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# Universal scaling relations for the energies of many-electron Hooke atoms

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A three-dimensional harmonic oscillator consisting of $N \geqslant 2$ Coulomb-interacting charged particles, often called a (many-electron) Hooke atom, is a popular model in computational physics for, e.g., semiconductor quantum dots and ultracold ions. Starting from Thomas-Fermi theory, we show that the ground-state energy of such a system satisfies a nontrivial relation: $E_{gs} = \omega N^{4/3} f_{gs}(\beta N^{1/2})$, where $\omega$ is the oscillator strength, $\beta$ is the ratio between Coulomb and oscillator characteristic energies, and $f_{gs}$ is a universal function. We perform extensive numerical calculations to verify the applicability of the relation. In addition, we show that the chemical potentials and addition energies also satisfy approximate scaling relations. In all cases, analytic expressions for the universal functions are provided. The results have predictive power in estimating the key ground-state properties of the system in the large-$N$ limit, and can be used in the development of approximative methods in electronic structure theory.

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## I. INTRODUCTION

Scaling relations obtained through the Thomas-Fermi approach [1,2] provide an efficient way to assess the energetic properties of many-particle systems, especially in the regime that is beyond the reach of first-principles electronic structure methods. On one hand, the prediction of energy components in atoms, molecules, and electron droplets brings generic information on the role of electron-electron interactions under varying particle numbers and confining potentials. On the other hand, the predictive power up to high particle numbers enables comparisons with experimental data, as well as benchmark results for the development of computational techniques.

The harmonic oscillator is one of the cornerstone models in various fields of physics. In material and condensed matter physics the three-dimensional harmonic oscillator consisting of two Coulomb-interacting particles is often called the Hooke atom (or hookium or harmonium). This system is analytically solvable, in contrast with its better known counterpart, a helium atom. The many-electron Hooke atom (HA) consisting of $N > 2$ interacting particles is much more complex, and the solution of its Schrödinger equation requires numerical methods. In practice, numerically accurate methods such as exact diagonalization, (quantum) Monte Carlo, and coupled-cluster schemes are restricted to the few-particle regime. For tens and hundreds of electrons other electronic structure methods such as density-functional theory [1,3,4] (DFT) are needed.

The many-electron Hooke atom is not only a curious physical example, but also a popular model for semiconductor quantum dots—alongside its numerically simpler two-dimensional (2D) counterpart—as well as for atomic clusters and ion plasmas [5]. In quantum dots, for example, it has been shown that the conduction band electrons are confined by harmonic potential in a good approximation [6,7]. In this case, the confinement arises from the semiconductor structure and external gate voltages.

In recent works, we have shown the existence of universal scaling relations for the ground-state energy [8], ionization potentials and electron affinities [9], and the correlation energy [10] of 2D parabolic quantum dots. Here we turn our attention to the energies of the three-dimensional (3D), many-electron Hooke atom. Previous studies on the energy scaling in 3D have mainly focused on atoms [2,11,12] and atomic ions [13,14]. Thus, in the present work we bridge the gap by considering scaling relations in a realistic 3D model that has general applicability for several classes of physical systems.

The paper is organized as follows. In Sec. II we present the general scaling relation for the ground-state energy of a Hooke atom based on the Thomas-Fermi approach. In Sec. III we, first, find a two-point Padé approximant for the ground-state energy based on an extensive set of reference results and, second, demonstrate the performance of the scaling against several sets of numerical results for different ranges of parameters. In Sec. IV we derive the scaling relations for the electrochemical potentials and addition energies and, again, compare the scaling against numerical results. The paper is summarized in Sec. V.

## II. SCALING RELATION FOR THE GROUND-STATE ENERGY

Here, a HA is defined as a system of $N$ electrons confined in a three-dimensional harmonic potential $v_{\text{ext}}(r) = \omega^2 r^2/2$, where $\omega$ is the oscillator strength. Following the procedure carried out in 2D systems in Ref. [8], the Thomas-Fermi (TF) energy functional [2] (in the units of $\omega$) can be written as

$$\frac{E_{\text{TF}}}{\omega} = \int dr \left( \alpha \rho^{5/3}(r) + \frac{\rho(r) r^2}{2} \right) + \beta \int \int dr\, dr' \frac{\rho(r)\rho(r')}{|\vec{r} - \vec{r}'|}, \tag{1}$$

where $\alpha$ is a numerical constant and $\beta = \omega^{-1/2}$ is the ratio of the Coulomb and harmonic-oscillator characteristic energies. We rescale the radial coordinate $r$ and the density $\rho(r)$ in such a way that the right-hand side of the normalization condition

$$\int \rho(r) dr = N \tag{2}$$

becomes equal to 1. This leads to the scaling relation

$$\frac{E_{gs}}{\omega N^{4/3}} = f_{gs}(\beta N^{1/2}) = f_{gs}(z), \tag{3}$$

where $f_{gs}$ is a *universal* function depending on $z = (N/\omega)^{1/2}$—a particular combination of the system parameters. As demonstrated below, the scaling relation in Eq. (3) is numerically consistent with previous results in the literature as well as our calculations.

## III. NUMERICAL RESULTS AND THE PADÉ APPROXIMANT

In order to corroborate the scaling property in Eq. (3), we carry out a large set of calculations within DFT [3,4] and path integral Monte Carlo [15–20] (PIMC) methods. In the DFT we apply the OCTOPUS software package [21–25] using the Perdew-Burke-Ernzerhof [26,27] (PBE) exchange-correlation functional. The PIMC method is used to obtain highly accurate many-electron reference data for the ground state. Since PIMC is a finite-temperature approach, we have chosen a simulation temperature that accurately describes the ground state, i.e., $T/T_F = 0.025$, for all simulations. In order to ensure high accuracy and an upper bound estimate, we have extrapolated our PIMC values to the zero time-step limit from the energetics of six different time steps. Fermi statistics is incorporated by the use of the so-called free particle nodes within the fixed-node PIMC formalism [20].

In the DFT calculations we consider the following combinations for the confinement strength and the number of electrons: $\{\omega = 0.1;\ N = 8,20,58,132,438,1502\}$, $\{\omega = 0.5;\ N = 106,198,398,1490\}$, and $\{\omega = 1;\ N = 106,198,440,790,1100\}$. With these combinations of $\omega$ and $N$ we cover a wide range of values for the scaling variable $z$ in Eq. (3), including the important large-$N$ limit. Additionally, for each system we also compute the ground-state energies $\{N_i - 1,\omega_i\}$ used in the calculations for the electrochemical potentials defined in Sec. IV.

An analytical expression for $f_{gs}(z)$ in Eq. (3) can be found with Padé approximants in the large-$N$ limit. We interpolate the strong-confinement limit with weak correlations as

$$\frac{E_{gs}}{\omega N^{4/3}} \underset{\lim_{x\to\infty}}{=} b_0 + b_3 x^3 + \cdots , \tag{4}$$

and the weak-confinement limit with strong correlations as

$$\frac{E_{gs}}{\omega N^{4/3}} \underset{\lim_{x\to\infty}}{=} x^2\left(a_2 + \frac{a_0}{x^2}\right) + \cdots , \tag{5}$$

where $x = \beta^{1/3} N^{1/6} = z^{1/3}$ [28,29]. Now, the $P_{3,2}$ approximant, for example, can be written as

$$P_{3,2} = b_0 + a_0 x^2\left(1 - \frac{1}{1 + q_1 x + q_2 x^2}\right), \tag{6}$$

where $q_1 = b_3/a_0 > 0$ and $q_2 = a_2/(b_0 - a_0) > 0$ with $b_0 = (3^{4/3})/4$ and $a_2 = 9/10$ [30]. The other two coefficients, $a_0$ and $b_3$, are determined numerically from a two-parameter fit to our main data set, i.e., a combination of the PBE results for "intermediate" confinements ($\omega = 0.5,1.0$) and PIMC results for $\{\omega = 0.5; 2 \leqslant N \leqslant 9, N = 40\}$. From the numerical fit, our scaling relation for the ground-state energy reads

$$\frac{E_{gs}}{\omega N^{4/3}} = \frac{3^{4/3}}{4} + \frac{(2.651 \times 10^{-7})z + 0.6197 z^{4/3}}{1 + (2.946 \times 10^{-7}) z^{1/3} + 0.6885 z^{2/3}},$$

which, after neglecting the low-order coefficients, leads to

$$\frac{E_{gs}}{\omega N^{4/3}} = \frac{1.571 + 1.0817 z^{2/3} + 0.9 z^{4/3}}{1.452 + 1.0 z^{2/3}}. \tag{7}$$

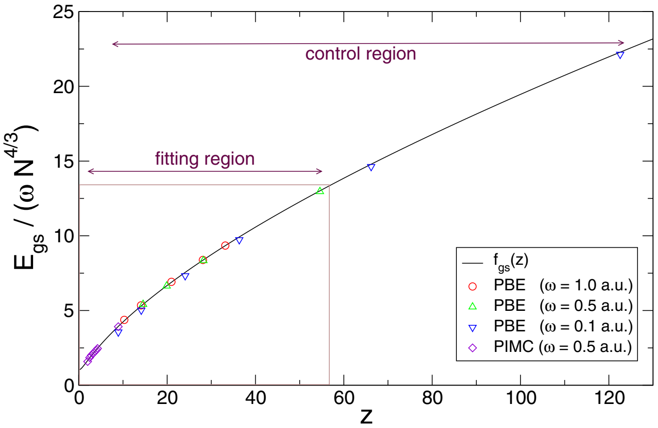

FIG. 1. Density-functional (PBE) and PIMC results for the scaled ground-state energies of HAs as a function of $z = (N/\omega)^{1/2}$ (symbols). The solid line represents the function $f_{gs}(z)$ of Eq. (7). The fitting region contains systems with $\omega = 1.0$ and $\omega = 0.5$. The control region contains systems with $\omega = 0.1$.

Figure 1 shows the DFT (PBE) and PIMC results for the scaled $E_{gs}$ (symbols) together with the function $f_{gs}$ (solid line) in Eq. (7). We can see that the scaling behavior is apparent and consistent across the parameter ranges of $\omega$ and $N$. Let us stress that the subset of systems with $\omega = 0.1$ was not used for the fitting but as "control cases". In terms of the variable $z$, the "control region" is twice the size of the "fitting region" (see Fig. 1), going from $z \approx 10$ to $z \approx 125$, i.e., deep into the strong correlation regime.

Figure 2 shows additional DFT results for $E_{gs}$ together with the function $f_{gs}$ in Eq. (7). We consider the local density approximation (LDA) results reported in Ref. [31]. The systems considered in this case are $\{\omega = 0.1;\ N = 8,20,58,100,132,438,800,1200,1500\}$, $\{\omega = 0.5;\ N = 100,200,400,800,1206,1490\}$, and $\{\omega = 1;\ N = 100,200,440,800,1200,1500\}$. With these combinations of $\omega$ and $N$ we cover a similar range of values for the scaling variable $z$ in Eq. (3) as for the PBE calculations. These numerical results agree remarkably well with the scaling relation.

The inset of Fig. 2 shows additional numerical results from three independent calculations: (1) coupled-cluster results of Yakobi *et al.* [32] ($\omega = 0.5$, $2 \leqslant N \leqslant 60$), (2) diffusion Monte Carlo (DMC) results for few-particle systems $\{\omega = 0.5, 2 \leqslant N \leqslant 9\}$ of Wilkens [33], and (3) DMC results for four-electron systems and $\omega = 0.5,0.04,0.034,0.028,0.024,0.020,0.014,0.010$ of Amovilli and March [34]. All additional data sets fit very well with the proposed scaling.

As an additional confirmation of the generality of our scaling relation, the results reported in Ref. [32] for the particular

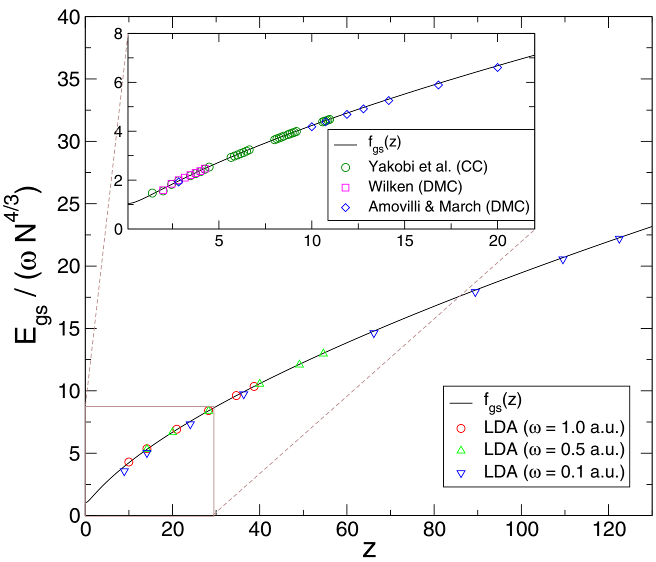

FIG. 2. LDA results (symbols) for the scaled ground-state energies of Hooke atoms with varying confinement strengths up to $N \approx 1500$ in comparison with the scaling function $f_{gs}(z)$ (solid line) of Eq. (7). Inset: Additional numerical results from Refs. [32–34].

case of $\omega = 0.5$, i.e., $E_{gs}(N,\omega = 0.5) = 0.5761N^{5/3}$, can be obtained from the large-$N$ expansion of Eq. (7):

$$E_{gs}(N,\omega = 0.5) \approx 0.5670N^{5/3} - 0.1127N^{4/3} + 0.7534N + \cdots O\left(\frac{1}{N}\right)^{1/3}.$$

Next, in order to assess the accuracy of our scaling relation, we analyze the relative error of some of our numerical results with respect to ground-state energies resulting from Eq. (7). The relative errors of PIMC results for $\{\omega = 0.1; N = 8,20\}$ are shown in the upper panel Fig. 3 together with some PBE results. The lower panel of Fig. 3 shows the corresponding LDA results. The large-$N$ limits were estimated by extrapolating from numerical fits, assuming that the dependence of relative error on $N$ follows simple power laws. The values are similar in all cases, meaning that the accuracy of ground-state energies calculated with Eq. (7) is surprisingly good even at very weak confinements. Equally surprising is that, in contrast to the two-dimensional case [35], in 3D the coefficient coming from the Thomas-Fermi theory, i.e., $a_2$ in Eq. (5), agrees with the scaling even for small $N$. We find that for $N \geqslant 500$ the relative error is always below 1%. In fact, the accuracy of the obtained scaling relation is so high that, in principle, it could be used not only to predict total energies of arbitrary Hooke atoms, e.g., in the large-$N$ limit, but also as a benchmark to assess the *convergence* of first-principles calculations.

To find the limits for the applicability of the scaling relation at very strong electron-electron correlations, we have compared the scaling against PIMC results for small $N$ and small $\omega$. In this regime the Coulomb interaction dominates over the other energy components and the system can be characterized by Wigner crystallization. In practice, we find that the computed ground-state energies deviates from the scaling in Eq. (7) for $N = 8$ and $0.01 > \omega > 0.001$, which means that a different value of $a_2$ in Eq. (5) is required to describe the Wigner regime. It is noteworthy, however, that these values for $\omega$ are much smaller than what has been estimated for semiconductor quantum dots, for example, where the confinement strengths are typically around $\omega \gtrsim 0.1$ [7].

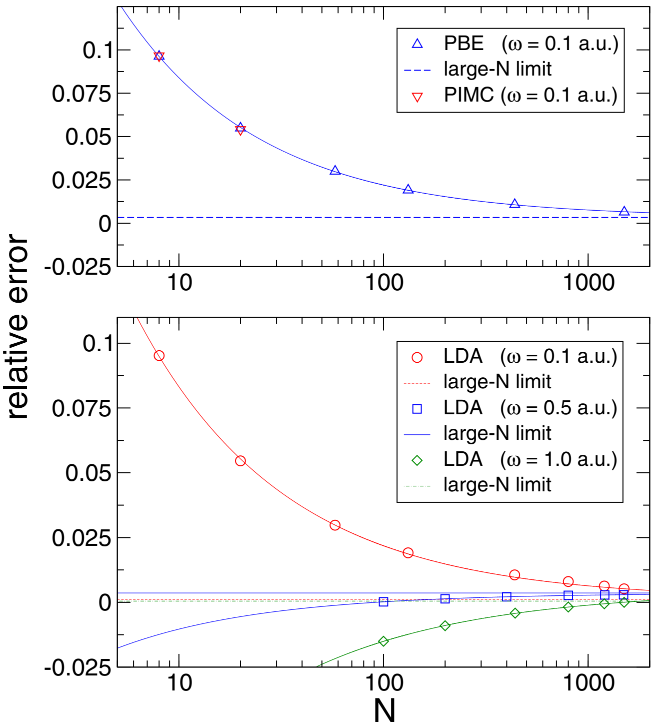

FIG. 3. Upper panel: Relative error of numerical PBE calculations with respect to ground-state energies resulting from Eq. (7). Lower panel: Same for LDA calculations. Hooke atoms with varying confinement strengths and particle numbers up to $N = 1500$ were considered (see main text for details).

## IV. SCALING RELATIONS FOR THE CHEMICAL POTENTIALS AND ADDITION ENERGIES

Next, we proceed with the scaling of the electrochemical potential defined as $\mu(N) = E_{gs}(N) - E_{gs}(N-1)$. The scaling relations for 2D systems have proven to be rather useful in the interpretation of Coulomb blockade experiments [9]. The behavior of chemical potentials—when measured or calculated from the first principles—also gives useful information of the shell structure of the system.

From Eq. (3) we obtain

$$\mu \sim \frac{\partial}{\partial N} E_{gs} = \frac{\partial}{\partial N}[\omega N^{4/3} f_{gs}(z)] \tag{8}$$

or

$$\frac{\mu}{\omega N^{1/3}} = f_\mu(z). \tag{9}$$

By approximating $f_{gs}(z)$ with Eq. (7) in Eq. (3) we can express $f_\mu(z)$ as

$$f_\mu(z) = \frac{3.0423 + 4.1893z^{2/3} + 4.05653z^{4/3} + 1.5z^2}{(1.4524 + 1.z^{2/3})^2}.$$

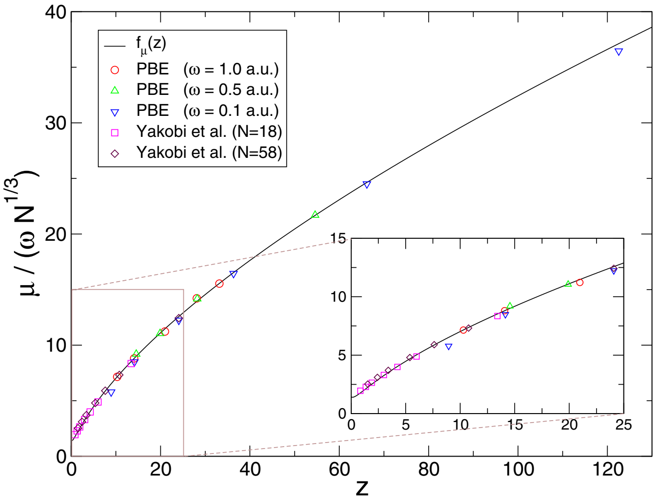

FIG. 4. Scaled chemical potentials (PBE results) of Hooke atoms as a function of $z$. The solid line represents the function $f_\mu$ in Eq. (10). Inset: Results from additional coupled-cluster (singles and doubles) calculations of systems with $\{N = 18,58\}$ and confinement strengths ranging from 0.1 to 25.0 a.u. [32].

Following the same reasoning, we can proceed with the addition energy defined as $\Delta\mu(N) = \mu(N) - \mu(N-1) = E_{gs}(N+1) - 2E_{gs}(N) + E_{gs}(N-1)$. We can now find an expression

$$\Delta\mu \sim \frac{\partial}{\partial N}\mu = \frac{\partial}{\partial N}[\omega N^{1/3} f_\mu(z)] \tag{10}$$

or

$$\frac{\Delta\mu}{\omega N^{-2/3}} = f_{\Delta\mu}(z). \tag{11}$$

Function $f_{\Delta\mu}(z)$ can also be expressed in terms of two polynomials, i.e., $f_{\Delta\mu}(z) = r(z)/s(z)$, where

$$r(z) = 1.4723 + 3.0423z^{2/3} + 5.8916z^{4/3} + 4.2569z^2 + 1.0z^{8/3} \tag{12}$$

and

$$s(z) = (1.4524 + 1.0z^{2/3})^3. \tag{13}$$

Figure 4 shows the scaled values of $\mu$ as a function of $z$, computed from our PBE results. No fitting process is performed in this case. Similarly to the previous results for the total energy, we find excellent agreement between the scaling relation, Eq. (10), and the calculated values of $\mu$. The additional numerical results calculated within the coupled-cluster (singles and doubles) method [32] correspond to the chemical potentials of systems with $N = 18,58$ and $\omega = 0.1,0.5,1.0,2.0,5.0,10.0,25.0$ for both $N$. This additional data set also agrees very well with the scaling relation (inset of Fig. 4).

In the case of the addition energies $\Delta\mu$ in Fig. 5, we add three data sets for small electron numbers and $\omega = 0.5$. The data sets correspond to the LDA, variational Monte Carlo (VMC), and DMC calculations for $\{\omega = 0.5, 2 \leqslant N \leqslant 9\}$ [33]. The solid line in Fig. 5 corresponds to

$$\Delta\mu(N,\omega = 0.5) = v(N)(1.1528N^{2/3} + 1.0N)^{-3} \tag{14}$$

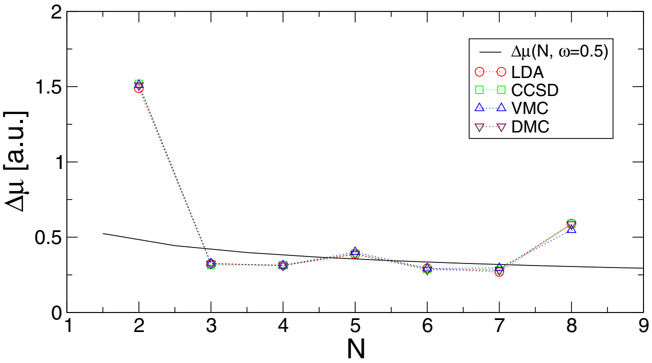

FIG. 5. Addition energies of few-particle Hooke atoms as a function of $zN$ (symbols). The results correspond to the local-density approximation (LDA) within density-functional theory, variational quantum Monte Carlo (VMC), and diffusion Monte Carlo (DMC). The solid line represents the function $\Delta\mu(N,\omega = 0.5)$ in Eq. (14).

with

$$v(N) = 0.3682 + 0.9583N^{1/3} + 2.3381N^{2/3} + 2.1285N + 0.6299N^{4/3}, \tag{15}$$

obtained from $f_{\Delta\mu}(z)$ by explicitly substituting $z = (N/\omega)^{1/2}$ and setting $\omega = 0.5$.

The agreement for the addition energies is good except for two outliers at $N = 2$ and $N = 8$, where all the reference results show large peaks. They correspond to completely filled energy shells, which are known to be energetically very stable [7]. The shell effects are beyond the reach of our model based on the Thomas-Fermi approach, where the kinetic energy is an explicit orbital-free functional of the density. We expect, however, that $f_{\Delta\mu}(z)$ performs much better in the large-$N$ limit, where, as in the 2D case [9], jumps in the additional energy are less pronounced.

## V. SUMMARY

In summary, we have used the Thomas-Fermi approach to derive scaling relations for several energetic quantities of many-electron Hooke atoms, i.e., three-dimensional harmonic electron droplets consisting of $N \geqslant 2$ interacting electrons. The analytic scaling relations have been supplemented by density-functional results to determine the parameter values in the scaling. The obtained full expressions for the total energy, electrochemical potential, and addition energy have then been compared to additional results obtained with alternative methods such as coupled-cluster calculations and variational, diffusion, and path-integral Monte Carlo methods. In most cases, excellent numerical agreement has been found throughout a large regime of parameter values, excluding extremely weak confinements (strong correlations).

The obtained scaling relations are useful to assess energetic quantities of very large harmonically confined systems that are beyond the reach of current electronic structure methods. Moreover, the accuracy of the scaling provides a way to assess the accuracy of the convergence obtained within a first-principles method. Given the general character of the scaling properties, they could be employed in the developments of density functionals for the exchange and correlation, or as a starting point for approximations in self-consistent orbital-free methods. The present work can be continued in different directions: for example, to study how the obtained scaling relations are affected by anharmonicity effects in the external potential.

## ACKNOWLEDGMENTS

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