Equation of State of Nuclear Matter with Gaussian Processes

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Abstract: In this work we employ a Gaussian Processes method to obtain a non-parametric description of the Equation of State (EoS) of cold dense matter that allows for rapid calculations and gives an estimation of the uncertainty of the theoretical model and related observables. The calculations are based on results derived in a Bruckner-Hartree-Fock approach. The non-parametric EoS is then used to study asymmetric β-stable neutron star matter, obtaining its composition, the pressure and the energy density at different baryonic densities. By solving the Tolman-Oppenheimer-Volkoff equations, we also determine the stellar structure parameters. Our results for the non-parametric EoS are consistent with those obtained with a traditional power-law fit to the data.
Keywords: Neutron Stars, Dense Matter, Gaussian Processes, Beta Equilibrium
SDGs: Industry, innovation and infrastructure, quality education

I. INTRODUCTION

Calculating the Equation of State (EoS) of dense nuclear matter is a fundamental problem of modern nuclear physics. Its correct determination is a key ingredient to understand the properties of neutron stars (NSs) such as their masses and radii[1]. Theoretically, the EoS can be obtained in different frameworks [1, 2]. Particularly interesting are the so called microscopic ones that are built up directly from the bare nucleon-nucleon (NN) interaction. Despite their accuracy, these methods are computationally expensive, which require the use of sophisticated parametric fits and interpolation techniques. Recently, non-parametric fitting procedures have been available with the development of Gaussian Processes (GPs) [3], allowing us to obtain a regression of some given data without the need to provide a particular functional form. In this work we will explore the usefulness of this procedure to reproduce an EoS for dense matter based on the results of a microscopic calculation that employed the Brueckner–Hartree–Fock (BHF) method [4]. We will compare the GPs results with the ones that we get from fitting the data to a parametric model commonly used in the literature. With the obtained EoSs we will be able to calculate the composition of NSs and consequently some of their properties.

II. GAUSSIAN PROCESSES

A GP is a probabilistic model that performs a regression to some data while also estimating how uncertain the predictions are. Imagine we are given some set of observed data $\{(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)\}$. Rather than assuming a specific analytical to fit these data points, like linear or polynomial models, GPs will treat our data as coming from a smooth relation, $y(x)$, that we are trying to figure out. In order to do so, this method assumes that the collections of possible functions that could represent our data is normally distributed ($\mathcal{N}$). Thus, a GP represents a multivariate normal distribution over all possible functions. In the same way that the normal distribution for a random variable is fully described by its mean value and its standard deviation, which measures the dispersion of points in the distribution, the multivariate normal distribution is also described by a mean *function* μ (which in this work will be assumed to be zero) and by what is called the covariance function K, also known as a kernel, which relates one observation to another. Going back to our given data set, the GP will thus provide a normal distribution $\mathcal{N}$ over the given values y and some function values y^* measured at the test points x^*:

$$\begin{bmatrix} y \\ y^* \end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} K(x,x)+\sigma^2 I & K(x,x^*) \\ K(x^*,x) & K(x^*,x^*)+\sigma^2 I \end{bmatrix}\right), \quad (1)$$

where σ^2 is the added noise variance. Intuitively, in order to obtain a smooth function, we would want the points that are nearby to be related with each other and not with the ones that are very far away. This is why in this present work the correlation between two points, x_i and x_j, is expressed with the *Square Exponential Kernel* [3]:

$$K_{ij} = \alpha \exp\left(-\beta |x_i - x_j|^2\right), \quad (2)$$

where α and β are the so called hyperparameters of the kernel. The parameter α is related with the vertical scale over which the function is varying, and the parameter β controls the rate of variation of the function. In this work, we have used a Python library called *gptools* in order to find the distribution that better fits the data using this method, as we will see in further sections. Using advanced machine learning techniques, this library provides the optimal values for the hyperparameters of the covariance function. The use of this method can have numerous advantages. First of all, as we have mentioned before, GPs are non-parametric, meaning they do not assume a fixed form for the function and can be adapted to the data. Secondly, GPs provide not only predictions but they also estimate the uncertainty, which can be very useful in scientific modelling.

III. EQUATION OF STATE OF DENSE MATTER

In a neutron star, nucleons are subjected to extreme densities. As a consequence, their interaction is not limited to a simple pairwise nucleon-nucleon (NN) force, which is often modeled using realistic potential models such as Argonne V18 (AV18)[4], but multi-body forces (such as three-body forces) start to be important. Thus, to obtain the EoS of infinite nuclear matter, one has to solve a complicated many-body problem. One of the most widely used methods in the literature is the Brueckner-Hartree-Fock (BHF) approximation. In this method, the key goal is to describe the interactions between nucleons beyond the simple Hartree-Fock approximation, which only accounts for the average field produced by the surrounding nucleons. The BHF method improves on this by including correlations between the nucleons that arise from realistic NN interactions. The resulting effective interaction between two nucleons in the BHF approximation is represented by the G-matrix, obtained from the solution of the following equation:

$$G(\omega)_{(N_1,N_2,N_3,N_4)} = V_{(N_1,N_2,N_3,N_4)} + \\ + \sum_{N_i,N_j} V_{(N_1,N_2,N_i,N_j)} \frac{Q_{N_i,N_j}}{\omega - E_{N_i} - E_{N_j}} G(\omega)_{(N_i,N_j,N_3,N_4)}, \tag{3}$$

known as the Bethe-Goldstone equation [4]. The parameter ω is the energy of the interacting pair, also known as starting energy and Q is the Pauli operator, which prevents the transitions to intermediate nucleon states that are already occupied. In the BHF approximation, the single particle potential energy U_{N_i} can be written as the sum of the different pair interactions between the different species (neutrons and protons in the present work):

$$U_{N_i}(\vec{k}) = \\ = Re \sum_{N_j} \sum_{\vec{k}'} n_{N_j}(|\vec{k}'|) \langle \vec{k}, \vec{k}'| G(E_{N_i}(\vec{k}) + E_{N_j}(\vec{k}')) | \vec{k}, \vec{k}' \rangle, \tag{4}$$

where $n_{N_j}(|\vec{k}'|)$ represents the occupation number of the state with a momentum $\vec{k}'$ for the j-th species. We need to perform a sum of the matrix elements over all occupied momentum states in order to obtain the single particle energy contributions from the G–matrix. Finally, to obtain the EoS, we need to find the total energy per particle, which is given by:

$$\frac{E}{A} = \frac{1}{A} \sum_{N_i} \sum_{\vec{k}} n_{N_i}(|\vec{k}|) \left(\frac{k^2}{2M_{N_i}} + \frac{U_{N_i}(\vec{k})}{2} \right), \tag{5}$$

	a	b	c	d
SNM	151.50	1.73	-52.77	0.45
PNM	44.44	0.53	207.03	1.95

TABLE I: Optimal parameters for the model in the Eq.(8) for symmetric nuclear matter and pure neutron matter.

where A is the total number of nucleons. For simplicity, in this section we will use natural units. As a starting point in this work, we will use results obtained in the BHF framework using the realistic Argonne V18 interaction for symmetric nuclear matter (SNM) and pure neutron matter (PNM) for 12 different densities in the range of $0.05\,\mathrm{fm}^{-3}$ up to $1\,\mathrm{fm}^{-3}$ [4]. With the aim of obtaining the energy per particle for an arbitrary composition, we approximate the energy per particle by means of a Taylor expansion around the symmetric case, where the particle fraction $x_i \equiv \rho_i/\rho$ for protons and neutrons is the same, $x_p = x_n = 1/2$. Thus, one can compute the energy per particle for a certain fraction of protons as:

$$\frac{E}{A}(\rho, x_p) = \frac{E}{A}(\rho, x_p = 1/2) + 4S(\rho)(x_p - 1/2)^2. \tag{6}$$

The symmetry energy, denoted as $S(\rho)$, is a term that arises from the difference in the energy contributions from neutrons and protons in the system, and it quantifies the energy cost of breaking the symmetry between neutron and proton populations [5] . Knowing the energy per particle for the SNM case ($x_p = 1/2$) and the PNM case ($x_p = 0$), the symmetry energy can be defined as a function of the baryonic density ρ:

$$S(\rho) = \frac{E}{A}(\rho, x_p = 0) - \frac{E}{A}(\rho, x_p = 1/2). \tag{7}$$

Given the data, our objective is to estimate an EoS that accurately represents the system's behaviour. To achieve this, we will employ two different methods. First, we will perform a regression using the GP method, as outlined in Section II. For comparison, we will also fit the data into the model

$$\frac{E}{A}(\rho)_{\mathrm{Fit}} = a\rho^b + c\rho^d, \tag{8}$$

commonly utilized in literature. In Table I we display the optimal values for the parameters a, b, c, d that are obtained using the least square method. Fig. 1 shows the results obtained with the two models (red curve - GP, blue curve - power law fit) for SNM and PNM along with the exact results obtained in the BHF framework (black dots). Both methods reproduce the data rather well. Furthermore, the saturation densities found for both methods are $\rho_{0(\mathrm{GP})} = 0.18\,\mathrm{fm}^{-3}$ and $\rho_{0(\mathrm{Fit})} = 0.15\,\mathrm{fm}^{-3}$, which are coherent with the typical values for nuclear matter around $\rho_0 \sim 0.16\,\mathrm{fm}^{-3}$.

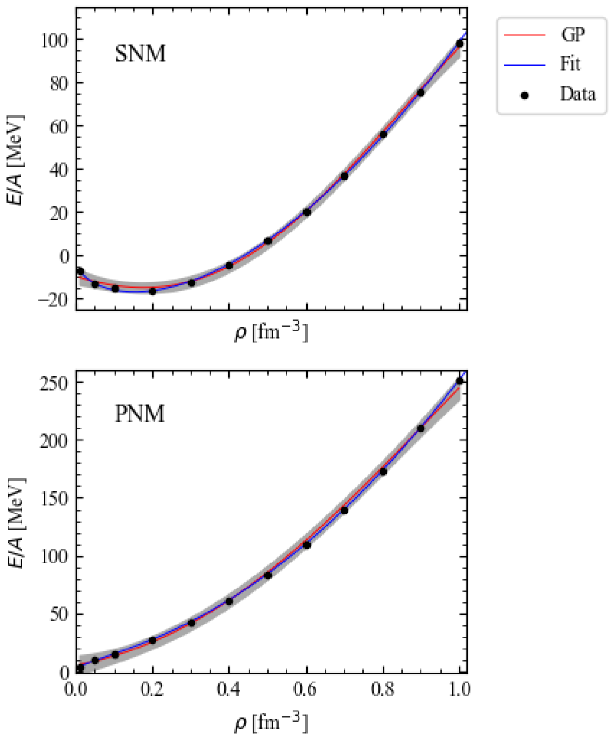

FIG. 1: Energy per particle of symmetric nuclear matter (SNM) and pure neutron matter (PNM) as a function of the baryonic density, computed using the GP method (red curve) and by fitting the data to the power-law model shown in Eq.(8) (blue curve). The grey band represents the uncertainty obtained in the GPs.

IV. BETA STABLE NEUTRON STAR MATTER

In the neutron star core, matter is expected to be composed of homogeneous nuclear matter and leptons in beta equilibrium. This balance ensures that all weak interaction processes are equilibrated. Inside the star, the neutron decay reaction:

$$n \to p + e^- + \bar{\nu}_e$$

is Pauli blocked since the the lowest levels of the proton and neutron Fermi seas are occupied [4]. That decay is balanced with the electron capture reaction:

$$p + e^- \to n + \nu_e.$$

Neutrinos can escape freely since their mean free path is usually larger than the radius of the neutron star. Hence, while the baryonic number is conserved,

$$\rho = \rho_p + \rho_n, \tag{9}$$

the leptonic number is not. In terms of the chemical potentials, the equilibrium condition can be written as:

$$\mu_n = \mu_p + \mu_e. \tag{10}$$

The definition of the chemical potential using the energy per particle is:

$$\mu_i = \frac{\partial(\frac{E}{A}\rho)}{\partial\rho_i}. \tag{11}$$

From this expression and employing Eq.(6) it can be shown that $\mu_n - \mu_p = 4S(\rho)(1-2x_p)$. Assuming ultralativistic electrons with $\mu_e = \hbar c k_{F_e} = \hbar c(3\pi^2\rho x_p)^{1/3}$, where $\hbar k_{F_e}$ is the Fermi momentum of the electrons, the $\beta-$equilibrium condition can be written as:

$$\hbar c(3\pi^2\rho x_p)^{1/3} = 4S(\rho)(1-2x_p). \tag{12}$$

At extremely high densities, the available energy is sufficient to produce particles heavier than electrons, such as muons. Thus, when the chemical potential of the electron equals the rest mass energy of the muon, $E_{0,\mu} = m_\mu c^2 = 105.65\,\text{MeV}$, this species will appear in matter. In weak equilibrium with no neutrinos, the chemical potential of the two leptonic species will be equal: $\mu_e = \mu_\mu$ [4]. Taking the muons into account we must consequently consider the following new expressions for the charge balance and the chemical potentials for the muons and the electrons, respectively:

$$\mu_e = \mu_\mu = \sqrt{{m_\mu}^2 c^4 + (\hbar c k_{F_\mu})^2}. \tag{13}$$

$$\rho_p = \rho_e + \rho_\mu. \tag{14}$$

Imposing the $\beta-$equilibrium condition we can rewrite the charge balance as follows:

$$\begin{aligned}&(\hbar c)^3 3\pi^2 x_p \rho = \\ &= [4S(\rho)(1-2x_p)]^3 + \{[4S(\rho)(1-2x_p)]^2 - m_\mu^2 c^4\}^{3/2}\end{aligned} \tag{15}$$

Solving this equation for x_p, the other particle fractions can be automatically computed using Eqs.(9), (12), (13) and (14). The results of the composition of the neutron star core is shown in Fig. 2. The upper panel represents the results obtained with GP, while the lower panel represents the results obtained with the power-law fit. Both approaches predict that matter is dominated by neutrons and the amount of protons does not surpass 30% of the nuclear matter, even at very high densities.
The energy density for the baryons is readily obtained, including the nucleon rest mass energy, from Eq.(6):

$$\varepsilon_B = \left[\frac{E}{A}(\rho, x_p = 1/2) + 4(x_p - 1/2)S(\rho) + m_N c^2\right]\rho, \tag{16}$$

where $m_N = (m_p + m_n)/2$ is the average nucleon mass. The pressure can then be computed according to the relation:

$$P_B = \rho\frac{\partial\varepsilon_B}{\partial\rho} - \varepsilon_B. \tag{17}$$

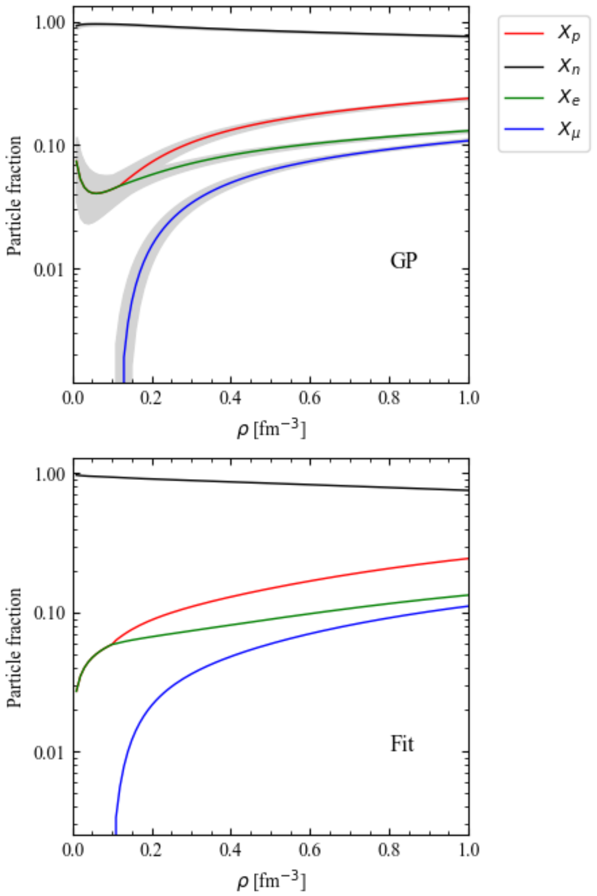

FIG. 2: Particle fractions of the protons, neutrons, muons and electrons in neutron star matter as a function of the baryonic density computed with values of the energy per particle $E/A(\rho)$ obtained with GP interpolation and with the fit.

To obtain the energy density of the leptons we must add their single particle energies up to the highest occupied state:

$$\varepsilon_l = \frac{1}{\pi^2}\int_0^{k_{F_l}} \sqrt{m_l^2c^4 + (\hbar c k)^2}\, k^2\, dk, \tag{18}$$

which gives rise to the following result:

$$\varepsilon_l = \frac{(m_l c^2)^4}{(\hbar c)^3 8\pi^2}\Big[x_{F_l}(1+2x_{F_l}^2)\sqrt{1+x_{F_l}^2} - \ln x_{F_l} + \\ + \sqrt{1+x_{F_l}^2}\Big] \tag{19}$$

with

$$x_{F_l} = \frac{\hbar c(3\pi^2\rho x_l)^{1/3}}{m_l c^2}. \tag{20}$$

Similarly, the pressure is given by:

$$P_l = \frac{3\hbar c\rho^{4/3}}{8}\left(\frac{3}{8\pi}\right)^{1/3}\left[\frac{1}{x_{F_l}^4}\left[x_{F_l}\sqrt{1+x_{F_l}^2}\left(\frac{2x_{F_l}^2}{3}-1\right)+ \\ + \ln x_{F_l} + \sqrt{1+x_{F_l}^2}\right]\right]. \tag{21}$$

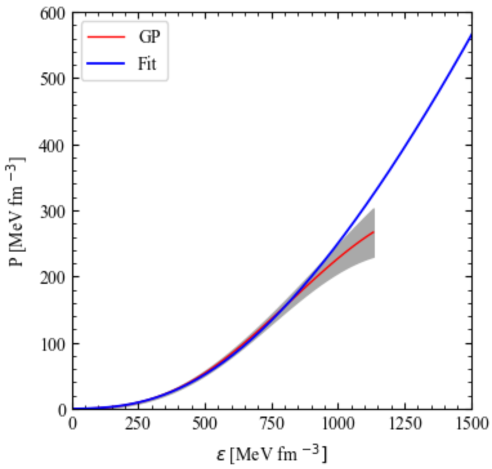

FIG. 3: Total pressure of matter in beta equilibrium as a function of the total energy density computed using GP interpolation (red curve) and by fitting the data into the traditional model shown by Eq.(8) (blue curve).

Thus, the total energy density and the total pressure will be, respectively:

$$\varepsilon = \varepsilon_B + \varepsilon_e + \varepsilon_\mu, \qquad P = P_B + P_e + P_\mu. \tag{22}$$

The results obtained for the pressure as a function of the energy density computed with the GP and the power-law fit are presented in Fig. 3. It is important to note that the values for the fit have been extrapolated to a density value of $\rho = 1.5\,\mathrm{fm}^{-3}$. In this high-density region, the parametric fitting procedure seems to do a better extrapolation, indicating that for the particular problem in this work the GP method does not appear to be the preferred regression procedure. However, we must keep in mind that the study of the nuclear EoS is not only needed at zero temperature. For instance, to describe supernova explosions or the merger of NSs, a larger range of temperatures, from 0 to 100 MeV, would be needed. In those conditions, the usefulness of GPs might prove more evident.

V. TOV EQUATIONS

The Tolman Oppenheimer Volkoff (TOV) equations

$$\frac{dP(r)}{dr} = -\frac{Gm(r)\varepsilon(r)}{r^2}\left(1+\frac{P(r)}{\varepsilon(r)}\right)\left(1+\frac{4\pi r^3 P(r)}{m(r)}\right), \tag{23}$$

$$\frac{dm(r)}{dr} = 4\pi r^2 \varepsilon(r) \tag{24}$$

describe the structure of an isotropic, spherically symmetric star in static gravitational equilibrium, within the general relativity framework [6]. Eq.(23) describes the evolution of the pressure in the star, and is obtained by imposing hydrostatic equilibrium. Eq.(24) describes the growth of the enclosed mass as one moves outwards from

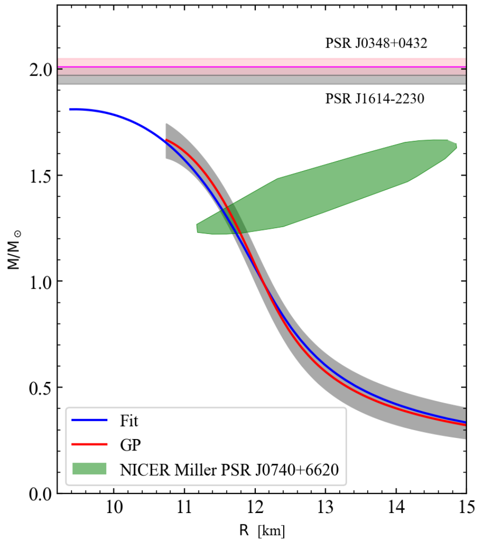

FIG. 4: Mass (in units of the solar mass, $M_\odot$) and radius (in km) for the family of neutron stars obtained using the EoS determined from the GP interpolation and the parametric fit. The thin horizontal bands indicate two of the heaviest observed masses $M = 1.97 \pm 0.04\,M_\odot$ and $M = 2.01 \pm 0.04\,M_\odot$ [8]. We also include the Miller analysis of the NICER PSR J0740+6620 mass-radius measurement.

the centre to the surface of the neutron star. In order to obtain the numerical solution to these coupled equations we have employed a Python module called *TOVsolver* [7] that proceeds as follows. Firstly, given the model of the EoS of the core, the module provides an EoS for the crust that serves as a low density extrapolation for the one we have provided. Secondly, a particular value of the central density, ρ_0, is selected which defines the initial $P(\rho_0)$ and $\varepsilon(\rho_0)$ at the centre of the star $(r = 0)$. Using small radial steps, the pressure and the enclosed mass are computed at every radius r, until the surface of the star, namely the radius R for which $P = 0$, is reached. Note that the EoS is not calculated at every pressure that is needed in the integration process, so a linear interpolation for the energy density is performed. Since the EoS is not calculated at every step, using interpolation methods is mandatory. One can then obtain the energy density corresponding to a specific pressure value and follow once again the steps described before. Varying the initial central density of the star, a family of stars with different masses and radii is obtained. The results are shown in Fig. 4. As we can see, the maximum mass for the fit is $M = 1.8\,M_\odot$ when the central density is $\rho_c = 1.48\,\text{fm}^{-3}$. We are unable to determine the maximum mass for the GPs case because we cannot extrapolate the calculations to higher densities.

VI. CONCLUSIONS

In this work we have obtained the equation of state of dense matter with a Gaussian Processes regression, based on Brueckner Hartree Fock calculations that use the realistic Argonne V18 nuclear force. We showed that the regression reproduces the results of the numerically costly microscopic calculation with a good precision. In addition it gives an estimation of the uncertainty in the regression procedure. To show the usefulness of the obtained EoS, different properties of the neutron stars have been computed. In particular, we showed the composition of the neutron star, as well as the mass-radius relation. For a comparison, all of the analysis has been also done with a traditional power law fit of the microscopic results and we have observed that the results from the two approaches are consistent. However, the GP procedure does not seem necessary for the chosen problem since the fit yields very good results and allows us to extrapolate. Even so, this work has allowed us to become familiar with the GP method, which we can improve in the future and apply it also to study the EoS in the context of violent astrophysical events, such as supernova explosions or binary neutron star mergers, which require a regression to a much larger data set, covering a wide range of temperatures. In this case, the use of typical parametric methods might not be as straightforward as in the present analysis.

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Equació d'Estat de la Matèria Nuclear amb Processos Gaussians

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Resum: En aquest treball utilitzem un mètode de processos gaussians per obtenir una descripció no paramètrica de l'Equació d'Estat (EoS) de la matèria freda i densa, que permet càlculs ràpids i proporciona una estimació de la incertesa del model teòric i dels observables associats. Els càlculs es basen en resultats derivats a partir de la teoria de Brueckner-Hartree-Fock. L'Equació d'Estat no paramètrica s'utilitza per estudiar la matèria de neutrons asimètrica i $\beta-$estable, obtenint-ne la composició, la pressió i la densitat d'energia per a diferents valors de la densitat bariònica. Resolent les equacions de Tolman-Oppenheimer-Volkoff, també determinem els paràmetres de l'estructura estel·lar. Els nostres resultats per a l'Equació d'Estat no paramètrica són consistents amb els obtinguts mitjançant un ajust tradicional segons una llei de potències.
Paraules clau: Estrelles de neutrons, matèria densa, processos gaussians, equilibri beta
ODSs: Indústria, innovació i infraestructura, educació de qualitat

Objectius de Desenvolupament Sostenible (ODSs o SDGs)

1. Fi de la es desigualtats		10. Reducció de les desigualtats	
2. Fam zero		11. Ciutats i comunitats sostenibles	
3. Salut i benestar		12. Consum i producció responsables	
4. Educació de qualitat	X	13. Acció climàtica	
5. Igualtat de gènere		14. Vida submarina	
6. Aigua neta i sanejament		15. Vida terrestre	
7. Energia neta i sostenible		16. Pau, justícia i institucions sòlides	
8. Treball digne i creixement econòmic		17. Aliança pels objectius	
9. Indústria, innovació, infraestructures	X		