

Tan's Two-Body Contact in a Planar Bose Gas: Experiment versus Theory

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We determine the two-body contact in a planar Bose gas confined by a transverse harmonic potential, using the nonperturbative functional renormalization group. We use the three-dimensional thermodynamic definition of the contact where the latter is related to the derivation of the pressure of the quasi-two-dimensional system with respect to the three-dimensional scattering length of the bosons. Without any free parameter, we find a remarkable agreement with the experimental data of Zou *et al.* [Tan's two-body contact across the superfluid transition of a planar Bose gas, *Nat. Commun.* **12**, 760 (2021).] from low to high temperatures, including the vicinity of the Berezinskii-Kosterlitz-Thouless transition. We also show that the short-distance behavior of the pair distribution function and the high-momentum behavior of the momentum distribution are determined by two contacts: the three-dimensional contact for length scales smaller than the characteristic length $\ell_z = \sqrt{\hbar/m\omega_z}$ of the harmonic potential and, for length scales larger than ℓ_z , an effective two-dimensional contact, related to the three-dimensional one by a geometric factor depending on ℓ_z .

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Introduction.—Relating the macroscopic properties of a physical system to microscopic interactions and degrees of freedom is one of the main goals of many-body quantum physics. In ultracold atomic gases not all details of the interaction potential between particles are required since low-energy collisions are generally fully described by the s -wave scattering length. As a result, the equation of state of a dilute gas takes a simple, universal, expression where the microscopic physics enters only through two parameters, the mass of the particles and the scattering length. Considering the latter as an additional thermodynamic variable, besides the usual variables (e.g., the chemical potential μ and the temperature T in the grand canonical ensemble), one can define its thermodynamic conjugate, the so-called Tan two-body contact C [1–3]. In a dilute gas, the contact relates the (universal) low-temperature thermodynamics to the (universal) short-distance behavior which shows up in the two-body correlations or the momentum distribution function [1–9]. This simple description fails in a strongly interacting Bose gas where other parameters (e.g., associated with three-body effective interactions) are required for a complete description of the universal thermodynamics and short-distance physics [10].

There have been few measurements of the two-body contact in Bose gases. Apart from experiments in the thermal regime [11,12] or the quasi-pure BEC one [11,13], the two-body contact has been determined in a planar Bose gas in a broad temperature range including the normal and superfluid phases as well as the vicinity of the Berezinskii-Kosterlitz-Thouless (BKT) transition [14].

The experimental data are in good agreement with theoretical predictions in the high-temperature limit (normal gas) and in the low-temperature limit (strongly degenerate superfluid). On the other hand, there is no theoretical explanation for the value of the contact obtained near the BKT transition. In particular, the experimental data seem at odds with the predictions of a classical field theory [15] used earlier successfully for the equation of state of a two-dimensional Bose gas [16,17].

In this Letter we compute the two-body contact in a planar Bose gas confined by a harmonic potential using the nonperturbative functional renormalization group (FRG), a modern implementation of Wilson's RG [18–20]. This approach has proven to be very accurate for determining the equation of state of such a system [21]. We consider the weak-coupling limit where the three-dimensional scattering length a_3 of the bosons is much smaller than the characteristic length $\ell_z = \sqrt{\hbar/m\omega_z}$ of the harmonic potential. We use the three-dimensional thermodynamic definition of the contact where the latter is expressed as a derivative of the pressure with respect to the three-dimensional scattering length a_3 and pay special attention to the quasi-two-dimensional structure of the system. We show that the short-distance behavior of the pair distribution function and the high-momentum behavior of the momentum distribution are determined by two contacts: the three-dimensional contact for length scales smaller than ℓ_z and, for larger length scales, an effective two-dimensional contact (obtained from the derivative of the pressure with respect to the effective two-dimensional scattering length of the

confined bosons), related to the three-dimensional one by a geometric factor depending on ℓ_z . We then compare our results with the experimental data of Ref. [14]. Without any free parameters, we find a remarkable agreement between theory and experiment from low to high temperatures, including the vicinity of the BKT phase transition. We also show how to reconcile these experimental data with the classical field simulations of Ref. [15].

Contact of a planar Bose gas.—We consider a quasi-two-dimensional system of surface L^2 obtained by subjecting a three-dimensional Bose gas to a confining harmonic potential of frequency $\omega_z = \hbar/m\ell_z^2$ along the z direction. In the low-temperature regime $k_B T \ll \hbar\omega_z$, the physical properties of the planar gas can be obtained from the effective two-dimensional Hamiltonian (from now on we set $\hbar = k_B = 1$)

$$\hat{H} = \int d^2r \left\{ \frac{\nabla\hat{\psi}^\dagger \cdot \nabla\hat{\psi}}{2m} + \frac{g}{2} \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \right\}, \quad (1)$$

with an ultraviolet momentum cutoff $\Lambda \simeq 0.54\ell_z^{-1}$ [22,23]. The effective interaction constant g is related to the three-dimensional scattering length a_3 by

$$mg = \sqrt{8\pi} \frac{a_3}{\ell_z}. \quad (2)$$

Computing the low-energy scattering amplitude from (1), one obtains the effective two-dimensional scattering length a_2 as a function of the microscopic parameters of the gas [22–24],

$$\frac{a_2}{\ell_z} \simeq 3.71 e^{-\sqrt{\frac{\pi\ell_z}{2a_3}} - \gamma}, \quad (3)$$

where $\gamma \simeq 0.577$ is the Euler constant.

In the low-temperature regime $T \ll \omega_z$, the pressure can be written in the scaling form characteristic of a two-dimensional system [21],

$$P(\mu, T) = -\frac{\Omega(\mu, T)}{L^2} = \frac{T}{\lambda^2} \mathcal{F}\left(\frac{\mu}{T}, \tilde{g}(T)\right), \quad (4)$$

where $\Omega(\mu, T)$ is the grand potential, \mathcal{F} a universal scaling function, $\lambda = \sqrt{2\pi/mT}$ the thermal de Broglie wavelength, and

$$\tilde{g}(T) = -\frac{4\pi}{\ln\left(\frac{1}{2}\sqrt{2ma_2^2 T}\right) + \gamma} \quad (5)$$

a temperature-dependent dimensionless interaction constant. Equation (4) is valid for $|\mu|$, $T \ll \Lambda^2/2m \sim \omega_z$. The corrections to the scaling form (4) are negligible when $ma_2^2 T$, $ma_2^2 |\mu| \ll 1$. The dependence of the scaling function \mathcal{F} on μ/T and $ma_2^2 T$ can be simply obtained by

dimensional analysis using the fact that the scattering length is the only characteristic length scale at low energies. Renormalization-group arguments show that the dependence on $ma_2^2 T$ arises only through $\tilde{g}(T)$ [21].

The pressure depending only on a_3 [through $a_2 \equiv a_2(a_3, \ell_z)$] and not on the details of the interaction potential between particles, it is natural to consider a_3 as an additional thermodynamic variable besides μ and T [1]. The quasi-two-dimensional two-body contact C is then essentially defined as the conjugate variable to a_3 ,

$$\frac{C}{L^2} = 8\pi m \left. \frac{\partial P}{\partial(1/a_3)} \right|_{\mu, T}. \quad (6)$$

C is an extensive quantity with dimension 1/length. It can equivalently be defined in the canonical ensemble by replacing the pressure by the energy density in (6) and taking the derivative at fixed particle number and entropy. The motivation for defining the contact from a derivative with respect to $1/a_3$ as in a three-dimensional system, rather than with respect to $\ln a_2$ as in a two-dimensional system, is that in the limit $a_3 \ll \ell_z$ the collisions keep their three-dimensional character at length scales smaller than ℓ_z .

Using the equation of state (4), we can write the contact as

$$\frac{C}{L^2} = -4(2\pi)^{5/2} \frac{T\ell_z}{\lambda^4} \mathcal{F}^{(0,1)}\left(\frac{\mu}{T}, \tilde{g}(T)\right) \tilde{g}'(T), \quad (7)$$

where we use the notation $\mathcal{F}^{(i,j)}(x, y) = \partial_x^i \partial_y^j \mathcal{F}(x, y)$. On the other hand, the scaling function \mathcal{F} determines the two-dimensional particle and entropy densities, $\bar{n} = \partial P / \partial \mu$ and $s = \partial P / \partial T$. This allows us to express $\mathcal{F}^{(0,1)}$ in terms of P , \bar{n} , s , which leads to a relation between the contact and the thermodynamic potentials P and E (as in isotropic systems [2])

$$\frac{C}{L^2} = 4(2\pi)^{5/2} \frac{\ell_z}{\lambda^2 T} \left(P - \frac{E}{L^2} \right), \quad (8)$$

where $E/L^2 = -P + Ts + \mu\bar{n}$ is the two-dimensional energy density.

In the weak-coupling limit, the scattering length a_2 is exponentially small with respect to ℓ_z and $\tilde{g}(T) \simeq \tilde{g} = 2mg$ is nearly temperature independent except for exponentially small temperatures $T \sim \omega_z e^{-\sqrt{\pi/2}(\ell_z/a_3)}$. For this reason it is often concluded that the two-dimensional Bose gas exhibits an approximate scale invariance [15–17] (with no characteristic energy scales other than μ and T): $\mathcal{F}[\mu/T, \tilde{g}(T)] \simeq \mathcal{F}(\mu/T, \tilde{g})$ [21], and the normalized contact $C\lambda^4/L^2\ell_z$ is a function of μ/T and \tilde{g} . However the assumption of approximate scale invariance cannot be used in the calculation leading to (8) since this would imply

$\hat{g}'(T) = 0$ and in turn $E = L^2 P$ and $C = 0$. The contact defined in (8) can thus be seen as a measure of the breakdown of scale invariance in the planar Bose gas [25]. The situation is different in an isotropic three-dimensional system; in the unitary limit $a_3 \rightarrow \infty$ where scale invariance is satisfied, $E_{3D} = (3/2)L^3 P_{3D}$, but the contact remains finite since $(3/2)P_{3D} - E_{3D}/L^3 = \mathcal{O}(1/a_3)$, whereas $C_{3D} \propto a_3[(3/2)P_{3D} - E_{3D}/L^3]$.

A remarkable feature of the contact defined from the pressure is that it also determines the short-distance behavior of the pair distribution function as well as the high-momentum limit of the momentum distribution function [1–9]. This property still holds in the planar gas. For the pair distribution function, averaged over the position $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ of the pair center of mass, one has [26]

$$g(\mathbf{r}) = \int d^3 R \langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) \rangle, \\ = \begin{cases} \frac{C}{(4\pi)^2} \left(\frac{1}{|\mathbf{r}|} - \frac{1}{a_3} \right)^2 & \text{if } |\mathbf{r}| \ll \ell_z, \lambda, d, \\ \frac{C}{\sqrt{2\pi}\ell_z} |\phi_0^-(z)|^2 \left(\frac{\ln|\rho/a_3|}{2\pi} \right)^2 & \text{if } \ell_z \ll |\rho| \ll \lambda, d, \end{cases} \quad (9)$$

where $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 = (\boldsymbol{\rho}, z)$ is the coordinate of the relative motion of the pair (with $\boldsymbol{\rho}$ a two-dimensional coordinate) and d the mean interparticle distance. ϕ_0^- denotes the ground state of a particle of reduced mass $m/2$ in an harmonic potential of characteristic frequency ω_z . The fact that the contact (6) determines the pair distribution function at short length scales, $|\mathbf{r}| \ll \lambda, \ell_z, d$, is not surprising since $C \propto \partial P / \partial(1/a_3)$ is defined as in the three-dimensional case. On the other hand, the effective contact that appears in the regime $\ell_z \ll |\rho| \ll \lambda, d$ can be written as

$$\frac{C}{\sqrt{2\pi}\ell_z L^2} = -4\pi m \frac{\partial P}{\partial \ln a_2}, \quad (10)$$

and thus coincides with the usual thermodynamic definition of a two-dimensional contact. Similarly, for the momentum distribution function $\bar{n}_{\mathbf{k},k_z}$, one finds

$$\bar{n}_{\mathbf{k},k_z} = \frac{C}{(\mathbf{k}^2 + k_z^2)^2} \quad \text{if } \frac{1}{a_3}, \frac{1}{d}, \frac{1}{\lambda} \ll \sqrt{\mathbf{k}^2 + k_z^2}, \quad (11)$$

and

$$\bar{n}_{\mathbf{k}}^{(2D)} = \int \frac{dk_z}{2\pi} \bar{n}_{\mathbf{k},k_z}, \\ = \frac{1}{\sqrt{2\pi}\ell_z} \frac{C}{|\mathbf{k}|^4} \quad \text{if } \frac{1}{d}, \frac{1}{\lambda} \ll |\mathbf{k}| \ll \frac{1}{\ell_z}, \quad (12)$$

where we assume the normalization $\frac{1}{L^2} \sum_{\mathbf{k}} \int (dk_z/2\pi) \bar{n}_{\mathbf{k},k_z} = N$ (with $N \equiv \langle \hat{N} \rangle$ the total number of particles). Equation (11) holds at any temperature while Eq. (12) is valid only in the low-temperature regime $T \ll \omega_z$. Note that a result similar

to (11), (12) has been obtained for fermions in quasi-one- and quasi-two-dimensional traps [37] (see also [38,39] for bosons in a quasi-one-dimensional trap).

FRG calculation of the contact.—Following Ref. [21] we compute the pressure of the planar Bose gas at low temperatures $T \ll \omega_z$ using the two-dimensional Hamiltonian (1). The main quantity of interest in the FRG approach is the effective action (or Gibbs free energy) Γ , defined as the Legendre transform of the Helmholtz free energy, and which is directly related to the pressure: $P = -(T/L^2)\Gamma$. We refer to Refs. [20,21] for a detailed description of the method. Once the pressure is known, the contact is obtained from (6).

The FRG approach to interacting boson systems has proven to be very accurate. In particular, the universal scaling function \mathcal{F} entering the equation of state (4) of the two-dimensional Bose gas has been computed using the FRG approach [21], and very good agreement with experimental data in planar gases [16,40,41], with or without an optical lattice, has been obtained [42].

In Fig. 1, we show the contact C normalized by $L^2 \ell_z / \lambda^4$ obtained for $2mg = 2\sqrt{8\pi}a_3/\ell_z = 0.32$ and $T/\omega_z \simeq 0.00145$ by computing the pressure P for two nearby values of a_3 and taking a numerical derivative. We find a very good agreement with two limiting cases [26], the zero-temperature limit in the superfluid phase where

$$\frac{C_{\text{Bog}}}{L^2} = \sqrt{2\pi} (m\mu)^2 \ell_z \quad (13)$$

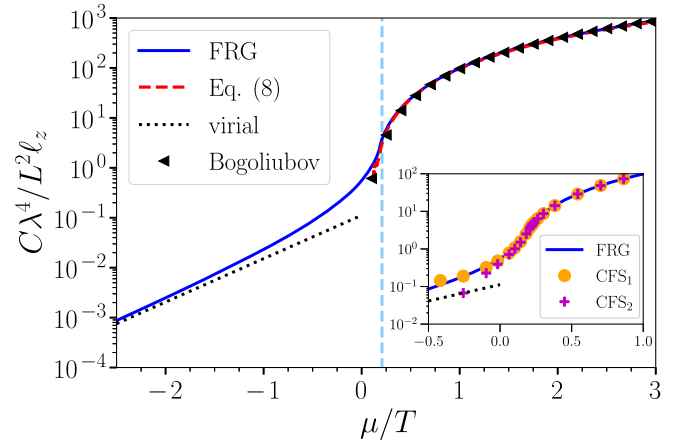


FIG. 1. Two-body contact $C\lambda^4/L^2\ell_z$ vs μ/T for $2mg = 0.32$ and $T/\omega_z \simeq 0.00145$ as obtained from the FRG [solid (blue) line]. The dashed (red) line shows the result obtained from (8) while the symbols correspond to the Bogoliubov result (13) and the virial expansion (14). The BKT transition occurs at $\mu/T \simeq 0.21$, shown as a vertical dashed line, as estimated from FRG. The inset shows a comparison between FRG and classical field simulations using the thermodynamic definition (6) [CFS₁, (orange) circles] and the relation between C and $\langle (\hat{\psi}^\dagger)^2 (\hat{\psi})^2 \rangle$ [CFS₂, (purple) crosses]; see text.

can be obtained from the Bogoliubov theory (including the Lee-Huang-Yang correction [46]), and the dilute normal gas where

$$\frac{C_{\text{virial}}}{L^2} = \frac{z^2 \ell_z}{\lambda^4} \frac{2(2\pi)^{5/2}}{|\ln(\frac{a_2}{\lambda} \sqrt{\frac{\pi}{2}} e^{\gamma})|^2} \quad (14)$$

(with $z = e^{\beta\mu}$ the fugacity) can be obtained from the virial expansion. The contact deduced from (8), the two-dimensional energy density $E/L^2 = -P + T\partial P/\partial T + \mu\partial P/\partial\mu$ being obtained from numerical derivatives, is also shown in the figure. The apparent disagreement for $\mu/T \lesssim 0.5$ is due to a lack of precision in the numerical calculation, the values of P and E/L^2 being extremely close and the normalized contact very small.

The inset of Fig. 1 shows the contact obtained from the classical field simulations of Ref. [15] using two different methods. The first one (CFS₁) is based on the thermodynamic definition (6) of the contact and the calculation of the pressure P , the second one (CFS₂) uses the definition $C/L^2 = 4(2\pi)^{3/2}(a_3^2/\ell_z)\langle(\hat{\psi}^\dagger)^2(\hat{\psi})^2\rangle$ [which follows from Eq. (6)]. Both P and $\langle(\hat{\psi}^\dagger)^2(\hat{\psi})^2\rangle$ are obtained from the results of Ref. [15] (see [26]). The first method has one fitting parameter, the value of the contact at the BKT transition, which we determine by minimizing the relative difference between the FRG and the classical field results. The first method CFS₁ and the FRG are in agreement with an accuracy better than 1% when $\mu/T \gtrsim 0.25$. In the range $0 \lesssim \mu/T \lesssim 0.25$, which includes the fluctuation region about the BKT transition, the agreement remains within 5% but deteriorates when $\mu/T < 0$. The second method, CFS₂, is clearly much less accurate when $\mu/T < 0$ and breaks down in the low-density limit since C becomes negative when $\mu/T \lesssim -0.3$.

Comparison with the experiment.—The thermodynamic definition (6) of the contact was realized experimentally by means of a Ramsey interferometric method [14]. The measurements were performed on a Bose gas of ⁸⁷Rb atoms confined by a harmonic potential with $2mg = 2\sqrt{8\pi}a_3/\ell_z = 0.32$ in a broad temperature range around the BKT transition. In Fig. 2 we compare the experimental data with the FRG and classical field results obtained for $2mg = 0.32$. Following Ref. [14] we show the contact normalized by the mean-field contact $C_0 = 4(2\pi)^{3/2}L^2\bar{n}^2a_3^2/\ell_z$ as a function of the phase-space density $\mathcal{D} = \bar{n}\lambda^2$. The FRG calculation is done at $T/\omega_z = 0.03$, low enough to be in the quasi-2D regime ($T \ll \Lambda^2/2m$) but high enough to minimize the logarithmic corrections (in the experiment, $T/\omega_z \in [0.05, 0.75]$). The normalized contact varies between [47]

$$\frac{C_{\text{Bog}}}{C_0} = \frac{\pi}{2} \frac{\ell_z^2/a_3^2}{|\ln(a_2\sqrt{\pi\bar{n}}e^{\gamma+1/2})|^2} \simeq 1 \quad (15)$$

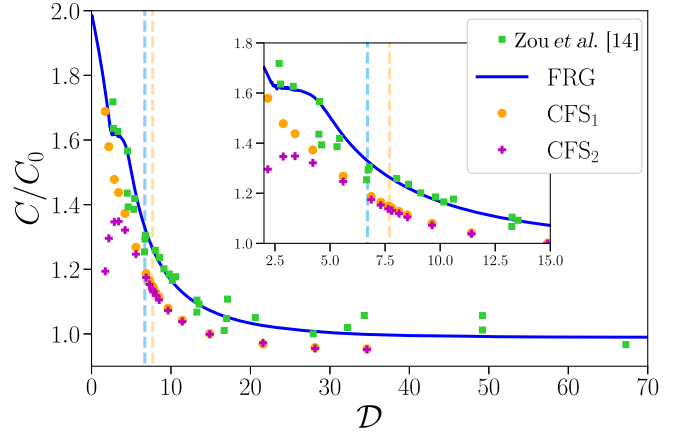


FIG. 2. Normalized two-body contact C/C_0 as a function of the phase-space density $\mathcal{D} = \bar{n}\lambda^2$ for $2mg = 0.32$. The square (green) symbols show the experimental data from Ref. [14] and the solid (blue) line the FRG result at $T/\omega_z = 0.03$. The (orange) circles and (purple) crosses are the estimate from classical field simulations, CFS₁ and CFS₂, respectively (see text). The vertical dashed lines correspond to the position of the BKT transition as estimated from FRG at $\mathcal{D} \simeq 6.7$ (blue line on the left) and classical field simulations at $\mathcal{D} \simeq 7.7$ (orange line on the right). The inset is an enlargement on the fluctuation region about the BKT transition.

for $\mathcal{D} \gg 1$ and

$$\frac{C_{\text{virial}}}{C_0} = \frac{\ell_z^2}{a_3^2} \frac{\pi}{|\ln(\frac{a_2}{\lambda} \sqrt{\frac{\pi}{2}} e^{\gamma})|^2} \simeq 2 \quad (16)$$

for $\mathcal{D} \ll 1$.

The agreement between FRG and the experimental data is very good in spite of the absence of any fit parameter. On the other hand, there is a downward shift of the classical field result with respect to the experimental data (only CFS₂ was compared to the experimental data in Ref. [14]). This does not come from the value of the contact, which is highly accurate for $\mu > 0$ as previously discussed (Fig. 1), but apparently from a lower accuracy of the density estimate and therefore the normalized contact C/C_0 . The relative difference between the FRG and CFS results for the density (for a given value of the chemical potential) is only about 5%, but this is enough to have a visible effect in the plot of C/C_0 . Normalizing the contact with C_{Bog} gives the same qualitative results [26]. The classical field result CFS₁, apart from this downward shift, provides us with a good fit of the experimental data except in the low-density limit $\mathcal{D} \lesssim 1.5$ where it becomes much too large (and therefore does not appear in Fig. 2). Note that there is no sign of the BKT transition, predicted to occur around $\mathcal{D} \simeq 7.7$ (classical field simulations [15]) and $\mathcal{D} \simeq 6.7$ (FRG), marked as vertical dashed lines in Fig. 2. The bump predicted by the FRG near $\mathcal{D} = 3$ is due to the rapid change of \bar{n} , and therefore C_0 , for small and positive values

of μ/T [16,17]. Although this bump also appears in the experimental data, the 3%–10% experimental uncertainty [48] does not allow us to assert that it is a real feature.

Conclusion.—The theoretical calculation of the two-body contact of a planar Bose gas in the framework of the nonperturbative FRG is in remarkable agreement with the experimental data of Ref. [14]. The FRG provides us with an accurate value of the contact over a broad temperature range including the vicinity of the BKT transition. We have also shown how the apparent contradiction between the experimental data of Ref. [14] and the classical field simulations [15] can be overcome. The FRG predicts a bump in the contact for a phase-space density $\mathcal{D} \simeq 3$, which requires improved-precision measurements to be confirmed.

An interesting aspect of the contact theory in a quasi-two-dimensional gas is that the high-momentum tail, $\sqrt{\mathbf{k}^2 + k_z^2} \gg 1/a_3, 1/\lambda, 1/d$, of the three-dimensional momentum distribution is controlled by the three-dimensional contact [as defined in (6)] while the intermediate momentum range, $1/d, 1/\lambda \ll |\mathbf{k}| \ll 1/\ell_z$, is controlled by the effective two-dimensional contact $C/\sqrt{2\pi}\ell_z$ [Eqs. (11), (12), and Refs. [37,39]]. A measure of the momentum distribution, for instance, by ballistic expansion of the atomic cloud or rf spectroscopy [49], would allow us to confirm this essential property of the contact theory.

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