The harmonically confined Tonks-Girardeau gas: A simulation study based on Nelson's stochastic mechanics

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Outline

- Nelson's stochastic mechanics
- Tonks-Girardeau gas
- Simulation method
- Results
- Conclusions

Stochastic Mechanics

Equation of motion:

$$dx(t) = v_f(x,t)\,dt + \sqrt{\hbar/m}\;\; dW_f(t)$$

Conservative diffusion process ⇒ time-reversed process exists

$$dx(t) = v_b(x,t)\,dt + \sqrt{\hbar/m}\;\; dW_b(t)$$

$$v(x,t) = \frac{v_f(x,t) + v_b(x,t)}{2} \;=\; \frac{1}{m}\nabla S(x,t) \;\rightarrow\; v_{cl}(x,t) \;\; for \;\; \hbar/m \rightarrow 0$$

$$u(x,t) = \frac{v_f(x,t) - v_b(x,t)}{2} \;=\; \frac{\hbar}{m}\nabla R(x,t) \;\rightarrow\; 0 \;\; for \;\; \hbar/m \rightarrow 0$$

E. Nelson, Phys. Rev. **150**, 1079 (1966)

Stochastic Mechanics

Stochastic Newton law for mean acceleration: $\bar{a} = \frac{1}{m} \nabla U(x,t)$

Madelung fluid

$$\frac{\partial R}{\partial t} + \frac{1}{2\mathrm{m}} \Delta S + \frac{1}{m} \nabla R \cdot \nabla S = 0$$

$$\frac{\partial S}{\partial t} + U + \frac{1}{2\mathrm{m}} (\nabla S)^2 - \frac{\hbar^2}{2\mathrm{m}} \left[(\nabla R)^2 + \Delta R \right] = 0$$

→ $$\psi(x,t) = \exp\left(R(x,t) + \frac{i}{\hbar} S(x,t) \right)$$

Tonks-Girardeau Gas

1d system of N hard-core bosons in harmonic external potential

$$H=\sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2}+\frac{1}{2}m\omega^2 x_i^2\right)$$

Length scale $\sqrt{\hbar/m\omega}$

Energy scale $\hbar\omega$

Constraint $\psi=0 \quad if \quad |x_i-x_j| < a, \quad 1\leqslant i\leqslant j\leqslant N$

Fermi-Bose mapping $\psi_B(x_1,\ldots,x_N)=|\psi_F(x_1,\ldots,x_N)|$

Limit $a \rightarrow 0$

$$\psi_B(x_1,\ldots,x_N)=2^{N(N-1)/4}\left[N!\prod_{n=0}^{N-1}n!\sqrt{\pi}\right]^{-1/2}\prod_{i=1}^{N}\exp\left(-\frac{x_i^2}{2}\right)\prod_{1\leqslant j\leqslant k\leqslant N}|x_k-x_j|$$

Simulation Methodology

Stationary state

$$S(x_1,\dots,x_N,t)=0$$

$$R(x_1,\dots,x_N,t)=\ln(C_N)-\frac{1}{2}\sum_{i=1}^{N} x_i^2+\sum_{1\leqslant j\leqslant k\leqslant N}\ln|x_k-x_j|$$

Equation of motion

$$dx_i(t)=\left[-x_i+\sum_{j=1,\,j\neq i}^{N}\frac{1}{|x_j-x_i|}\,sign(x_j-x_i)\right]dt+dW_i(t)$$

Scaled velocity (momentum) $u_i(t)$

Draw $dW_i(t)$ from uniform distribution with correct first 4 moments

Observables

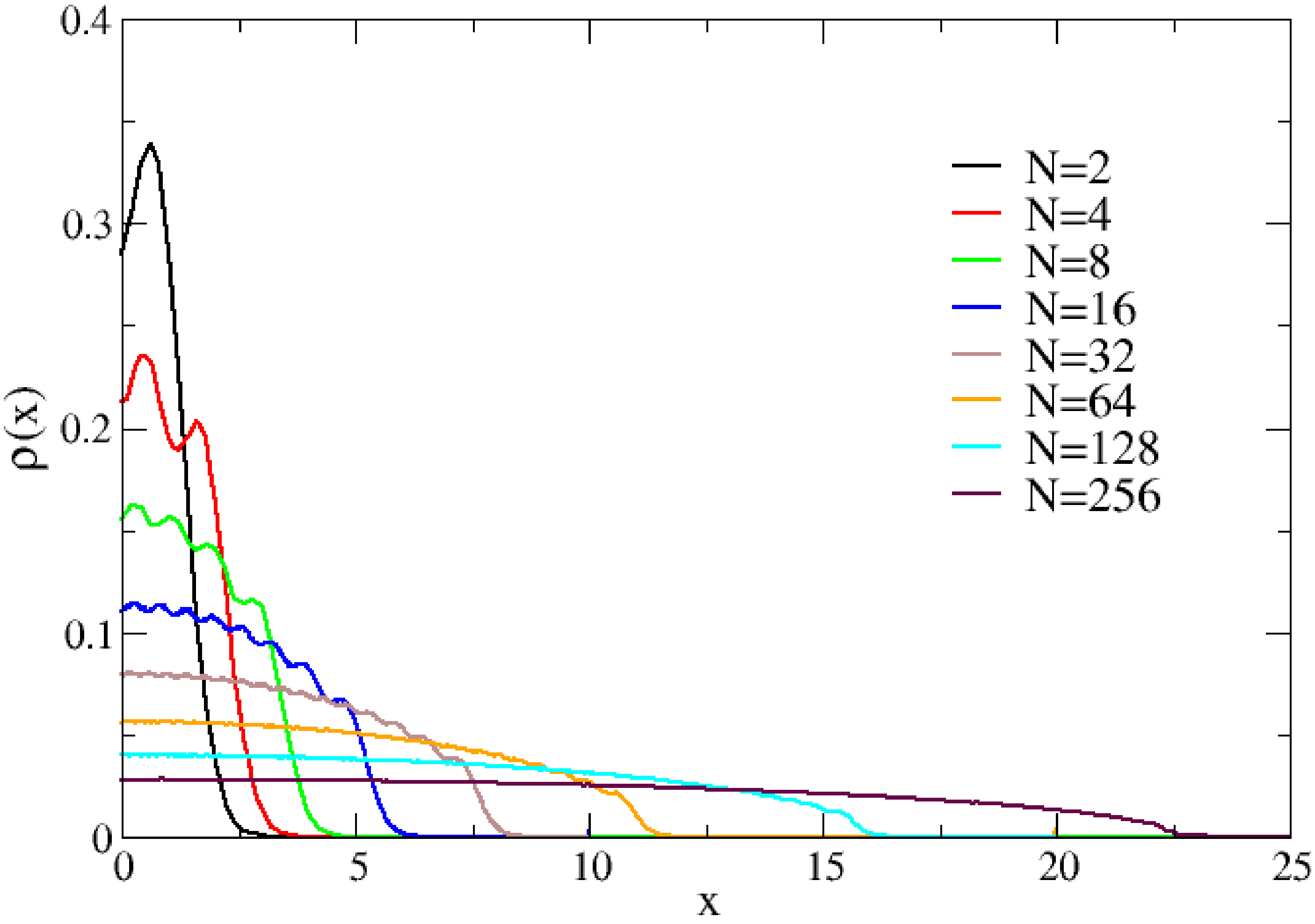
- Local density $\rho(x)=N\int|\psi_B(x,x_{2,}\dots,x_N)|^2 dx_2\dots dx_N=\frac{1}{\sqrt{\pi}}\sum_{n=0}^{N-1}\frac{1}{2^n n!}H_n^2(x)\exp(-x^2)$
- Momentum distribution $p(u)$
- Reduced single particle density matrix

$$\rho_1(x,x')=N\int dx_2\dots dx_N\,\psi_B(x,x_{2,}\dots,x_N)\psi_B(x',x_{2,}\dots,x_N)$$

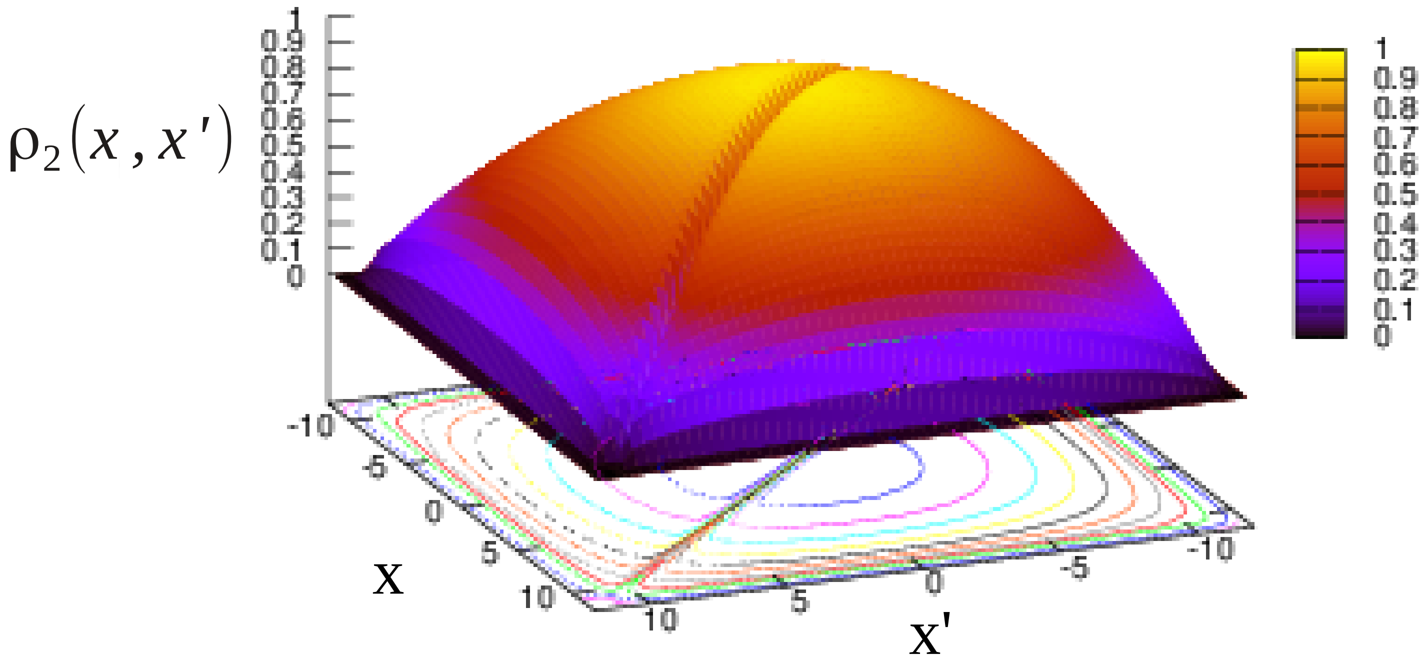
- Effective single particle states

$$\int\rho_1(x,y)\Phi_j(y)dy=\lambda_j\Phi_j(x)\quad j=0,1,2,\dots$$

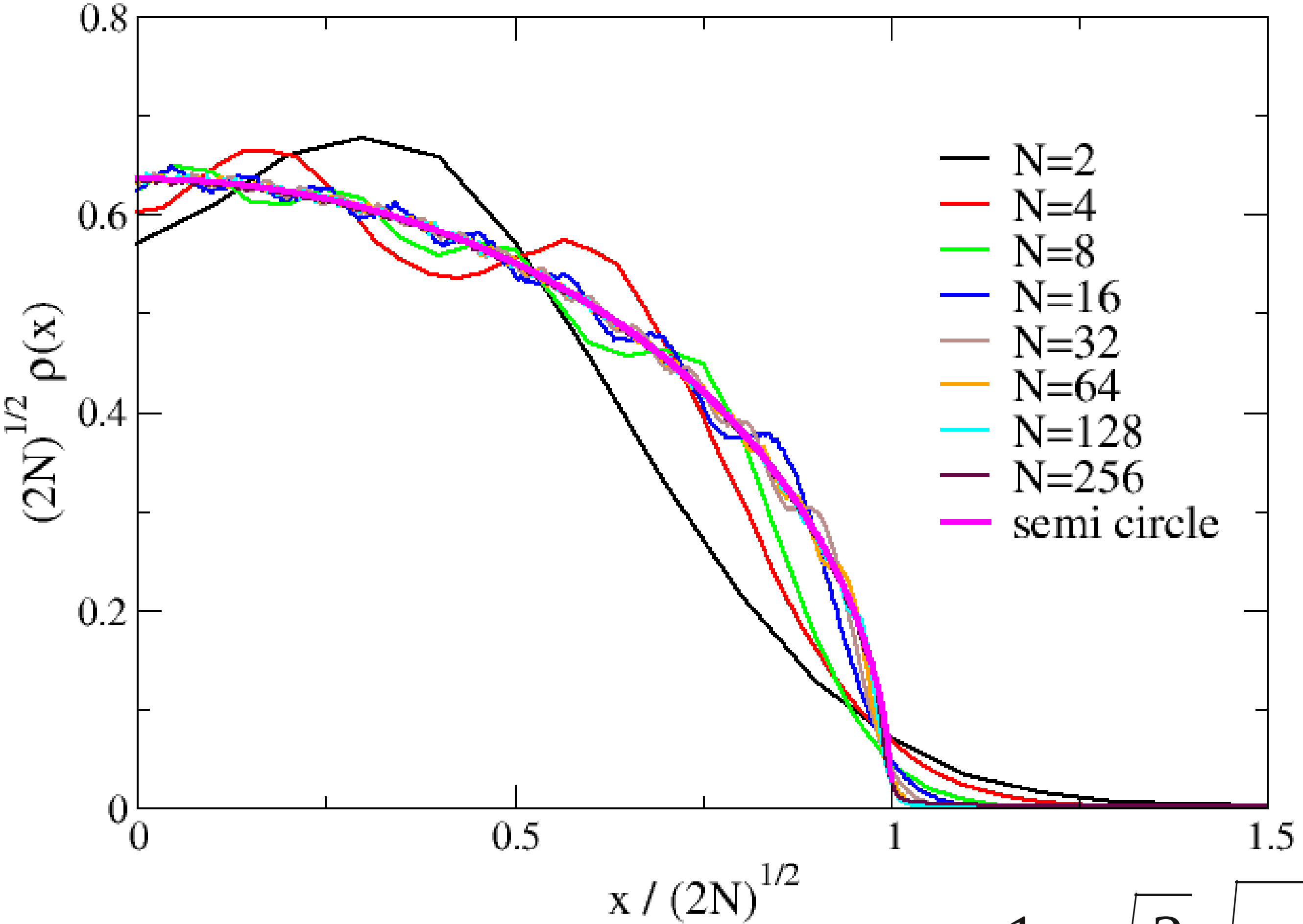
Real-space density



Two-particle density



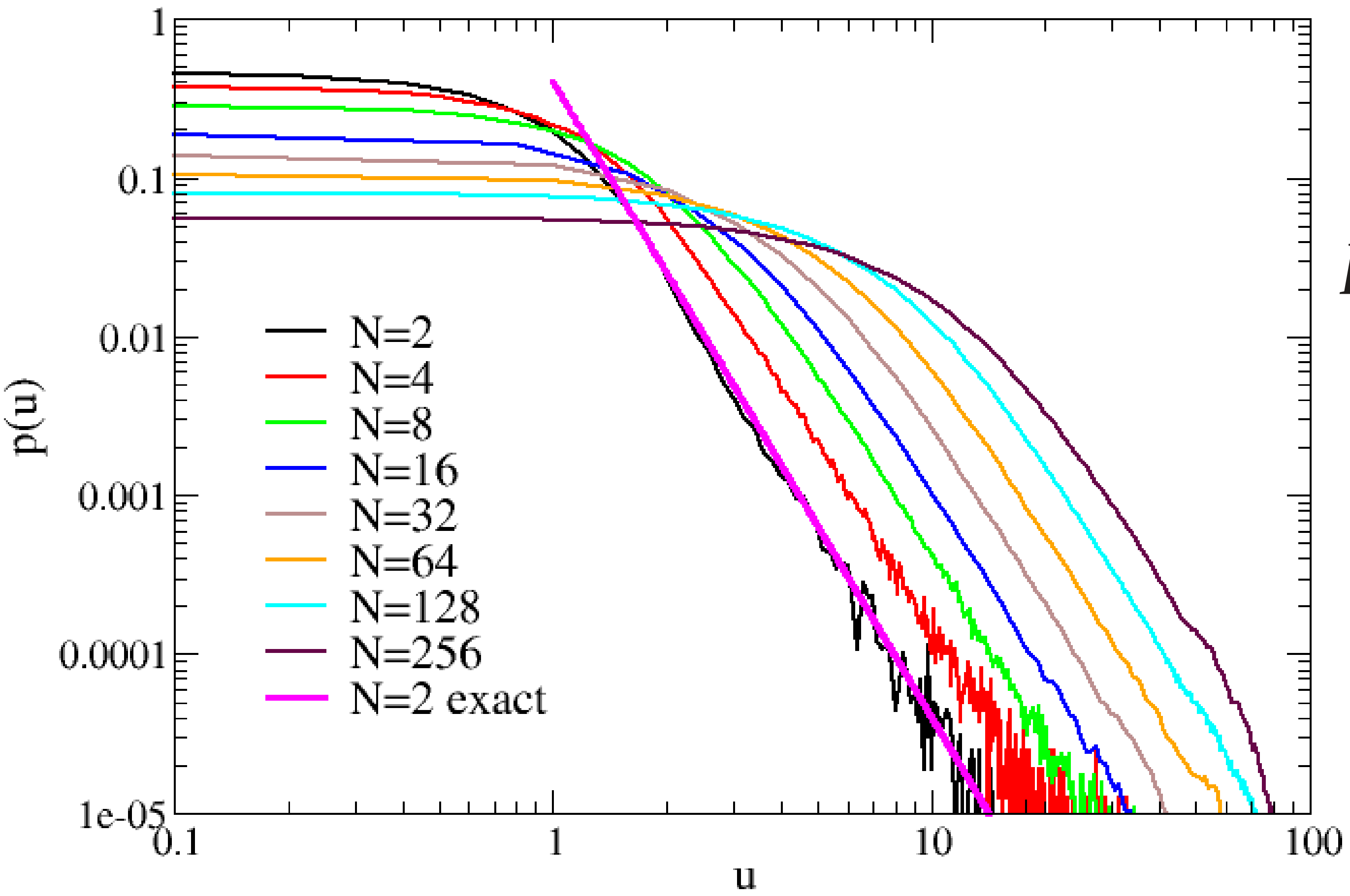
Real-space density: scaled



Wigner semi-circle law

$$\rho(x)=\frac{1}{\sqrt{2N}}\sqrt{\frac{2}{\pi}}\sqrt{1-\frac{x^2}{2N}}$$

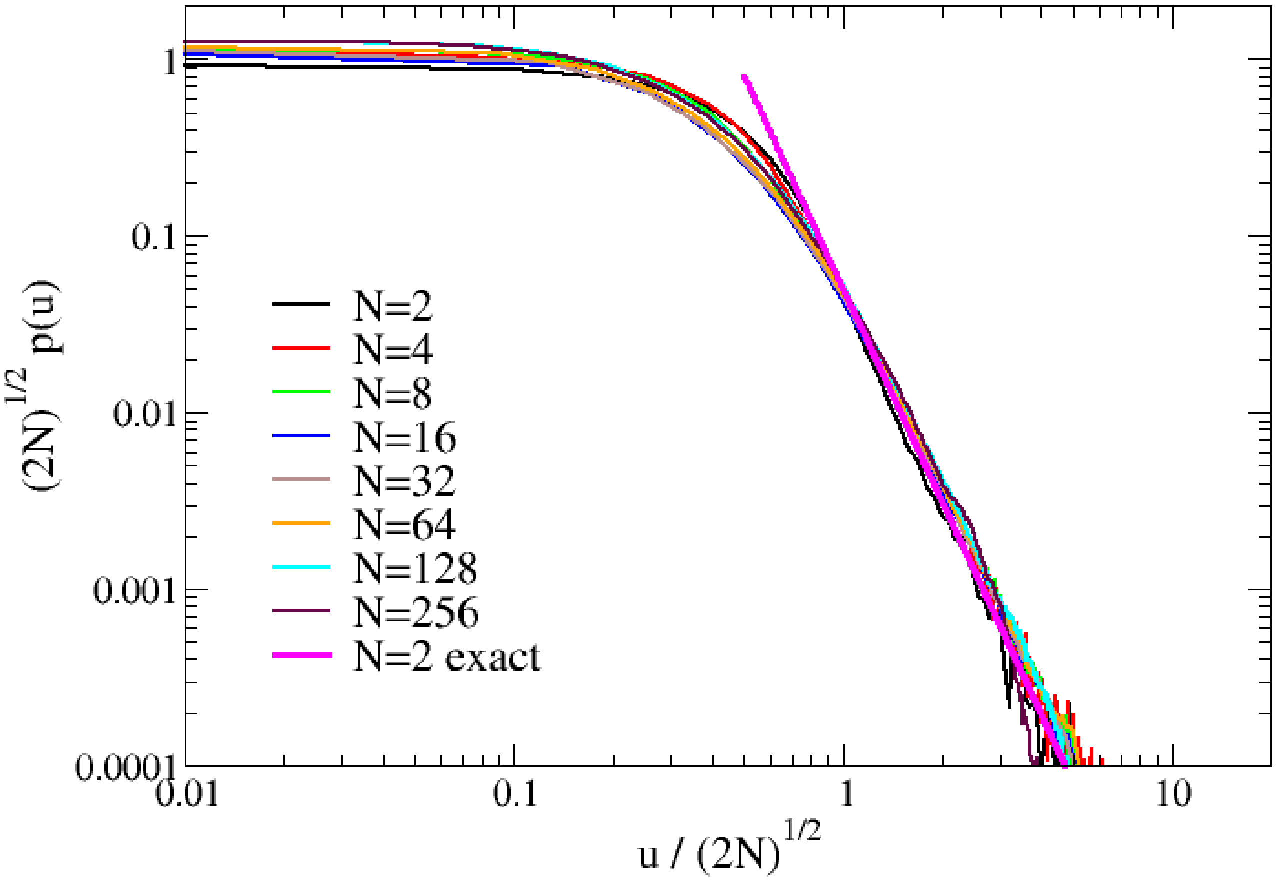
Momentum distribution



$$p_2(u) = \frac{1}{2}\sqrt{\frac{2}{\pi}}\,u^{-4}$$

A. Minguzzi, P. Vignolo, and M. P. Tosi, Phys. Lett. A **294**, 222 (2002)

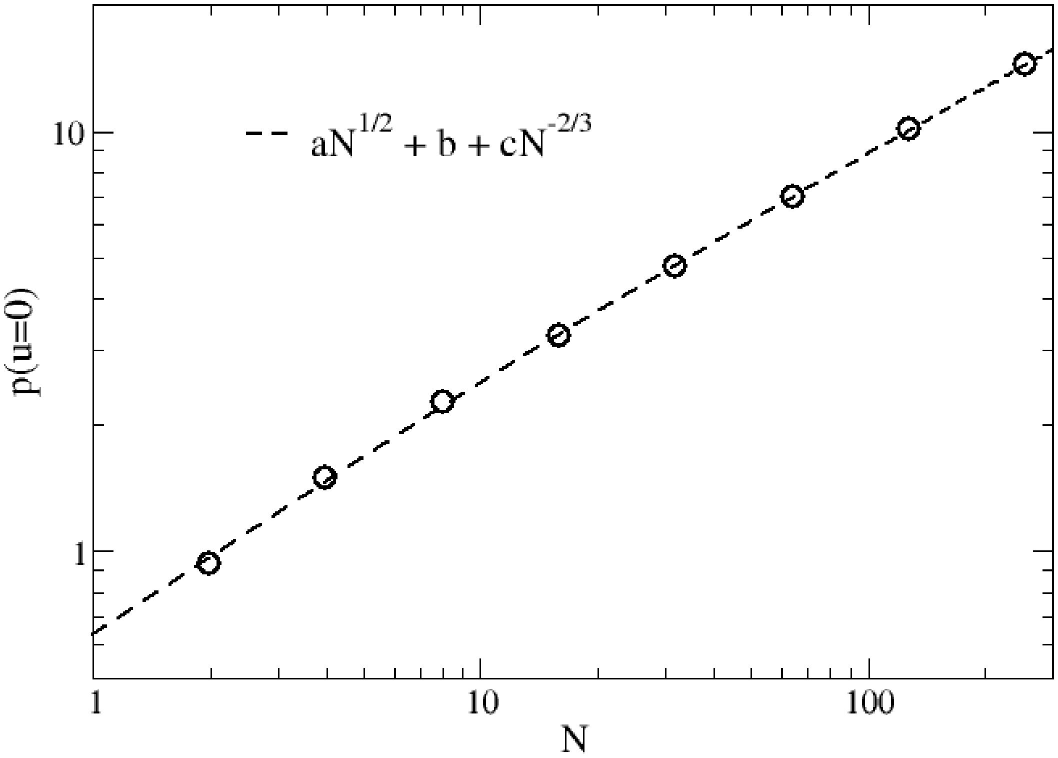
Momentum distribution: scaled



$$p_N(u) = \frac{1}{4}\sqrt{\frac{2}{\pi}} N^{3/2} u^{-4}$$

Test for BEC behavior

$$\int dk_2 n_1(k,-k_2)\tilde{\Phi}_j(k_2)=\lambda_j\tilde{\Phi}_j(k)$$



$n_1(k,-k)$ is the Momentum distribution

Occupation numbers should scale as the momentum distribution

Functional form: P. J. Forrester et al., Phys Rev. A **67**, 043607 (2003)

Conclusions

- All exactly known results reproduced
- New scaling behavior found for momentum distribution
- Prefactor of asymptotic scaling for momentum inferred
- Relation between momentum distribution and occupation number of natural orbitals established

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Diffusion paths of quantum particles make sense

W. Paul, Phys. Rev. A **86**, 013607 (2012)