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

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References: **Physical Review 130, 2518 (1963)**

(0.58 centuries later)

Physical Revew A, 103, 053309 (2021)

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New definition of the N-point function

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

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

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 limit case is the hard-core V of radius (and scattering length) a

The new n-body density, which is *not quadratic in* Ψ, 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 $\boxed{2e/\rho = \int g(x)V(x)dx}$. Next, we integrate Ψ over $(N-2)$ $x's$ and get

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

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

We write $\boxed{g(x) := 1-u(x)}$.

To make progress we now make assumptions about how g^3, g^4 are related to g^2. These 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 similarly for g^4. Then (in the limit $|\Lambda| \to \infty$)

$$\int g^3(1,2,3)V(2,3)dx_3 = g^2(1,2)\left[2e/\rho - \int u(1,3)g^2(2,3)V(2,3)dx_3\right]$$

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

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

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

$$K(1,2) = \int u(1,3)\, g(2,3)V(2,3)\, d3 = (u * gV)(x_1 - x_2).$$

This is quite a complicated 'differential-integral' equation. It is the 'BIG simple equation'. We have investigated it numerically and the results agree with the less accurate 'SMALL simple equation' which is obtained from this big equation 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) $u(x) \to 0$ as $x \to \infty$;

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

We also expect to find that $u(x) \leq 1$, otherwise $g = 1-u$ is not non-negative.

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 prove.

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 ρ_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: $u_n(x) \leq 1$ (miracle) and $u_{n+1}(x) \geq u_n(x)$, $\rho_{n+1} \geq \rho_n \quad \forall n \geq 0, \forall x$.

The proof is then by iteration. It is not very long but is omitted for lack of time.

We prove uniqueness too. That is, for each e there is one and only one $\rho(e)$. Unfortunately, we do not known how to prove that there is only one e for a given ρ, although the numerical solution makes this evident.

Small equation challenges

(A) We have seen that e determines ρ, but we need to prove that ρ 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 $\rho \to \rho e(\rho)$ must be *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 $e \to 1/\rho(e)$ must be *convex.*

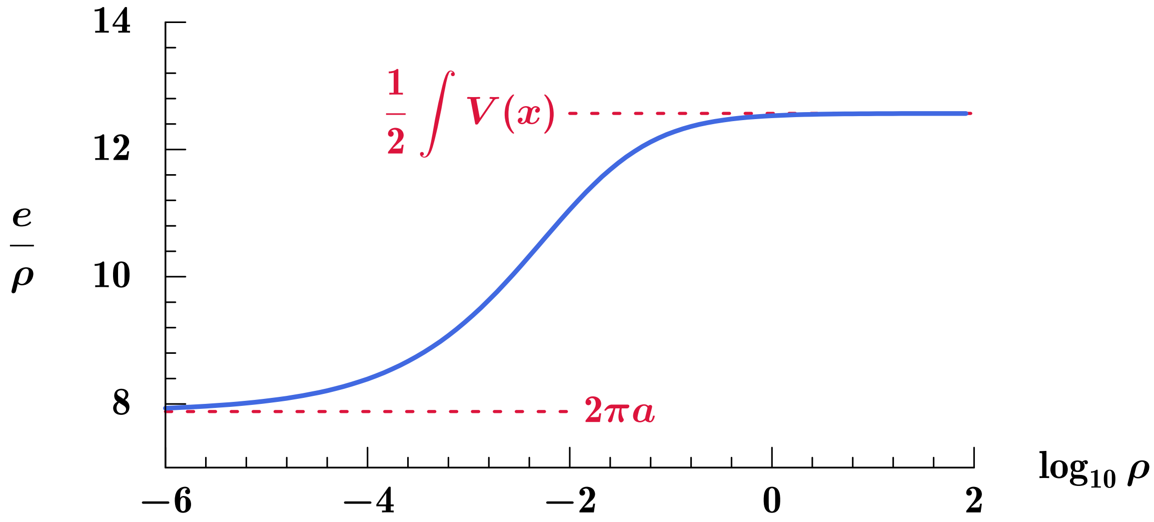
Numerical solution of the equation shows unambiguously that A and B are true.

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

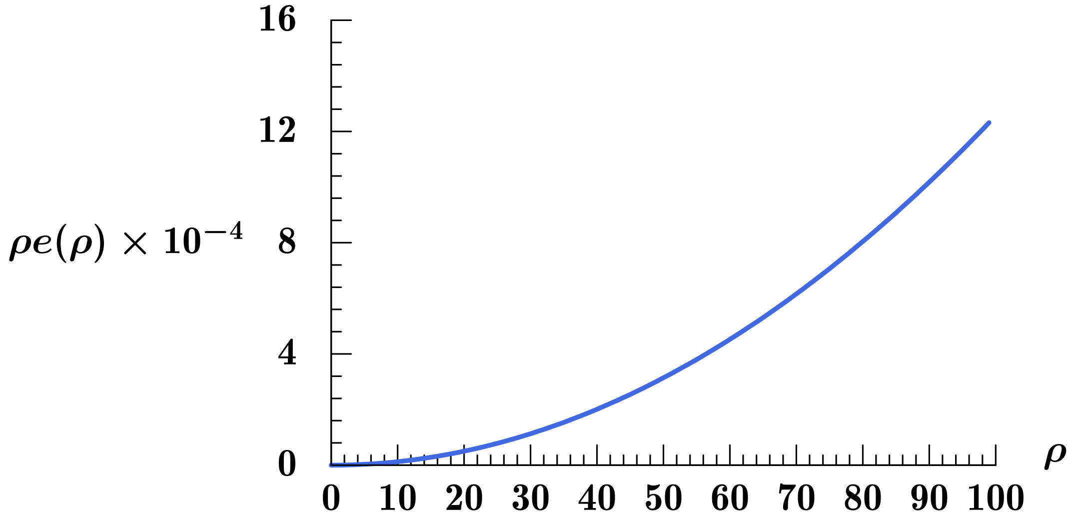
$$(-\Delta + V(x))u(x) = \rho g(x)\{2K(x) - \rho L(x)\}.$$

Some numerical results

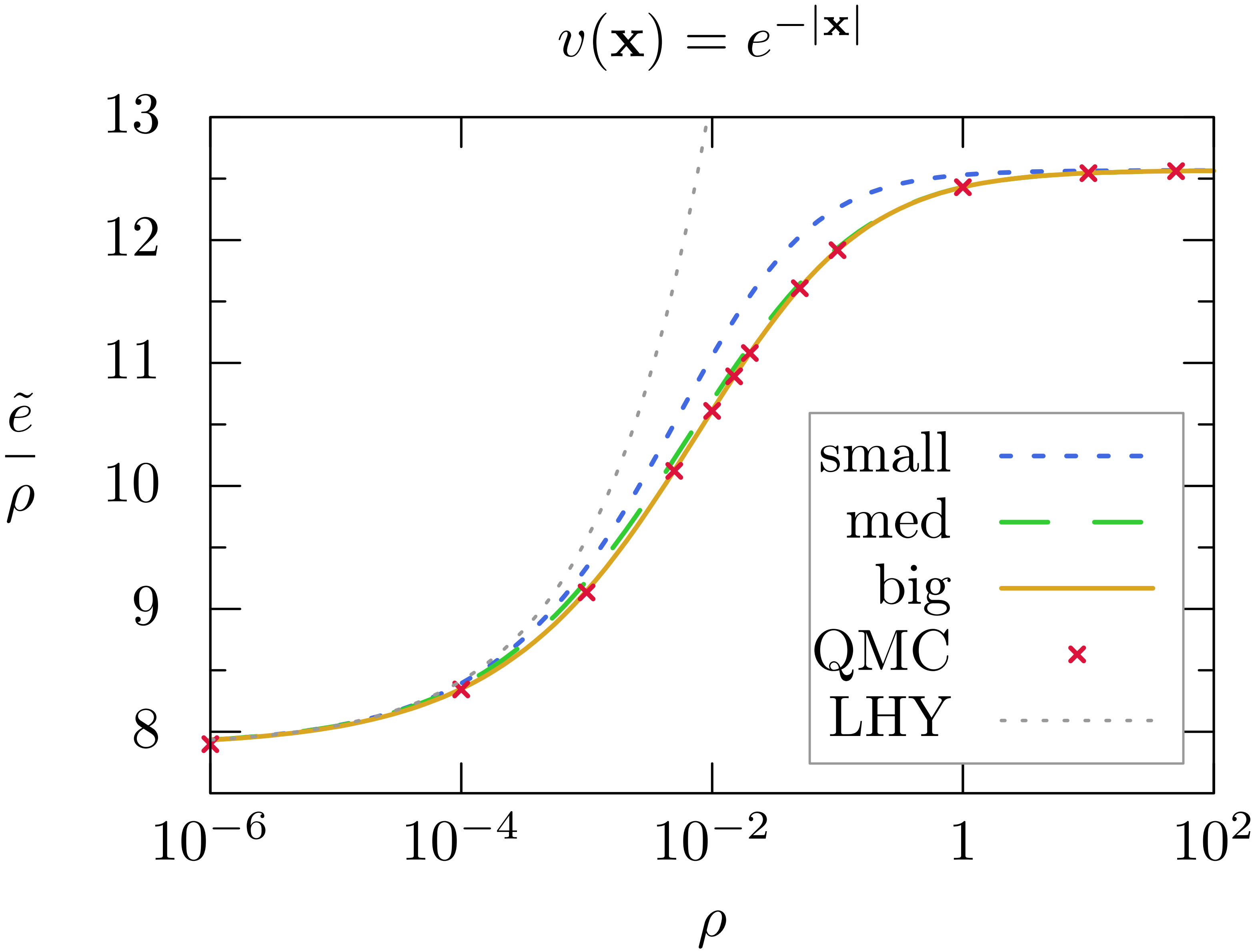
To get accurate numerical solutions is surprisingly tricky. Here are results for $V(x) = \exp(-|x|)$ in 3D. We find $a \approx 1.2544$. Graph #1 shows that $e(\rho)$ starts as $2\pi\rho a$ and ends as $\frac{1}{2}\rho \int V$.



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



Energy comparison with quantum Monte Carlo



Analytic solution for small ρ

We solve the small equation analytically for small ρ. 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

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

proved by Fournais & Solovej!!

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.

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

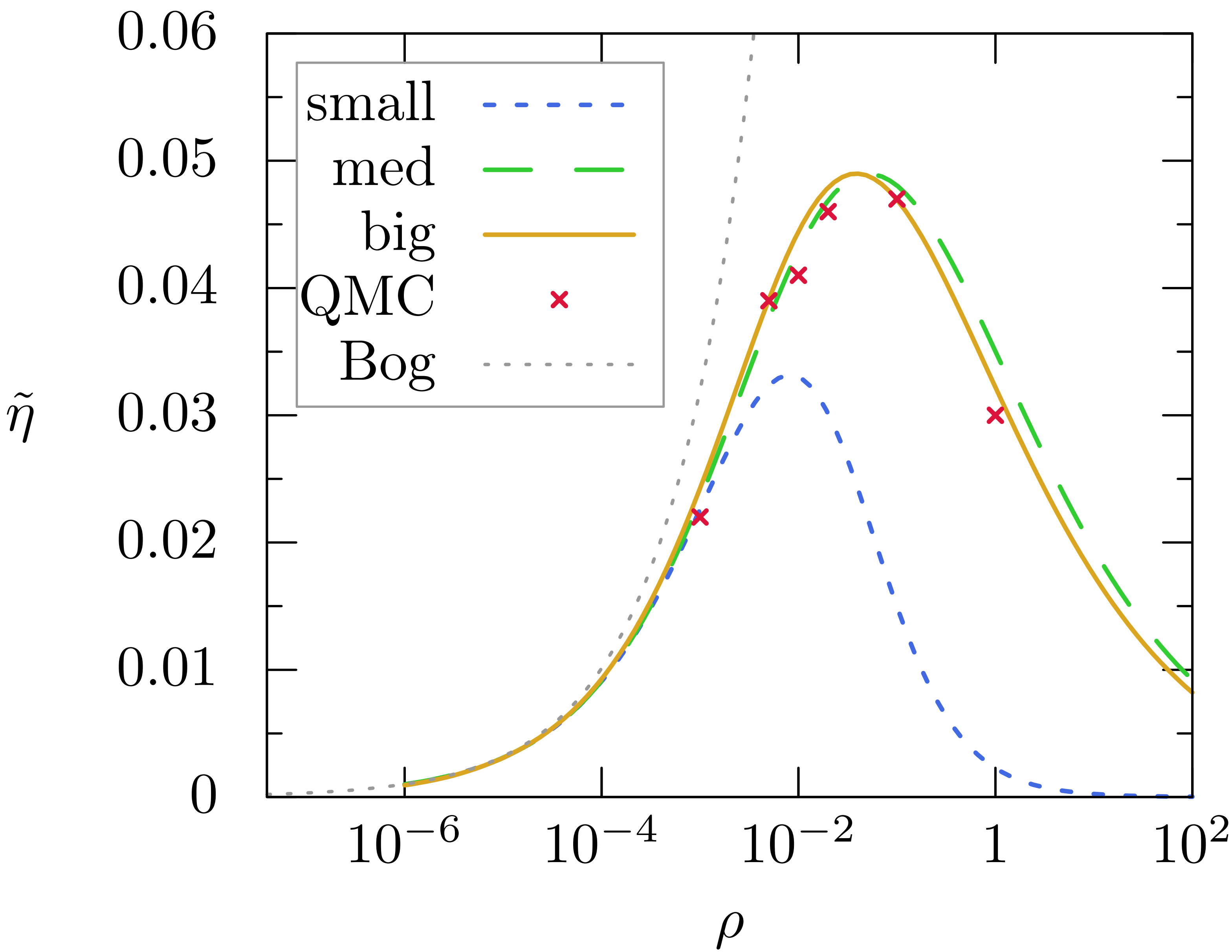
Condensate fraction

The usual way to define the condensate fraction (the fraction of particles in the 1-body ground state $\phi_0(x) = |\Lambda|^{-1/2}$) is $N^{-1}\times$ the largest eigenvalue of the 1-body density *matrix*. In our case, we use that our integral over Ψ measures the overlap of Ψ with the totally condensed state $\phi_0^{\otimes N}$.

Define the projector P_i by $P_i\Psi = |\Lambda|^{-1}\int \Psi dx_i$. So, if we add $\mu\sum_i P_1$ to the Hamiltonian H, and then differentiate the energy w.r.t. μ at $\mu = 0$, we will have computed the expected number of zero-momentum particles in the ground state.

In the next slide we graph $\tilde{\eta}$, which is the fraction of particles predicted to be <u>not condensed</u> and compare this number with what Quantum Monte Carlo tells us. The 2-body potential is $V(x) = \frac{1}{2}\exp(-|x|)$. The agreement is excllent! Note that $\tilde{\eta}$ is small for both small *and large* ρ, as it should be!!!

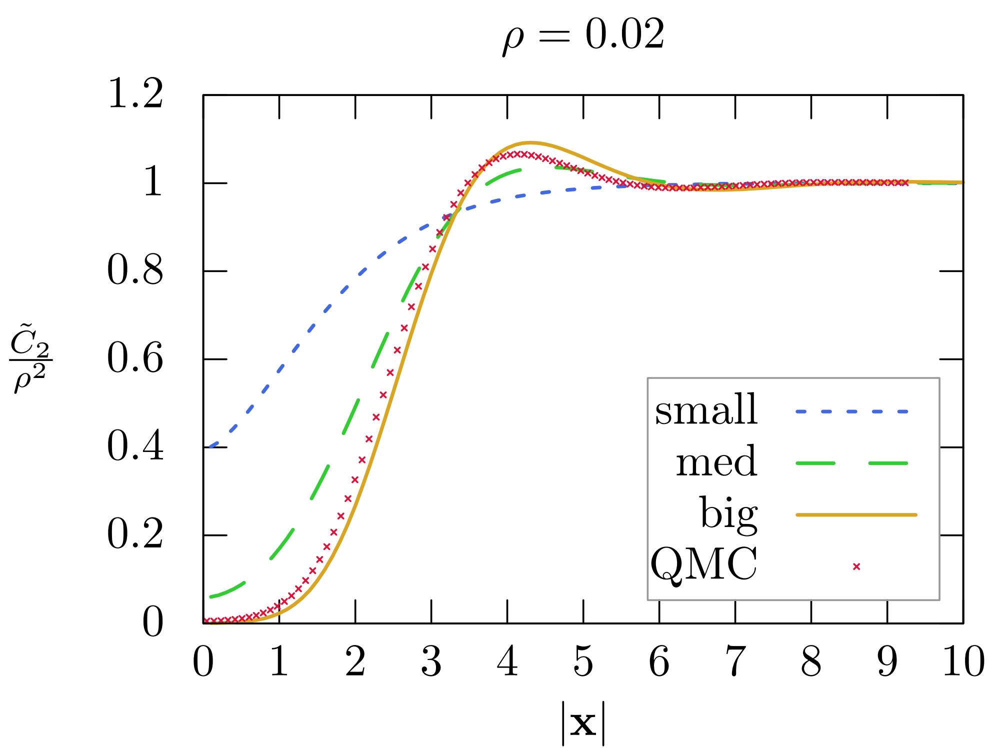
Condensate fraction



2-particle correlation function

In a similar fashion we can define the 2-particle correlation function $\tilde{C}_2$ by functionally differentiate the energy with respect to the 2-body potential V. We compute it from the solution to the (Small or Big)-equation.

Here is a result for 2 exponential potentials potentials, with comparison to Monte Carlo. The accuracy of the Big equation is unexpectedly good – even to the little extra bump at medium density.



Summary

- **We have analyzed a 'Theoretical Physics' approach to the ground state of a Bose gas. It utilizes the wave function itself as a probability distribution.**

- **The approach is unusual, even by 'Theoretical Physics' standards, but produces exceptionally good agreement with Quantum Monte Carlo calculations for the Energy, Condensate fraction, and Pair correlation functions in many cases.**

- **Much remains to be done on the pure mathematical physics level with regard to justification, and possible connection to Feynman–Kac integrals.**

- **Of special interest is the fact that the approach reveals properties at intermediate densities. It might be said that 'new physics' is revealed, which might lead to interesting new physics accessible to experiments.**

$\boxed{\boldsymbol{THANKS\ \ FOR\ \ LISTENING!}}$