# A study of a simple equation that describes the ground-state energy of a Bose gas at low and high density and in dimensions one, two and three

**Elliott Lieb**
**Princeton University**



**Joint work with**
**Eric Carlen, and Ian Jauslin**

**Reference:** *Physical Review* **130**, *2518-2528 (1963) (+ 2 more).*

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# New definition of the $N$-point function

The usual $N$-particle translation-invariant Hamiltonian in a box $\Lambda$ of volume $|\Lambda|$, and particle density $\rho = N/|\Lambda|$, is

$$H = -\frac{1}{2}\sum_{1\le j\le N}\Delta_j + \sum_{1\le i<j\le N} V(|x_i - x_j|).$$

Its ground-state wave function $\Psi(x_1 \ldots, x_N)$ is unique and positive, and we normalize it by $\int_{\Lambda^N}\Psi = 1$.

We assume the 2-body potential $V$ is *positive, radial and integrable.*

A special case is the hard-core $V$ of radius (and scattering length) $a$

The new $n$-body density, which is *not quadratic in* $\Psi$, is

$$g^n(x_1,\ldots x_n) = |\Lambda|^n \int_{\Lambda^{N-n}} \Psi(x_1,\ldots, dx_N)\, dx_{n+1}\ldots x_N.$$

By translation invariance, $g^0$ and $g^1$ equal 1, and $g^2(x_1, x_2) =: g(|x_1 - x_2|)$.

We want to find suitable equations for $g$ and hence for $e := E/N$, the ground-state energy/particle.

# Quick 'derivation' of simple equation, 1963

From Schrödinger's equation $H\Psi = Ne\,\Psi$, we integrate to obtain $2e/\rho = \int g(x)V(x)dx$. Next, we integrate over $(N-2)$ $x's$ and get

$$[-\tfrac{1}{2}(\Delta_1 + \Delta_2) + V_{12}]g^2(1,2) = eg^2(1,2) - 2\rho \int g^3(1,2,3)V_{2,3}dx_3 - \tfrac{1}{2}\rho^2 \int\int g^4(1,2,3,4)V_{3,4}dx_3dx_4.$$

This is motivated by a similar equation in classical stat mech where the role of $\Psi$ is played by the Boltzmann factor $e^{-\beta H}$.

We write $g(x) := 1 - u(x)$.

To make progress we make assumptions about how $g^3$, $g^4$ are related to $g^2$. They are presumably quite reliable to leading order when $\rho \ll 1$ . For example $g^3(1,2,3) \approx [1-u(1,2)][1-u(1,3)][1-u(2,3)]$ and Then (in the limit $|\Lambda| \to \infty$)

$$\int g^3(1,2,3)V(2,3)d3 = g^2(1,2)\left[2e/\rho - \int u(1,3)g^2(2,3)V(2,3)d3\right]$$

# Quick 'derivation' of simple equation, 1963

I confess to having been sloppy by leaving out $O(1/|\Lambda|)$ corrections. They play no role in the calculation of $g^3$ above, but they do play a role in the calculation of $g^4$ in terms of $g^2$. All these approximations remain to be proved. But they work quite well, as we shall see.

The final equation for the 2-body function $g = 1 - u$ is:

$$(-\Delta + V(x))g(x) = \rho g(x)\{2K(x) - \rho L(x)\} \qquad \text{with}$$

$$L(1,2) = \int\int \Big\{ u(1,3)u(2,4)\{g(1,4)g(2,3) - \tfrac{1}{2}u(1,4)u(2,3)\}g(3,4)V(3,4) \Big\} d3d4$$

$$K(1,2) = \int u(1,3)\, g(2,3)V(2,3)\, d3 \qquad \text{or} \qquad K(x) = (u * gV)(x).$$

This is quite a complicated 'differential-integral' equation– the 'big equation'. We have investigated it numerically and the results agree with the slightly less accurate 'small equation' which is obtained from this by taking leading terms from the big equation–as follows:

# The 'small simple equation'

Recalling $g = 1 - u$ and $\int V(1-u) = \int Vg = 2e/\rho$, and taking the main terms from the big equation:

$$\boxed{\Big(-\Delta + 4e + V(x)\Big)u(x) = V(x) + 2e\rho(u * u)(x).} \qquad **$$

There are 2 supplementary conditions: (a) $0 \le u(x) \to 0$ as $x \to \infty$;

(b) $\int V(1-u) = 2e/\rho$.

We also expect to find that $u(x) \le 1$, otherwise $g = 1 - u$ is not nonegative. If there is such a solution then, by integrating the equation, $\int u = 1/\rho$.

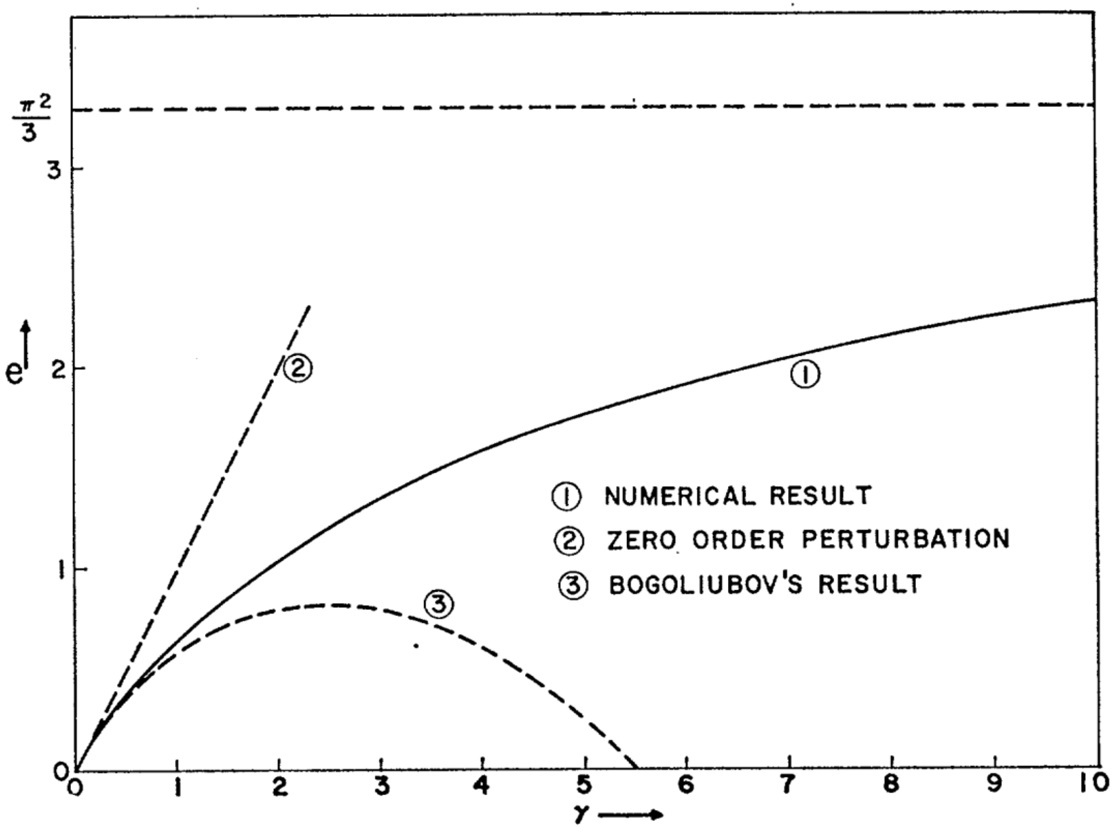
*There is a unique solution that satisfies these conditions,* as we will prove.

But let us first demonstrate the accuracy of this enterprise in the case where the exact $e(\rho)$ is known — the 1D $\delta$-function gas:

# Lieb-Liniger model 1963

Here, $V(x) = c\delta(x)$ with $c \geq 0$. The dimensionless parameter is $\gamma = c/\rho$, and the energy/particle (denoted by $e$ before) is $\rho^2 e(\gamma)$.

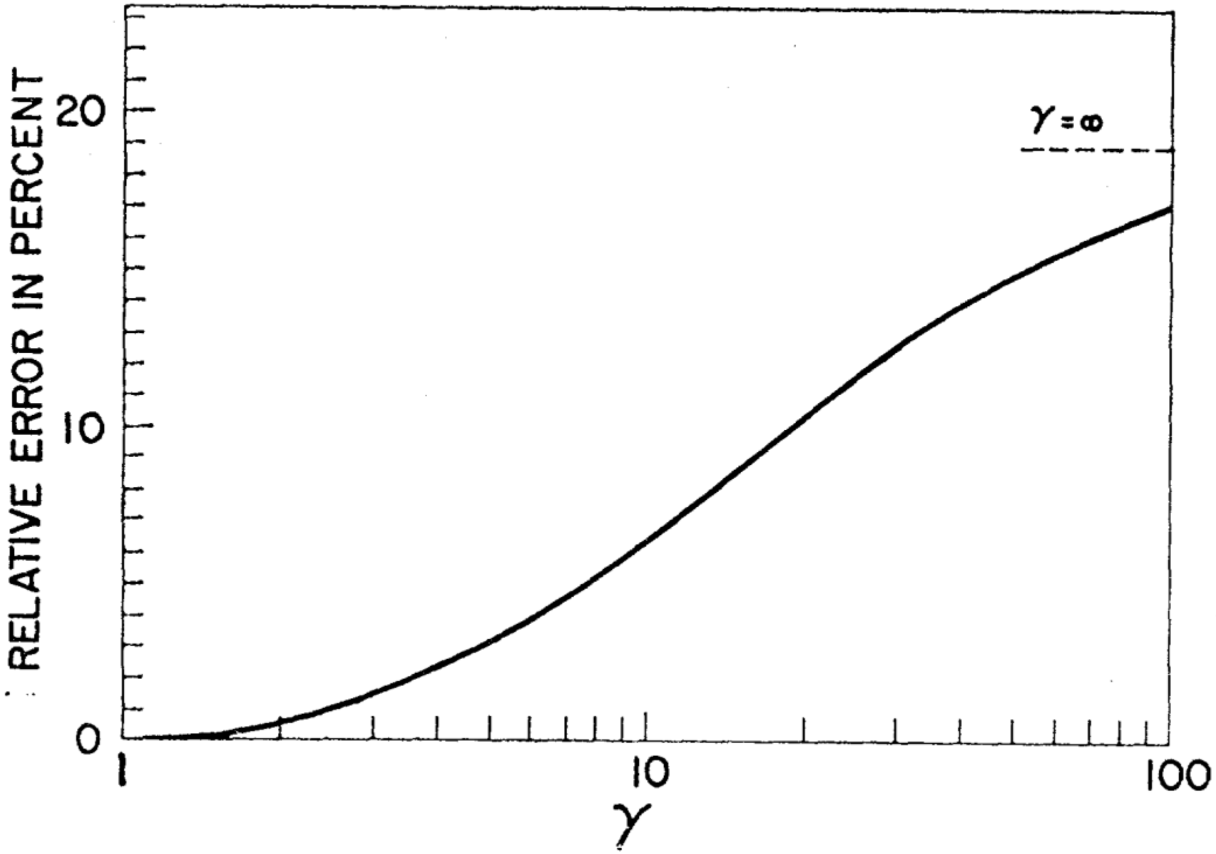
*Note:* The easy, perturbation theory side corresponds to large $\rho$. The graphic compares the exact $e$ with Bogolubov's and with simple perturbation theory. As $\gamma \to \infty$, $e(\gamma) \to \pi^2/3$, a fact 'proved' not long ago.



**The $\delta$-function and 1D makes things easy, even the Big equation, which becomes (in dimensionless units)** $\ddot{u} = e(1-u)\left\{2u - u*u + 2u^2*u - \frac{1}{2}u^2*u^2\right\}$.

**The Small equation is simply** $\ddot{u} = e(\gamma)\left\{2u - u*u\right\}$.

**The maximum error with the Big eqn is only 19%. The Small eqn can be solved exactly with Fourier transforms and its error is 69%.**



# Existence and uniqueness

We fix $e$ and proceed by iteration of the $u * u$ term.

$u_0 := (-\Delta + 4e + V(x))^{-1} V$. $\qquad u_{n+1} := (-\Delta + 4e + V(x))^{-1} \Big[ V + 2e\rho_n u_n * u_n \Big]$

where $\rho_n$ is defined by $\qquad 2e/\rho_n := \int V(1 - u_n)$ ,

and is exact if there is a solution. Note that $(\cdots)^{-1}$ is a positive kernel.

(Important:We might have used $\int u_n =: 1/\rho_n$, but that doesn't work!)

**LEMMA:** $u_n(x) \le 1$ (miracle) and $u_{n+1}(x) \ge u_n(x)$, $\rho_{n+1} \ge \rho_n \quad \forall n \ge 0, \forall x$.

Proof: Let $A_n = \{x : u_n(x) > 1\}$. Clearly, $u_{n+1} \ge u_n \Rightarrow \rho_{n+1} \ge \rho_n$.

We start with $A_0$. $(-\Delta)u_0 = V(1-u) - 4eu_0 \Rightarrow u_0$ is subharmonic on $A_0$ and $u_0 \to 0$ at $\infty$. Therefore, $\max u_0 = 1$ in $A_0$, which implies $A_0 = \emptyset$.

Now we turn to $u_{n+1}$, $n > 0$. By induction, $\rho_n \ge \rho_{n-1}$ and $u_n * u_n \ge u_{n-1} * u_{n-1}$, so $u_{n+1} \ge u_n$. Moreover, $(u_n * u_n)(x) \le \int u_n$

We claim $\int u_n \le 1/\rho_n$. By induction, $\qquad 4e \int u_{n+1} =$

$2e/\rho_{n+1} + 2e\rho_n (\int u_n)^2 \le 2e/\rho_{n+1} + 2e\rho_n \int u_n \int u_{n+1} \le 2e/\rho_{n+1} + 2e \int u_{n+1}$.

To prove $u_{n+1} \le 1$, i.e. $A_n = \emptyset$, use the subharmonicity argument. On $A_n$, $(-\Delta)u_{n+1} = V(1 - u_{n+1}) - 4eu_{n+1} + 2e\rho_n u_n * u_n = (< 0) + (\le -4e) + (\le 2e)$.

□

# Existence and uniqueness (cont.)

**We now have an increasing sequence of $u's$ and $\rho's$ for each fixed $e$, which are uniformly bounded in every $L^p$ for $0 \leq p \leq \infty$. By monotone convergence (or whatever) this has a limit that satisfies the 'small' simple equation**

$$\Big(-\Delta + 4e + V(x)\Big)u(x) = V(x) + 2e\rho(u*u)(x).$$

**(We have not tried to do this for the big equation, but we are hopeful.)**

**This solution gives us a unique function $\rho(e)$. While there are other solutions, there is only one $\rho \geq 0$, $u \geq 0$ that satisfies the condition $\int V(1-u) = 2e/\rho$.**

**Proof of uniqueness:** **We suppose $\widetilde{u}$, $\widetilde{\rho}$ is another solution. From the equation $\widetilde{u} = (\cdots)^{-1}(V+2e\widetilde{\rho}\widetilde{u}*\widetilde{u})$ we see that $\widetilde{u} > u_0$ and, since $\int V(1-\widetilde{u}) = 2e/\widetilde{\rho}$, we have $\widetilde{\rho} > \rho_0$. By inserting this into the equation for $u_1$, we also have $\widetilde{u} > u_1$ and $\widetilde{\rho} > \rho_1$. Continuing to $\infty$, we have that $\widetilde{u} \geq u$ and $\widetilde{\rho} \geq \rho$. Since $\int \widetilde{u} = 1/\widetilde{\rho}$ we have a contradiction unless there is equality everywhere.** □

# Small equation challenges

**(A) We have seen that $e$ determines $\rho$, but we need to prove that $\rho$ determines $e$ uniquely. This would lead to Monotonicity of the function $e(\rho)$, which is required for physics. (We are able to prove continuity.)**

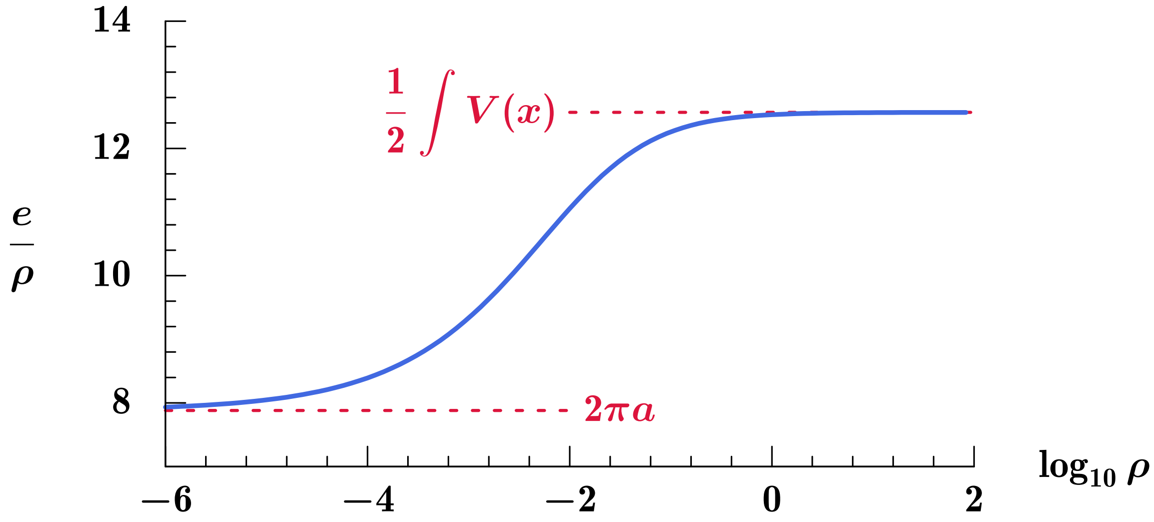
**(B) The physical requirement of stability (i.e., remove a partition and the density equilibrates) means that the function $\rho \to \rho e(\rho)$ is *convex.* In terms of the inverse function $e \to \rho(e)$, this means that $\dot{\rho}(e)^2 - \rho\ddot{\rho} \geq 0$. This is equivalent to $e \to 1/\rho(e)$ is *convex.***

**Numerical solution of the equation shows unambiguously that A and B are true.**

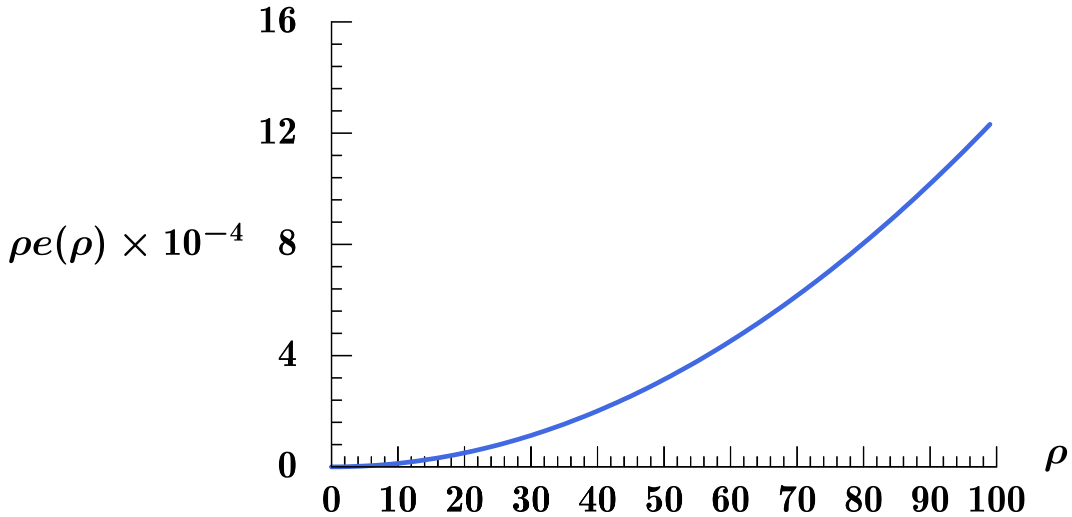
**(C) Repeat this whole story for the 'Big' simple equation.**

$$(-\Delta + V(x))u(x) = \rho g(x)\{2K(x) - \rho L(x)\}.$$

To get accurate numerical solutions is surprisingly tricky. Here are results for $V(x) = \exp(-|x|)$ in 3D. We find $a \approx 1.2544$. Graph #1 shows that $e(\rho)$ starts as $2\pi\rho a$ and ends as $\frac{1}{2}\rho \int V$. (Note: $\int V > 4\pi a$ when $V \geq 0$.) It displays the monotonicity (as a function of $\log \rho$)




Graph #2 shows the convexity of $\rho e(\rho)$ as a function of $\rho$.



# Analytic solution for small $\rho$

**We try to solve the small equation analytically for small $\rho$. First, $D = 3$.**

**Step 1: To leading order $(-\Delta + V)g_1 = 0$, so $g_1 = 1 - u_1$ is the zero energy scattering solution with scattering length $a$. Then $e_1 \approx 2\pi\rho a$.**

**Step 2: In the full equation, replace $V(1-u)$ by $2\pi\rho a\delta(x)$ and solve it by Fourier transforms. The result is: $\widehat{u}_2(k) = \frac{4e^{3/2}}{\pi^2\rho}\left(k^2 + 1 - k(k^2+2)^{1/2} - \frac{1}{2}k^{-2}\right)$ The second term, $e_2$, is obtained by inserting $e_1$ in this formula and integrating $V u_2$, which is essentially $2\pi\rho\, a\, \widehat{u}_2(0)$. We can integrate $\widehat{u}_2(k)$. This is a familiar integral and the final result (for D=3) is the famous**

$$e \approx 2\pi\rho a\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3}\right).$$

**Something similar can be done for D=2, and we obtain Schick's formula, which he obtained (as late as 1971 !) using Bogolubov's method, but only after summing infinitely many diagrams. A rigorous proof was given (in 2001 !) by L–Yngvason.**

$$e \approx 2\pi\rho / \log(\rho a^2).$$

# Condensate fraction

The usual way to define the condensate fraction (the fraction of particles in the 1-body ground state $\phi(x) = |\Lambda|^{-1/2}$) to be $N^{-1}\times$ the largest eigenvalue of the 1-body density *matrix*. In our case, we note that our integral over $\Psi$ measures the overlap of $\Psi$ with the totally condensed state $\phi^{\otimes N}$.

Define $\eta$ to be the probability that two particles are *not* in the state $\phi$ while $N-2$ *are condensed.* This is our substitute for the usual $\eta =$ probability that the other $N-2$ are in *any state*. This leads to our

*First Guess:* $\eta = \rho \int u^2 = \rho \int \frac{dk}{(2\pi)^3}\ \widehat{u}^2(k)$. A *more Refined Guess* is

$$\boxed{\eta = \int \frac{dk}{(2\pi)^3}\ \frac{\rho \widehat{u}^2(k)}{1-\rho^2\widehat{u}^2(k)}.}$$

(Recall: $1 = \rho\widehat{u}(0) > |\widehat{u}(k \neq 0|$)

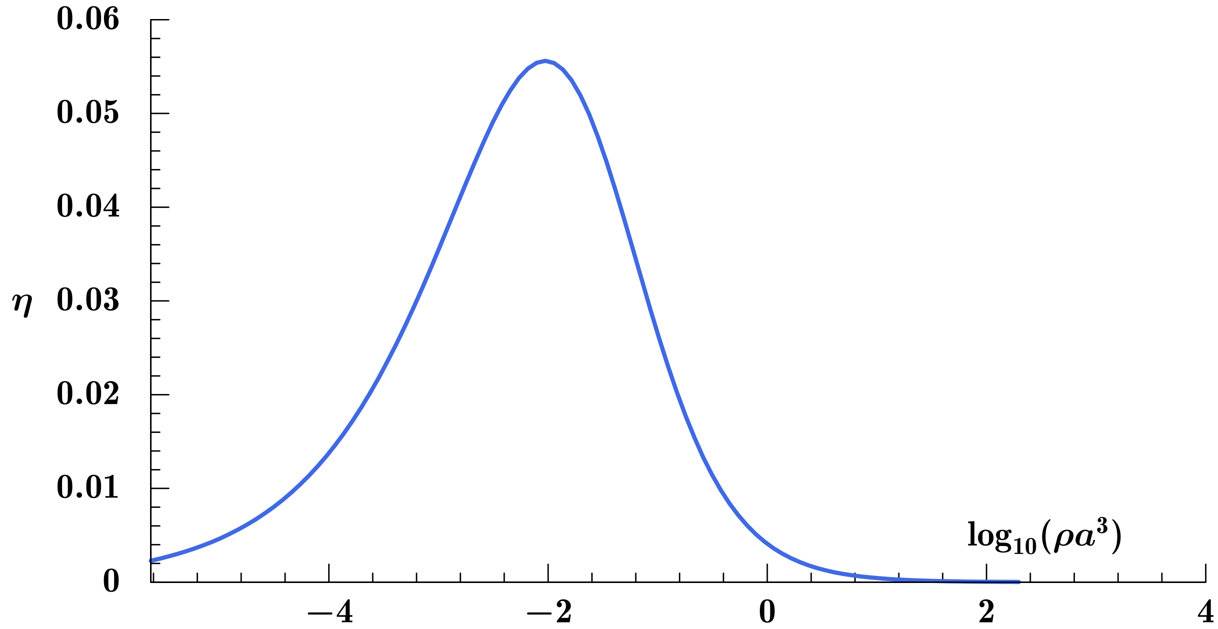
If we use our small $\rho$ asymptotics, $\rho\widehat{u}(k) \approx 1 + \frac{k^2}{2e} - \sqrt{\left(1+\frac{k^2}{2e}\right)^2 - 1}$, the Refined Guess gives: $(2/3)\sqrt{\frac{2}{\pi}\rho a_0^3}\,(1 + O(\sqrt{\rho}))$, which agrees perfectly with the Bogolubov estimate.

Our First Guess is only 9% smaller: $(64/105)\sqrt{\frac{2}{\pi}\rho a_0^3}\,(1+O(\sqrt{\rho}))$.

# Condensate fraction for large $\rho$

Since our 'small' equation is supposed to be reasonably good for all $\rho$, we took $V = \exp(-|x|)$, solved the equation numerically, (found that $a \approx 1.2544$), and found that $\eta$ increased with $\rho$ and then decreased. This was surprising until we realized that as $\rho \to \infty$ the energy $e$ moves from $e \approx 2\pi\rho a$ to $2\pi\rho \int V$. The particles are then all over each other, the problem becomes 'mean field', and correlations disappear. The gas becomes 'ideal', and all particles shelter in $\phi$.

Here is the numerical plot of our Refined $\eta$ as a function of $\log_{10} \rho a^3$ in 3D. Is it reasonable? Has this been noted earlier?



***THANKS FOR LISTENING!***