sat}} = 0.15 \pm 0.01\ \mathrm{fm}^{-3}$ [45].

used in conjunction with Skyrme forces (see, e.g., Ref. [18] and references therein), leads to complex, highly nonlinear EL equations for the particle densities, which are difficult to solve exactly [53, 57]. To avoid these difficulties and speed up computations, the ETF energy functional is most often minimized explicitly within a family of *parametrized* nucleon density profiles $n_{\rm n}(\mathbf{r})$ and $n_{\rm p}(\mathbf{r})$ (examples will be given below). This *restricted variational method* drastically simplifies and accelerates calculations. At the same time, it can be very accurate, as was demonstrated by Bartel et al. [57].

The ETF method is subject to different kinds of divergences. Being based on expansions in powers of $\hbar$ around the classical values, the gradient corrections can only be calculated inside the classically allowed region of particle motion. In the case of finite or semi-infinite classical orbits, the semiclassical expansions of the number density $n(\mathbf{r})$ and kinetic energy density $\tau(\mathbf{r})$ are not defined at the classical turning points and beyond, and they diverge near such points. However, this is not a problem, because such divergences are integrable and allow one to obtain nondiverging expressions of the gradient corrections to τ as functions of n [11, 12, 49]. Thus, the ETF number densities can be understood as generalized distributions with well-defined integrals and moments [4, 12]. It is also of interest that a nonzero temperature in the TEFT model removes the divergence of the ETF densities and allows their extension to the classically forbidden regions [14].

Other divergences are related to the asymptotic nature of the gradient expansion. The sixth- and higher-order gradient terms diverge for densities which fall exponentially to zero as functions of $\mathbf{r}$, and must therefore be left out [12, 14], at least in calculations of the properties of isolated atoms or nuclei. Thus, only the terms up to the fourth order constitute the converging part of the ETF expansion.

However, this part can still diverge within the restricted variational method if the trial density distributions $n_q(\mathbf{r})$ are not sufficiently smooth. The goal of the present paper is to clarify the smoothness conditions for the applicability of this method to the fourth-order ETF theory in spherical, cylindrical, and plane-parallel WS cells.

In Section 2, we recall the basic ETF expressions for the kinetic energy of nucleons. In Section 3, we review the most common parametrizations of the local density of nucleons which were employed in the variational calculations of the atomic nuclei and non-uniform matter in the crust and mantle of neutron stars. In Section 4, we discuss the divergences of the ETF energy functionals for different kinds of kinks of the parametrized density distribution. In Section 5, we derive an associated accuracy limit for numerical discrete-mesh ETF calculations. In Section 6, conclusions are summarized.

2. Extended Thomas–Fermi energy density

The nuclear energy in volume V is given by the integral

$$E_{\rm nuc} = \int_V \mathcal{E}_{\rm nuc}\,{\rm d}V, \tag{3}$$

where $\mathcal{E}_{\rm nuc}$ is given by Eqn (2). The kinetic energy contribution in Eqn (3) can be written as

$$\mathcal{T}_q = \int_V \frac{\hbar^2}{2M_q^*}\,\tau_q\,{\rm d}V, \quad \tau_q = \tau_q^{(0)} + \tau_q^{(2)} + \tau_q^{(4)}, \tag{4}$$

where $\tau_q^{(0)}$ is the TF contribution, while $\tau_q^{(2)}$ and $\tau_q^{(4)}$ are the second and fourth order gradient corrections, respectively.

For simplicity, let us disregard the difference between the effective mass M_q^* and the bare nucleon mass M_q and omit the spin-orbit terms. Then, in the zero temperature limit [11, 28],

$$\tau_q^{(0)} = \frac{3}{5}\,(3\pi^2)^{2/3}\,n_q^{5/3}, \tag{5}$$

$$\tau_q^{(2)} = \frac{1}{3}\,\nabla^2 n_q + \frac{1}{36}\,\frac{(\nabla n_q)^2}{n_q}, \tag{6}$$

$$\begin{aligned}\tau_q^{(4)} = {}& \frac{n_q^{1/3}}{(3\pi^2)^{2/3}}\left\{\frac{1}{180}\,\frac{\nabla^4 n_q}{n_q} - \frac{1}{72}\,\frac{\nabla n_q\,\nabla(\nabla^2 n_q)}{n_q^2}\right.\\ & - \frac{7}{1080}\,\frac{(\nabla^2 n_q)^2}{n_q^2} - \frac{7}{2160}\,\frac{\nabla^2(\nabla n_q)^2}{n_q^2} + \frac{7}{324}\,\frac{(\nabla n_q)^2\nabla^2 n_q}{n_q^3}\\ & \left. + \frac{23}{810}\,\frac{(\nabla n_q\,\nabla)^2\,n_q}{n_q^3} - \frac{1}{45}\,\frac{(\nabla n_q)^4}{n_q^4}\right\}.\end{aligned} \tag{7}$$

The fourth and third derivatives of $n_q(\mathbf{r})$ can be eliminated from $E_{\rm nuc}$ by partial integration with the use of the Ostrogradsky–Gauss theorem [10, 12]. For example, the second term in Eqn (7) can be transformed as follows:

$$\begin{aligned}\int_V \phi\nabla n_q\,\nabla(\nabla^2 n_q)\,{\rm d}V &= \int_V \left\{\nabla\left[(\phi\,\nabla^2 n_q)\nabla n_q\right]\right.\\ &\quad \left. - \frac{{\rm d}\phi}{{\rm d}n_q}\,(\nabla n_q)^2\,\nabla^2 n_q - \phi\,(\nabla^2 n_q)^2\right\}{\rm d}V\\ &= \oint_S (\phi\,\nabla^2 n_q)\nabla n_q\,\mathbf{n}\,{\rm d}S\\ &\quad - \int_V \left[\frac{{\rm d}\phi}{{\rm d}n_q}\,(\nabla n_q)^2\,\nabla^2 n_q + \phi\,(\nabla^2 n_q)^2\right]{\rm d}V,\end{aligned} \tag{8}$$

where $\mathbf{n}$ is the outer normal to the surface S of the considered domain V, and we have denoted $\phi \equiv -(1/72)(3\pi^2)^{-2/3} n_q^{-5/3}$ for brevity. This method gives

$$\mathcal{T}_q^{(4)} \equiv \frac{\hbar^2}{2M_q}\int_V \tau_q^{(4)}(\mathbf{r})\,{\rm d}V = \mathcal{T}_{q,{\rm v}}^{(4)} + \mathcal{T}_{q,{\rm s}}^{(4)}, \tag{9}$$

where $\mathcal{T}_{q,{\rm v}}^{(4)}$ and $\mathcal{T}_{q,{\rm s}}^{(4)}$ can be written as

$$\mathcal{T}_{q,{\rm v}}^{(4)} \equiv \frac{\hbar^2}{2M_q}\int_V \tau_{q,{\rm v}}^{(4)}(\mathbf{r})\,{\rm d}V, \quad \mathcal{T}_{q,{\rm s}}^{(4)} \equiv \frac{\hbar^2}{2M_q}\oint_S \tau_{q,{\rm s}}^{(4)}(\mathbf{r})\,{\rm d}S, \tag{10}$$

and $\tau_{q,{\rm v}}^{(4)}(\mathbf{r})$ includes only first- and second-order derivatives of number density. Its explicit form is [49]

$$\begin{aligned}\tau_{q,{\rm v}}^{(4)} = {}& \frac{n_q^{1/3}}{(3\pi^2)^{2/3}}\left\{\frac{1}{270}\left(\frac{\nabla^2 n_q}{n_q}\right)^2 - \frac{1}{240}\,\frac{\nabla^2 n_q}{n_q}\left(\frac{\nabla n_q}{n_q}\right)^2\right.\\ & \left. + \frac{1}{810}\left(\frac{\nabla n_q}{n_q}\right)^4\right\},\end{aligned} \tag{11}$$

which is equivalent to Eqn (30) of Hodges [10]. Usually, one assumes $\mathcal{T}_{q,{\rm s}}^{(4)} = 0$, so that $\tau_q^{(4)}$ can be replaced by $\tau_{q,{\rm v}}^{(4)}$ in Eqn (4). To this end, Hodges [10] and Brack et al. [12] integrated over the whole space, considering in the context of an isolated atomic nucleus in a vacuum that $n_q(\mathbf{r})$ vanishes at $r \to \infty$ together with its derivatives. In the WS approximation, one can drop the surface term $\mathcal{T}_{q,{\rm s}}^{(4)}$, for example, under the condition that the normal density derivative to the WS cell

surface S equals zero:[2]

$$\mathbf{n}\cdot\nabla n_q(\mathbf{r})\Big|_{\mathbf{r}\in S}=0\,. \tag{12}$$

An analogous boundary condition was used by Wigner and Seitz [46] for electron wave functions; it naturally follows from the symmetry and periodicity of $n_q(\mathbf{r})$ under the assumption that ∇n_q is continuous.

The continuity of ∇n_q was previously shown for the density distributions that provide the exact minimum of $E_{\rm nuc}$ within the fully variational Euler–Lagrange approach [50]. We will see that the same continuity may be also required for parametrized nucleon density distributions within the restricted variational approach in order to ensure convergence of the volume integral in Eqn (3).

3. Parametrizations of nucleon density distributions

When matter is strongly compressed so that the mean nucleon number density $\bar{n}\equiv N/V$ exceeds the neutron-drip density $n_{\rm drip}\sim(2-3)\times10^{-4}$ fm^{-3}, neutrons start to drip out of nuclei. Such huge densities occur in the inner crust of neutron stars, where the nuclei are immersed in a 'sea' of unbound neutrons. One of the most microscopic and tractable methods of describing such dense matter so far is the ETF theory with shell corrections for the protons (which remain bound in the nuclei) and with pairing corrections.

We will consider spherical, cylindrical, and slab-like WS cells and assume that n_q is symmetric with respect to the rotations around the center of the sphere or the axis of the cylinder, or to the reflection with respect to the central plane of the slab. This means that the density n_q depends only on radial coordinate r or $r_\perp$ in the first and second cases, respectively, and only on $|z|$ in the third case, where z is the coordinate measured in the normal direction from the central plane of the cell. The phases with spherical, cylindrical, and plane-parallel symmetry are often called three-, two-, and one-dimensional (3D, 2D, and 1D) structures, respectively. However, one should keep in mind that such notation concerns only the type of symmetry of the density distribution, whereas the motion of particles (electrons and nucleons) remains three-dimensional. Such '2D' and '1D' structures should not be confused with true 2D and 1D systems, which were considered, e.g., in Ref. [6] and which are described by the ETF equations that differ from Eqns (5)–(7), and (11).

It is convenient to write a symmetric parametrization of the density distribution in a WS cell in the form

$$n_q(\xi)=n_q^{\rm out}+n_{\Lambda q}\hat{f}_q(\xi)\,, \tag{13}$$

$$\hat{f}_q(\xi)\equiv\frac{f_q(\xi)-f_q(R)}{f_q(0)-f_q(R)}\,, \tag{14}$$

where ξ is the radial coordinate for a spherical or cylindrical cell of radius R, or the distance from the central plane of a slab of half-size R ($\xi=r$, $r_\perp$, or $|z|$ for the three respective cases). The function $f_q(\xi)$ describes the shape of the density profile, which can depend on adjustable parameters, and $\hat{f}_q(\xi)$ is the normalized density profile, so that the parameter $n_q^{\rm out}$ has the meaning of nucleon density outside the 'nuclei' (the nucleonic clusters), and more generally at the cell boundary. In the bulk of the inner crust, free protons are absent and the nucleons are clustered near the center of the WS cell; in this case, $n_{\rm p}^{\rm out}=0$. However, free protons may appear near the transition to the core of the star [58]. We assume $f_q(0)>f_q(R)\geqslant0$, while $n_{\Lambda q}$ can be positive for the normal phases or negative for the inverse phases. Accordingly, $n_{\Lambda q}=n_q^{\rm cen}-n_q^{\rm out}$ is the central number density excess, $n_q^{\rm cen}$ being the density at the center of the cell. Hereafter, we will mark different parametrizations of $f_q(\xi)$ by abbreviations in superscripts.

Oyamatsu [59] studied nuclear shapes in the neutron star mantle using the Bethe theory [27] and assuming the shapes of neutron and proton number density distributions in the form

$$f_q^{\rm O}(\xi)=\begin{cases}\left[1-\left(\dfrac{\xi}{r_q}\right)^{t_q}\right]^3\,, & \xi<r_q\,,\\ 0\,, & \xi\geqslant r_q\,.\end{cases} \tag{15}$$

An analogous parametrization, but with $t_{\rm n}=t_{\rm p}$, $r_{\rm n}=r_{\rm p}$, and with the power index 2 instead of 3, was previously introduced by Arponen [60]. Parameters t_q control the sharpness of the local density profiles, while r_q determine the neutron and proton radii of a nucleus ($0<r_q<R$). In this case, $\hat{f}_q^{\rm O}(\xi)=f_q^{\rm O}(\xi)$. With increasing density $\bar{n}$, the profiles become smoother, approaching the limit of uniform matter; therefore, the parameters t_q decrease.

Parametrization (15) was widely used in TF and second-order ETF calculations [61–64]. However, real local density distributions of neutrons and protons in a neutron star crust are not cut off at a certain distance from the center of a WS cell. Therefore, $r_{\rm n}$ and $r_{\rm p}$ can be treated only as convenient fit parameters. Near the bottom of the crust, the local density distribution is rather smooth, and the boundary between the free and bound neutrons becomes rather uncertain. More importantly, this parametrization leads to divergences for the fourth-order ETF energy.

In a number of applications of the ETF methods to finite nuclei (with $n_q^{\rm out}=0$; e.g., [65]) and neutron-star mantles (e.g., [49, 66]), the simple Fermi-function form (also known as the Woods–Saxon shape [61, 67]) was adopted, which can be written as

$$f_q^{\rm F}(\xi)=\frac{1}{1+\exp\left[(\xi-r_q)/a_q\right]}\,, \tag{16}$$

where r_q is the half-height nuclear radius and a_q accounts for the diffuseness of the nuclear surface. This parametrization was criticized on the grounds that it cannot capture the asymmetry of nucleon density profiles on the surface of a nucleus [54]. To overcome this constraint, a modification of Eqn (16) was used in a number of ETF calculations [68–71],

$$f_q^{\rm MF}(\xi)=\frac{1}{\left\{1+\exp\left[(\xi-r_q)/a_q\right]\right\}^{v_q}}\,, \tag{17}$$

where the power index v_q is an additional fit parameter. A still more general modification, which allows additional enhancement or depression of the nucleon density at the center of the WS cell, was considered in Refs [12, 72], but the minimized energy was found to be insensitive to such an additional degree of freedom. Meanwhile, an increase in the power index v_q from 1 to 3 decreases the calculated energy in a heavy

[2] For instance, Onsi et al. [49] stressed: "it should be noted that the fourth-order expressions are valid only on integrating over the whole of space, or more generally, over a region on the surface of which the density gradients vanish."

nucleus by ~ 8 MeV [72], although it does not substantially change the results for the inner crust and mantle of a neutron star [71].

It is easy to see that neither f_q^{F} nor f_q^{MF} can provide trial functions $n_q(\mathbf{r})$ satisfying condition (12). Below, we will consider other modifications of Fermi-like parametrization (16), which can be written in the generic form

$$f_q(\xi) = \frac{1}{1 + h(\xi; r_q, a_q) \exp\left[(\xi - r_q)/a_q\right]} \,. \tag{18}$$

The first example of such parametrization with

$$h^{\mathrm{DF}}(\xi; r_q, a_q) = \exp\left[\left(\frac{r_q - R}{\xi - R}\right)^2 - 1\right] \tag{19}$$

was introduced by Onsi et al. [22]. The resulting 'damped Fermi parametrization' $f_q^{\mathrm{DF}}(\xi)$, which has *all* derivatives vanishing at $\xi = R$, was consistently used for trial density profiles in calculations of the properties of the neutron-star inner crust and mantle by the Brussels–Montreal group (e.g., Ref. [73] and references therein).

Density profiles $n_q(\mathbf{r})$ parametrized with the shape forms $f_q^{\mathrm{F}}(\xi)$, $f_q^{\mathrm{MF}}(\xi)$, and $f_q^{\mathrm{DF}}(\xi)$ do not have well-defined gradients at the centers of the WS cells. This fact is often neglected by considering only the interval $\xi \in (0, R]$ without including the origin. The gradient corrections can be defined in the entire WS cell if $n_q(\mathbf{r})$ is treated as a generalized distribution or is meant to be locally smoothed in a negligibly small neighborhood of the center [74]. Nevertheless, such parametrizations can cause potential problems, discussed in the next sections. Furthermore, in the case of the 'lasagna' phase, the nonzero derivative of $n_q(z)$ at $z \to 0$ hampers the aforementioned replacement of $\tau_q^{(4)'}$ by $\tau_{q,\mathrm{v}}^{(4)}$ in Eqn (4), because $\mathcal{T}_{q,\mathrm{s}}^{(4)}$ does not vanish on the surface $z = 0$.

In the same ('lasagna') case, there was also a symmetry argument disfavoring parametrization (19). Unlike the distinction between the normal quasi-spherical nuclei and 'Swiss cheese' or between 'spaghetti' and 'anti-spaghetti' phases, there is no physical distinction between 'lasagna' and 'anti-lasagna': a configuration with a maximum at the center of the WS cell can be transformed into a configuration with a minimum at the center by simple translation of the coordinate system. In practice, distinct 'lasagna' and 'anti-lasagna' parametrizations can give very close energy minima producing a spurious instability of a numerical minimization procedure. To avoid it, both 'lasagna' and 'anti-lasagna' should be described equally well by the chosen parametrization, meaning that, for any profile $n_q(\xi)$ determined by a parameter set $\boldsymbol{\chi}$, there should exist a set of parameters $\boldsymbol{\chi}'$ such that the inverted profile $n_q(R - \xi)$ obtained from a space inversion followed by a translation is also allowed [75]:[3]

$$\forall \boldsymbol{\chi}\ \exists \boldsymbol{\chi}' \colon \quad n_q(\xi, \boldsymbol{\chi}) = n_q(R - \xi, \boldsymbol{\chi}') \,. \tag{20}$$

If $n_q(\xi, \boldsymbol{\chi})$ satisfies condition (12) for any $\boldsymbol{\chi}$, then condition (20) ensures that $\mathrm{d}n_q/\mathrm{d}\xi \to 0$ at $\xi \to 0$, so that the gradient of the trial density distribution does exist and equals zero at the WS cell center.

Parametrizations of the form (18) are symmetric with respect to 'lasagna' and 'anti-lasagna' configurations, provided

$$h(\xi; r_q, a_q) = \frac{1}{h(R - \xi; R - r_q, a_q)} \,. \tag{21}$$

Constraint (20) is then satisfied with $n'_{\Lambda q} = -n_{\Lambda q}$, $n_q^{\mathrm{out}\prime} = n_q^{\mathrm{out}} + n_{\Lambda q}$, $a'_q = a_q$, and $r'_q = R - r_q$.

The particular form $h^{\mathrm{DF}}(\xi; r_q, a_q)$ in Eqn (19) does not satisfy condition (21). A straightforward generalization to fulfill this condition reads

$$h^{\mathrm{2DF}}(\xi; r_q, a_q) = \exp\left[\left(\frac{r_q - R}{\xi - R}\right)^2 - \left(\frac{r_q}{\xi}\right)^2\right] . \tag{22}$$

In particular, it ensures that all derivatives of $n_q(\mathbf{r})$ vanish not only at the boundary, but also at the center of the WS cell. However, a comparison of the ETF calculations with different density profile parametrizations [75] indicates that even the one-sided 'strong damping' defined by Eqn (19), let alone the two-sided damping in Eqn (22), is too restrictive, because a noticeably lower minimum of E can be obtained with a weaker ('soft') damping, defined by

$$h^{\mathrm{WDF}}(\xi; r_q, a_q) = \left(\frac{r_q - R}{r_q}\right)^2 \left(\frac{\xi}{\xi - R}\right)^2 . \tag{23}$$

The corresponding density profile not only satisfies condition (12) but also has a zero gradient at the center of the WS cell. Meanwhile, higher-order density derivatives do not vanish at the WS cell center or boundary.

In the next section, we will show that the parametrizations, which do not have the zero gradient at $\xi = 0$, lead to a divergence of the ETF energy functional E in the cylindrical and plane-parallel symmetries.

4. Divergences of nonsmooth parametrizations

4.1 Symmetric parametrizations in pasta phases

Let us assume that $f_q(\xi)$ is finite and differentiable at $\xi > 0$. We can then write

$$n_q(\mathbf{r}) = n_{q0} + n'_{q0}\, \xi + O(\xi^2) \,, \tag{24}$$

where $n_{q0} = n_q^{\mathrm{out}} + n_{\Lambda q}$ and

$$n'_{q0} = n_{\Lambda q} \left.\frac{\mathrm{d}\hat{f}_q(\xi)}{\mathrm{d}\xi}\right|_{\xi \to +0} .$$

If $n'_{q0} \neq 0$, then the distribution n_q has a kink at the center of the cell, and ∇n_q is not well defined at this point.

Let us evaluate a contribution to integral (4) from the first term on the right-hand side of Eqn (11),

$$\tau_{q,\mathrm{v}}^{(4a)} = \frac{\hbar^2}{2M_q} \frac{n_q^{1/3}}{(3\pi^2)^{2/3}} \frac{1}{270} \left(\frac{\nabla^2 n_q}{n_q}\right)^2 \propto n_q^{1/3} \left(\frac{\nabla^2 n_q}{n_q}\right)^2 , \tag{25}$$

in a small neighborhood $\xi < \varepsilon$ of the center of the cell (V_ε). In the case of cylindrical or plane-parallel symmetry, we will consider WS cells of finite volume V, respectively cylinders of unit length and slabs of unit area. The volume of the ε-neighborhood of their center will be denoted by V_ε. For the plane-parallel, cylindrical, or spherical symmetry, $\nabla^2 n_q = \xi^{1-D}\, (\partial/\partial\xi)(\xi^{D-1} \partial n_q/\partial\xi)$, where $D = 1$, 2, or 3, respectively.

[3] Alternatively, one can avoid the lasagna-anti-lasagna distinction by imposing the condition $n_{\Lambda q} > 0$.

In the case of spherical symmetry, Eqn (24) gives

$$\int_{V_\varepsilon} n_q^{1/3}\left(\frac{\nabla^2 n_q}{n_q}\right)^2 \mathrm{d}V = 4\pi\int_0^\varepsilon n_q^{-5/3}(\nabla^2 n_q)^2 r^2\,\mathrm{d}r = 16\pi\, n_{q0}^{-5/3}\,(n'_{q0})^2\,\varepsilon + O(\varepsilon^2)\,. \tag{26}$$

Here, the right-hand side tends to zero at $\varepsilon \to 0$. Therefore the kink at $r = 0$ can be safely isolated by removing a sphere of sufficiently small radius ε around the center without an appreciable effect on integral (4).

In the case of cylindrical symmetry,

$$\int_{V_\varepsilon} n_q^{1/3}\left(\frac{\nabla^2 n_q}{n_q}\right)^2 \mathrm{d}V = 2\pi\int_0^\varepsilon n_q^{-5/3}(\nabla^2 n_q)^2 r_\perp\,\mathrm{d}r_\perp = 2\pi n_{q0}^{-5/3}\,(n'_{q0})^2\int_0^\varepsilon \frac{\mathrm{d}r_\perp}{r_\perp} + O(\varepsilon)\,. \tag{27}$$

The last integral diverges. Therefore, the contribution of this gradient correction to E_{nuc} is infinite, unless $n'_{q0} = 0$. This result shows that the energy of a cylindrical WS cell (per unit length of the cylinder), calculated according to the ETF theory, can be made finite only by such a density distribution $n_q(r_\perp)$ in which

$$\lim_{r_\perp \to 0}\frac{\mathrm{d}n_q}{\mathrm{d}r_\perp} = 0\,. \tag{28}$$

For plane-parallel WS cells, we have $\xi = |z|$. Taking into account that $\mathrm{d}|z|/\mathrm{d}z = 2\theta(z) - 1$, where $\theta(z)$ is the Heaviside step function, and $\mathrm{d}\theta(z)/\mathrm{d}z = \delta(z)$, where $\delta(z)$ is the Dirac delta function, we obtain $\nabla^2 n_q = 2n'_{q0}\,\delta(z) + O(1)$. Now,

$$\int_{V_\varepsilon} n_q^{1/3}\left(\frac{\nabla^2 n_q}{n_q}\right)^2 \mathrm{d}V = \frac{(2n'_{q0})^2}{n_{q0}^{5/3}}\int_{-\varepsilon}^{\varepsilon}\left[\delta(z)\right]^2\mathrm{d}z + O(1)\,. \tag{29}$$

Since the squared delta function is not integrable, the integral is finite only if $n'_{q0} = 0$, that is

$$\lim_{z\to 0}\frac{\mathrm{d}n_q}{\mathrm{d}z} = 0\,. \tag{30}$$

4.2 Continuity across a surface

Condition (30) can be generalized. Let us consider a continuous distribution $n_q(\mathbf{r})$ which has a kink (i.e., a discontinuous first derivative) at the plane $z = 0$: $n_q(\mathbf{r}) = n_{q0}(x,y) + n'_+(x,y)\,z + O(z^2)$ at $z > 0$ and $n_q(\mathbf{r}) = n_{q0}(x,y) + n'_-(x,y)\,z + O(z^2)$ at $z < 0$. It can be written as

$$n_q(\mathbf{r}) = n_{q0}(x,y) + \frac{n'_+(x,y) + n'_-(x,y)}{2}\,z + \frac{n'_+(x,y) - n'_-(x,y)}{2}\,|z| + O(z^2)\,. \tag{31}$$

By analogy with Eqn (29), a contribution of the term containing $|z|$ to the integral of $\tau_q^{(4a)}$ over an ε-neighborhood $V_\varepsilon = \Delta S \otimes [-\varepsilon, \varepsilon]$ of any finite element ΔS of the plane $z = 0$ (for example, parallelepiped $V_\varepsilon = \{x, y, z : |x| < \Delta x, |y| < \Delta y, |z| < \varepsilon\}$) is proportional to

$$\int_{V_\varepsilon} n_q^{1/3}\left(\frac{\nabla^2 n_q}{n_q}\right)^2 \mathrm{d}V = A_{\Delta S}\int_{-\varepsilon}^{\varepsilon}\left[\delta(z)\right]^2\mathrm{d}z + O(1)\,, \tag{32}$$

where

$$A_{\Delta S} = \int_{\Delta S}\frac{\left[n'_+(x,y) - n'_-(x,y)\right]^2}{n_{q0}^{5/3}(x,y)}\,\mathrm{d}S\,. \tag{33}$$

If $A_{\Delta S} \neq 0$, integral (32) diverges. Since the surface element ΔS is arbitrary, the divergence can be excluded only if $n'_+(x,y) \equiv n'_-(x,y)$, except possibly a zero-measure submanifold of points (x,y). This means the absence of a kink across the plane.

If $n_q(\mathbf{r})$ has a kink on a smooth surface, which is not plane, one can approximate a sufficiently small area around an arbitrary point on this surface by the tangent plane and apply the above considerations to prove the divergence. Thus, we conclude that $n_q(\mathbf{r})$ should not have a kink on a smooth surface. As a particular case, it should not have a kink on the WS cell boundary, if instead of spheres and cylinders one considers the true polyhedral WS cells filling the space and minimizes E in two or more adjacent cells together. Assuming that $n_q(\mathbf{r})$ is symmetric and periodic, this leads to Eqn (12).

Although we have considered only one term in Eqn (11), obtained with the use of the Ostrogradsky–Gauss theorem, the drawn conclusions are general and do not assume fulfillment of condition (12) in advance. Indeed, we can isolate a kink location by a surface, across which $n_q(\mathbf{r})$ is smooth, and apply this theorem only to the contribution to integral (9) from the domain surrounded by this surface. Then, the volume integral of $\tau_{q,\mathrm{v}}^{(4)}$ over the considered domain contains the above-discussed divergence, whereas the corresponding surface integral is finite and cannot cancel it. Moreover, the third term in the original expression (7), being proportional to $\tau_q^{(4a)}$ (25), contains the same divergence.

5. Accuracy limit for nonsmooth parametrizations

One can try to circumvent the smoothness conditions, such as Eqn (28) or Eqn (30), by introducing a local modification of $n_q(\mathbf{r})$ in a small neighborhood V_ε around the origin, so that the modified trial density distribution $\tilde{n}_q(\mathbf{r})$ coincides with $n_q(\mathbf{r})$ outside V_ε and has a continuous gradient everywhere. Since ε is small and $\tilde{n}_q$ is symmetric and differentiable, we have $\tilde{n}_q|_{\xi\leqslant\varepsilon} = n_{q0} + O(\varepsilon)$ and $\nabla\tilde{n}_q|_{\xi=\varepsilon}\cdot\mathbf{n}_\varepsilon = n'_{q0} + O(\varepsilon)$, where $\mathbf{n}_\varepsilon$ is the outer normal to the surface of V_ε, which we denote S_ε. Then, the average of $\nabla^2\tilde{n}_q$ in V_ε equals

$$\left\langle\nabla^2\tilde{n}_q\right\rangle \equiv \frac{1}{||V_\varepsilon||}\int_{V_\varepsilon}\nabla^2\tilde{n}_q\,\mathrm{d}V = \oint_{S_\varepsilon}\nabla\tilde{n}_q\Big|_{\xi=\varepsilon}\cdot\mathbf{n}_\varepsilon\,\frac{\mathrm{d}S}{||V_\varepsilon||} = \left[n'_{q0} + O(\varepsilon)\right]\frac{||S_\varepsilon||}{||V_\varepsilon||} = \frac{n'_{q0}D}{\varepsilon} + O(1)\,, \tag{34}$$

where $||V_\varepsilon|| = ||S_\varepsilon||\,\varepsilon/D = \pi^{D/2}\,\varepsilon^D/\Gamma(D/2+1)$ and the angle brackets denote the averaging. Assuming that $n_{q0} \neq 0$ and using the inequality $\langle x^2\rangle \geqslant \langle x\rangle^2$, we obtain

$$\int_{V_\varepsilon}\frac{(\nabla^2\tilde{n}_q)^2}{\tilde{n}_q^{5/3}}\,\mathrm{d}V \approx \frac{||V_\varepsilon||}{n_{q0}^{5/3}}\left\langle(\nabla^2\tilde{n}_q)^2\right\rangle \geqslant \frac{||V_\varepsilon||}{n_{q0}^{5/3}}\left\langle\nabla^2\tilde{n}_q\right\rangle^2 \approx \frac{D^2||V_\varepsilon||}{\varepsilon^2 n_{q0}^{5/3}}\,|n'_{q0}|^2\,, \tag{35}$$

where the approximate equality implies an accuracy up to the factor of $1 + O(\varepsilon)$. Thus, in the limit of small ε, the leading contribution of the integral of $\tau_q^{(4)}$ over V_ε to the kinetic

energy correction $\mathcal{T}_q^{(4)}$ can be bounded from below as

$$\mathcal{T}_{q,\varepsilon}^{(4a)} \equiv \int_{V_\varepsilon} \tau_q^{(4a)}\, \mathrm{d}V \gtrsim \frac{\hbar^2}{540 M_q} \frac{D^2 ||V_\varepsilon||}{(3\pi^2)^{2/3}} \frac{|n'_{q0}|^2}{\varepsilon^2 n_{q0}^{5/3}}\,. \tag{36}$$

When considering a WS cell fragment in the 'lasagna' phase ($D = 1$), Eqn (36) leads to the following inequality for the contribution of the kink to the kinetic energy per nucleon:

$$\frac{\mathcal{T}_{q,\varepsilon}^{(4a)}}{N} \gtrsim \frac{\hbar^2}{540 M_q} \frac{1}{(3\pi^2)^{2/3}} \frac{n_{q0}^{1/3}}{\bar{n} R} \left(\frac{n'_{q0}}{n_{q0}}\right)^2 \varepsilon^{-1}\,. \tag{37}$$

The right-hand side of Eqn (37) tends to infinity at $\varepsilon \to 0$, unless $n'_{q0} = 0$. Thus, the accuracy of a discrete-mesh calculation of the fourth-order ETF energy has a fundamental limit for nonsmooth trial functions, because the mesh cannot be arbitrarily refined: the smaller the interval $(-\varepsilon, \varepsilon)$ over which the smoothing is performed, the larger its contribution.

For example, the pasta phases were studied in Ref. [74] using the BSk24 nuclear energy-density functional with the damped Fermi (DF) parametrization, defined by Eqns (18) and (19). The 'lasagna' phase was found to exist in the density range $\bar{n} \sim 0.07-0.08$ fm^{-3}. In this range, the optimal variational parameters were, respectively, $R \approx 13.7$–13.0 fm, $r_\mathrm{p} \approx 4.7-6.6$ fm, $r_\mathrm{n} - r_\mathrm{p} \sim 0.5$ fm, $a_{\mathrm{n,p}} \approx 1.0-1.3$ fm, $n_{\Lambda\mathrm{n}} \approx 0.028-0.019$ fm^{-3}, $n_\mathrm{n}^\mathrm{out} \approx 0.058-0.065$ fm^{-3}, and $n_{\Lambda\mathrm{p}} \approx 0.007-0.005$ fm^{-3}. For such values, Eqns (13), (14), (18), (19), and (37) give $(\mathcal{T}_{\mathrm{n},\varepsilon}^{(4a)} + \mathcal{T}_{\mathrm{p},\varepsilon}^{(4a)})/N \gtrsim 0.034$–$0.007\,\mathrm{eV\ fm}/\varepsilon$. In the considered density range, energies of different pasta phases differ typically by a few hundreds of eV per nucleon. Therefore, the accuracy limitation would be essential when performing numerical integration of the ETF equations with steps $\varepsilon \lesssim 10^{-3}$ fm. In fact, a much coarser mesh was used in Ref. [74], which provided practical imperceptibility of the results of that study to the accuracy limit (37).

6. Conclusions

We considered the smoothness conditions on trial density distribution $n_q(\mathbf{r})$ for the applicability of the fourth-order ETF theory in the approximations of spherical, cylindrical, and plane-parallel WS cells. We have shown that a gradient discontinuity (a kink) of a trial density distribution on any smooth surface (which can be a WS cell surface) or on the center of a cylindrical or plane-parallel WS cell makes the fourth-order ETF gradient correction divergent. On the other hand, a kink in $n_q(\mathbf{r})$ at the center of a spherical WS cell does not result in a divergence, in which case the second and fourth order gradient corrections can be treated as distributions and remain integrable.

In previous discrete-mesh calculations, a kink in $n_q(\mathbf{r})$ was sometimes understood (e.g., Ref. [74]) as an approximation to a sufficiently smooth function $\bar{n}_q(\mathbf{r})$, which was not explicitly defined but was meant to coincide with the employed trial function $n_q(\mathbf{r})$ at the mesh nodes. In Section 5, we demonstrated a fundamental limitation of the accuracy inherent to this approach.

Such an accuracy limitation, however, does not invalidate the previously reported results [73, 74], because it lies well below their actual accuracy. According to these calculations, in order to correctly determine the structural phase transitions between the nuclear pasta phases, it is sufficient to calculate energy per nucleon with an accuracy of $\lesssim 0.1$ keV. Meanwhile, the minimal contribution of the smoothed-out central kink in the DF parametrization (19), evaluated according to Eqn (37), does not exceed 0.1 keV per nucleon in the 'lasagna' phase, if $\varepsilon \gtrsim 10^{-3}$ fm. As mentioned in Ref. [74], the integrals calculated with a mesh size of 0.1 fm correspond to the kink having been smoothed out locally over the region $\xi \lesssim 0.01$ fm, which is sufficient for the required accuracy.

We should emphasize that the above numerical example pertains to the concrete implementation of the ETF theory, based on the BSk24 energy density functional [74]. What is more, we have used the approximation $M_q^* = M_q$, which means that our numerical estimates are only valid by order of magnitude, but not exact. The limit on the step in ξ can be different with another nuclear interaction model. The result can also depend on the interval of the scanned parameters in the minimization procedure. For instance, because of the divergences, a numerical minimization can sometimes result in unrealistic values of parameters with a much bigger error in the energy in comparison with optimal parameters.

Anyway, the implicit smoothing-out of the divergences entails a risk of spoiling the results through the dependence on the rather arbitrary smoothing function. For example, a numerical integration of the kinetic energy density with an automated choice of an integration step might occasionally 'feel' the contribution from the kink, which would result in unlimited refinement of the mesh to ever smaller step sizes ε near the kink points, thus leading to the divergence evaluated in Section 5. Therefore, we conclude that using trial functions with continuous first derivatives everywhere, including the center of a WS cell, should be recommended for solving fourth order ETF equations using the restricted variational method.

Acknowledgments

A.P. thanks D.G. Yakovlev for useful remarks on a draft of the paper. The work of A.P. and A.C. was supported by the Russian Science Foundation, grant no. 22-12-00048. The work of N.S. was financially supported by the FWO (Belgium) and the Fonds de la Recherche Scientifique (Belgium) under the Excellence of Science (EOS) programme (project no. 40007501). The work of N.C. received funding from the Fonds de la Recherche Scientifique (Belgium) under grant no. IISN 4.4502.19.

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