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Polaron interactions and bipolarons in one-dimensional Bose gases in the strong coupling regime

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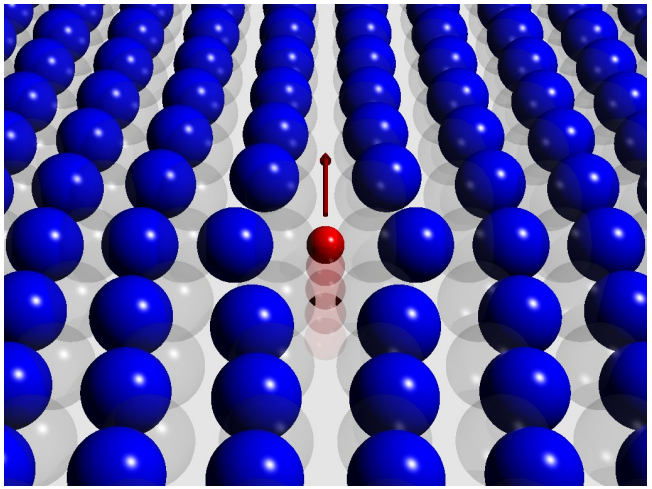
QUANTUM 2021: DYNAMICS AND LOCAL CONTROL
OF IMPURITIES IN COMPLEX QUANTUM ENVIRONMENT

MOTIVATION

The quantum problem of a single impurity is very interesting:



•polaron - quasiparticle with an effective mass

•Ultracold gases are fantastic for studying impurities:
-the system is extremely pure / defects free
-atom-atom and atom-impurity interactions can be fine tuned
-controllable geometry

•1D geometry: regimes of strong interactions accesible

HAMILTONAIN OF A 1D GAS

- Hamiltonian of N particles interacting via contact interaction

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + g\sum_{i<k}^{N}\delta(\mathbf{r}_i - \mathbf{r}_k)$$

- where $g>0$ is the strength of interaction (coupling constant)
- and $\delta(\boldsymbol{r})$ is the delta-function with the usual normalization

$$\int \delta(r) d^D r = 1$$

- Units of a delta-function in D dimensions:

$$[\delta(\boldsymbol{r})] = [1\ / r^{\mathrm{D}}]$$

- 1D: $[\delta(\mathrm{r})] = [1\ /\ \mathrm{length}]$
- 2D: $[\delta(\mathrm{r})] = [1\ /\ \mathrm{length}^2]$
- 3D: $[\delta(\mathrm{r})] = [1\ /\ \mathrm{length}^3]$

COUPLING CONSTANT

Relation between the s-wave scattering length a and the coupling constant g?

Interaction potential $g\,\delta(r)$ has units of energy: $\left[\dfrac{\hbar^2}{m\ (length)^2}\right]$

Units of g are :

- 3D: $\left[\dfrac{\hbar^2 a_{3D}}{m}\right] \rightarrow g_{3D} = 4\pi\dfrac{\hbar^2 a_{3D}}{m}$ i.e. $g_{3D} \propto a_{3D}$

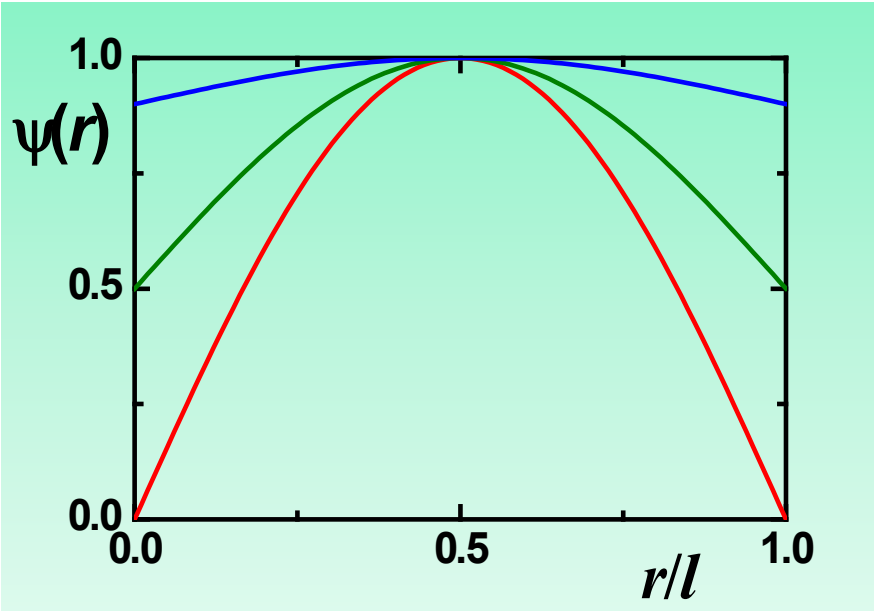
- 1D: $\left[\dfrac{\hbar^2}{m a_{1D}}\right] \rightarrow g_{1D} = -2\dfrac{\hbar^2}{m a_{1D}}$ i.e. $g_{1D} \propto -1/a_{1D}$

- 2D: $\left[\dfrac{\hbar^2}{m}\right] \rightarrow g_{2D} = 4\dfrac{\hbar^2}{m}\dfrac{1}{|\ln n a^2|}$ weak logarithmic dependence

POTENTIAL ENERGY: TYPICAL SCALING WITH DENSITY

Quantum effects are enhanced in low-dimensionality. Typical contribution from a short-range potential $V_{int}(r) = g\delta(r)$ to the potential energy $E/N \propto g|\psi(r_1 = r_2)|^2$,

- is decreased when the value of the w.f. is decreased at a contact $\psi(r_1 = r_2) \to 0$
- for a weakly interacting Bose gas $|\psi(r_1 - r_2)|^2 \approx n$ and the chemical potential is linear in density $\mu \propto g|\psi(r_1 - r_2)|^2 \propto gn$



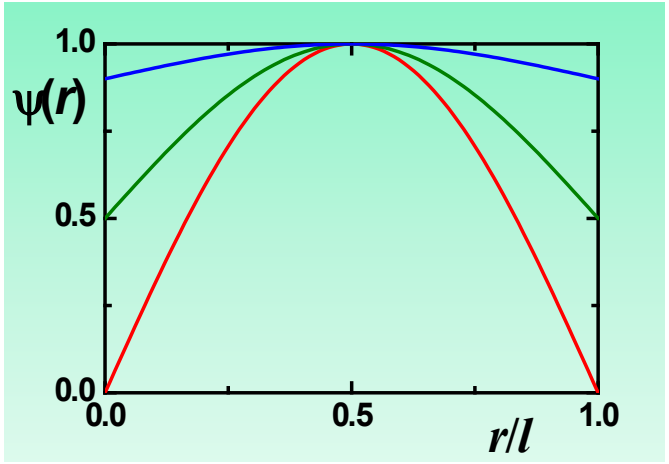
KINETIC ENERGY: TYPICAL SCALING WITH DENSITY

Kinetic energy is related to the curvature of the w.f. through the second derivative $\hat{p}^2/2m = -\hbar^2\Delta/2m$

- contains $\hbar$ and is finite even at zero temperature describing quantum fluctuations
- is increased when the value of the w.f. is decreased at a contact $\psi(r_1 = r_2) \to 0$

when the kinetic energy is dominant, it is related to the mean interparticle distance l as $E/N \propto \hbar^2/ml^2$

- in 3D system $l \propto n^{-1/3}$, $E/N \propto n^{2/3}$
- in 2D system $l \propto n^{-1/2}$, $E/N \propto n$
- in 1D system $l \propto n^{-1}$, $E/N \propto n^2$

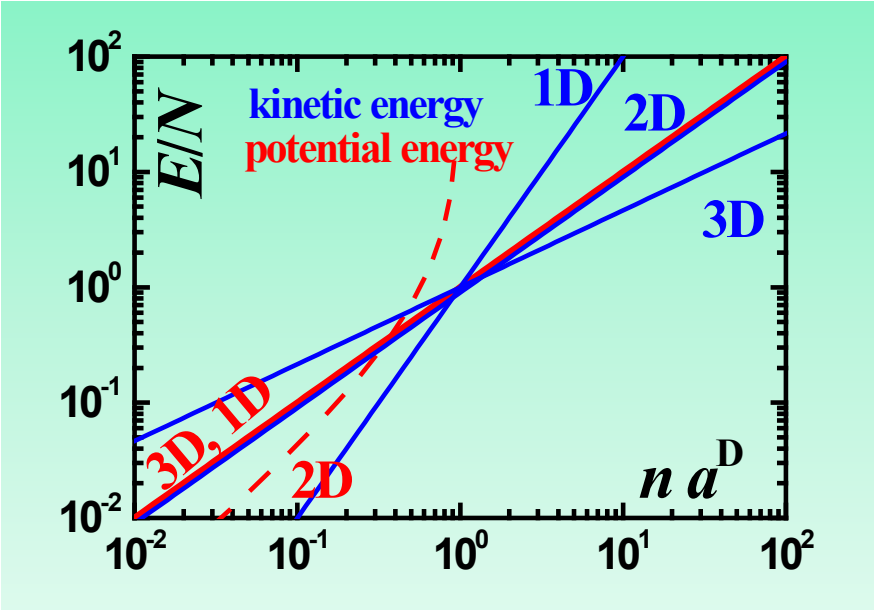


The increase in kinetic energy/quantum effects with density is larger in low-dimensional systems.

POTENTIAL vs KINETIC ENERGY

The value of the w.f. at a contact can be large or small depending on the dimensionality and if the density is high or low.

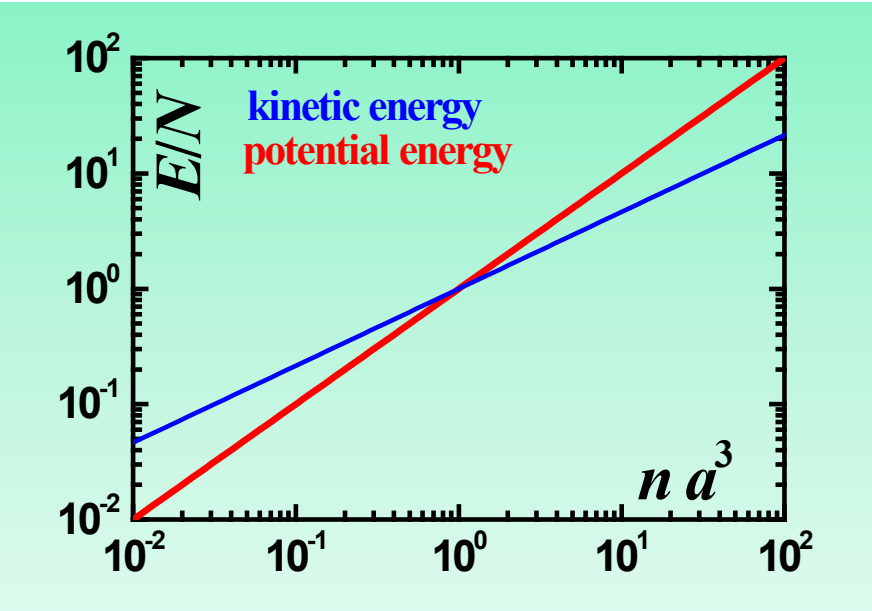
	potential energy $\propto gn$	kinetic energy
3D	$g_{3D}n = \frac{4\hbar^2 a_{3D}}{m} \times n$	$\frac{\hbar^2}{m} \times n^{2/3}$
2D	$g_{2D}n = \frac{4\pi\hbar^2}{m} \times \frac{n}{\lvert \ln n a_{2D}^2 \rvert}$	$\frac{\hbar^2}{m} \times n$
1D	$g_{1D}n = \frac{2\hbar^2}{m\lvert a_{1D} \rvert} \times n$	$\frac{\hbar^2}{m} \times n^2$



THREE-DIMENSIONAL GEOMETRY

In a three-dimensional geometry, minimal energy of a Bose system is obtained for the mean-field $\mu = gn$ solution at low densities.

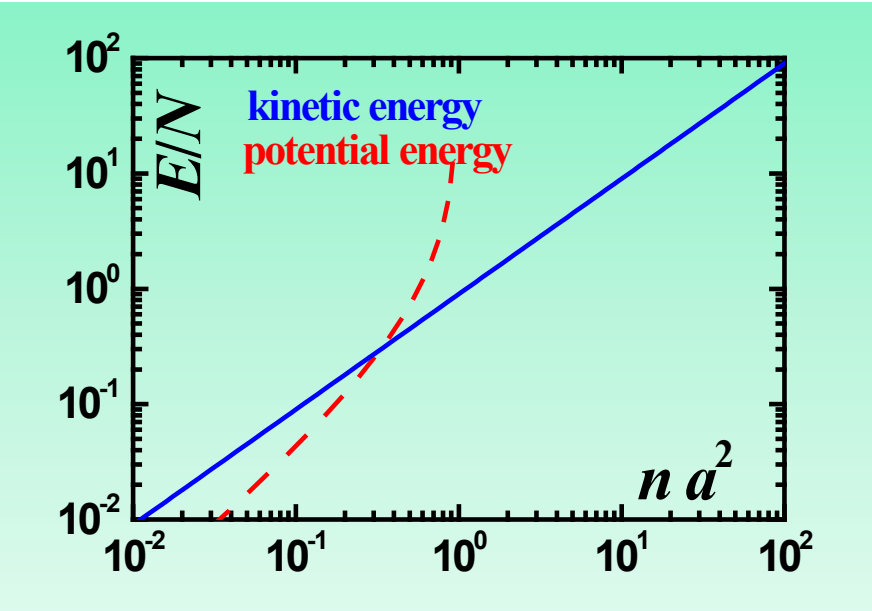
	potential energy $\propto gn$	kinetic energy
3D	$g_{3D}n = \frac{4\hbar^2 a_{3D}}{m} \times n$	$\frac{\hbar^2}{m} \times n^{2/3}$



TWO-DIMENSIONAL GEOMETRY

In a two-dimensional geometry, minimal energy of a Bose system is obtained for the mean-field $\mu = gn$ solution at low densities.

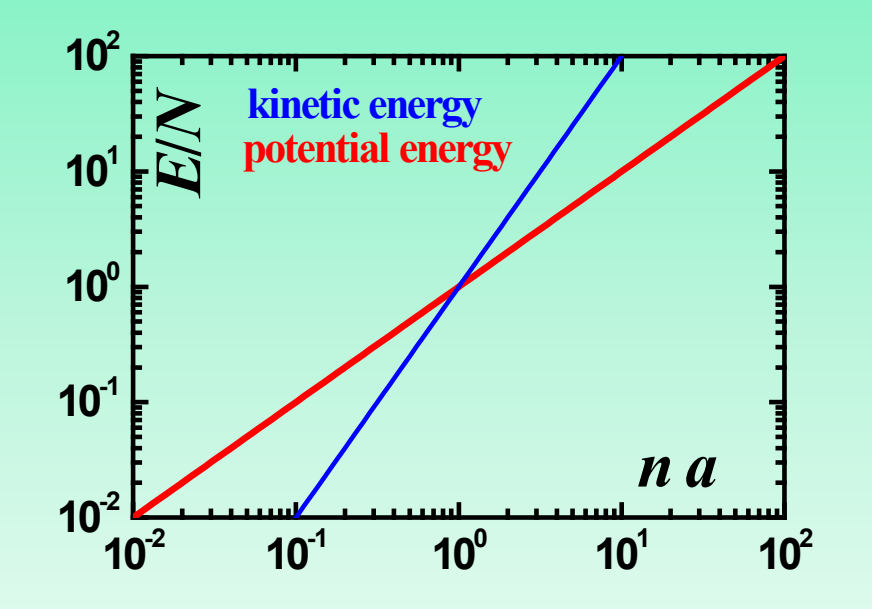
	potential energy $\propto gn$	kinetic energy
2D	$g_{2D}n = \frac{4\pi\hbar^2}{m} \times \frac{n}{\lvert \ln n a_{2D}^2 \rvert}$	$\frac{\hbar^2}{m} \times n$



ONE-DIMENSIONAL GEOMETRY

In a one-dimensional geometry, minimal energy of a Bose system is obtained for the mean-field $\mu = gn$ solution at **large** densities.

	potential energy $\propto gn$	kinetic energy
1D	$g_{1D}n = \frac{2\hbar^2}{m\lvert a_{1D}\rvert} \times n$	$\frac{\hbar^2}{m} \times n^2$



MEAN-FIELD vs QUANTUM REGIMES

The value of the w.f. at a contact can be large or small depending on the dimensionality and if the density is high or low.

	potential energy $\propto gn$	kinetic energy
3D	$g_{3D}n = \frac{4\hbar^2 a_{3D}}{m} \times n$	$\frac{\hbar^2}{m} \times n^{2/3}$
2D	$g_{2D}n = \frac{4\pi\hbar^2}{m} \times \frac{n}{\lvert \ln n a_{2D}^2 \rvert}$	$\frac{\hbar^2}{m} \times n$
1D	$g_{1D}n = \frac{2\hbar^2}{m\lvert a_{1D} \rvert} \times n$	$\frac{\hbar^2}{m} \times n^2$

The mean-field regime ($\mu = gn$) realizes

- in 3D and 2D geometry at small density $n \to 0$
- in 1D geometry at large density $n \to \infty$

CHARACTERISTIC PARAMETERS IN 1D

- Hamiltonian of N particles interacting via contact interaction of strength g
- coupling constant $g = -\frac{2\hbar^2}{ma} > 0$
- s-wave scattering length $a<0$
- linear density $n = N/L$ or mean interparticle distance $1/n$
- Healing length ξ related to chemical potential $\mu = \hbar^2/(2m\,\xi^2)$
- Size of the box L (often assumed to be large)

The system properties are governed by the following dimensionless parameter

- gas parameter na
- or Lieb – Liniger parameter $\gamma = -2/na$

THEORIES OVERVIEW

Most common methods used to address the problem of 1D gas

- *Bethe ansatz* method (1D)
- Gross-Pitaevskii mean-field theory (1D, 2D, 3D)
- Bogoliubov theory (1D, 2D, 3D)
- Luttinger liquid approach (1D)
- DMRG (1D)
- Monte Carlo methods (1D,2D,3D)
- ...

BETHE ANSATZ

Applies to contact delta-function interactions in 1D

- Constructs the wave function from plane waves with appropriate boundary condition at the contact
- Is exact for any interaction strength g
- Repulsive interactions: ground state energy (Lieb – Liniger, 1963), excitation spectrum (Lieb, 1963), thermodynamics (Yang-Yang, 1969)
- Local correlation functions (Gangardt & Shlyapnikov, 2003), dynamical density-density correlations (Caux & Calabrese, 2006)
- Attractive interactions: bright soliton ground state energy (McGuire, 1964), density profile (Calogero – Degasperis, 1975)

BETHE-ANSATZ SOLUTION

The Hamiltonian can be diagonalized exactly via a Bethe ansatz (Lieb and Liniger, 1963). The idea is that the wave function in each region is a superposition of plane waves with appropriate boundary conditions. By matching the wave functions on the interfaces between different regions a system of equations is obtained: For a given parameter λ, solution of

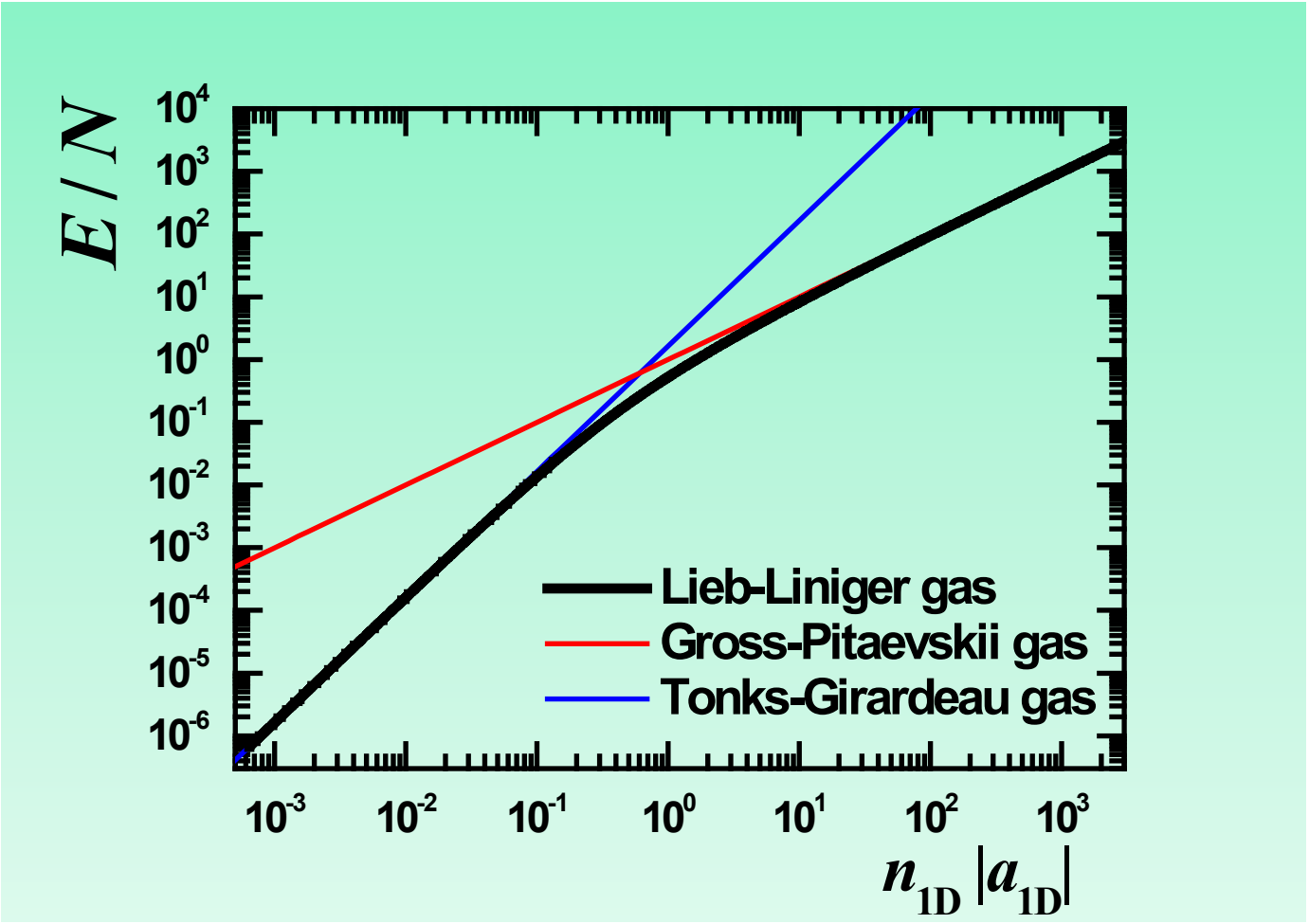
$$\rho(k) = \frac{1}{2\pi} + \int_{-1}^{1} \frac{2\lambda\rho(\varkappa)}{\lambda^2 + (k-\varkappa)^2} \frac{d\varkappa}{2\pi} \tag{1}$$

$$\gamma = \int_{-1}^{1} \rho(k)\, dk, \tag{2}$$

$$e(n_{1D}|a_{1D}|) = \frac{\gamma^3}{\lambda^3} \int_{-1}^{1} k^2 \rho(k)\, dk \tag{3}$$

integral Eq. (1) gives $\rho(k)$. Normalization of this function, Eq. (2), is denoted as γ and is related to the density as $n|a_{1D}| = 2/\gamma$. The energy per particle $E/N = n^2 e(n_{1D}|a_{1D}|)\hbar^2/2m$ is obtained from integral (3) and is a universal function of the dimensionless gas parameter $n_{1D}|a_{1D}$.

ENERGY OF LIEB-LINIGER GAS



- weak interactions $g_{1D} \to 0$ $(n_{1D}|a_{1D}| \to \infty)$ correspond to the mean-field interaction (Gross-Pitaevskii) with linear scaling with density $\mu = g_{1D} n$; $E/N = 1/2\, g_{1D} n_{1D}$

- strong interactions $g_{1D} \to \infty$ $(n_{1D}|a_{1D}| \to 0)$ correspond to the Tonks-Girardeau limit with quadratic dependence on the density, $\mu = \pi^2 \hbar^2 n_{1D}^2 / 2m$; $E/N = \pi^2 \hbar^2 n_{1D}^2 / 6m$

GROSS-PITAEVSKII THEORY

Within the mean-field description all bosons are considered to be condensed and described by the same (condensate) wave function

•In 1D where true Bose-Einstein condensation is absent (Mermin1966,Hohenberg1967) but GP theory is still applicable when the healing length ξ exceeds the mean interparticle distance

•Is applicable for weak interactions, $g \to 0$, or in terms of the one dimensional gas parameter, $na \to \infty$, i.e. large density (!)

•Chemical potential linear with density, $\mu = gn$

•Energy per particle linear with density, $E/N = gn/2$

•Can be used for prediction of time dynamics

BOGOLIUBOV THEORY

Bogoliubov approach makes is a perturbative one assuming that a small amount of bosons drop out of the condensate

- Provides a correction to the energy (Lee-Huang-Yang in 3D)
- Second order correction to the ground-state energy is always negative.
- Correction is negative in 1D, energy per particle:
  $E/N = gn/2 \cdot (1 - \text{const} \ / \ (n|a|)^{1/2} + \ldots)$.

NB1 In 3D, the LHY correction is positive due to renormalization, i.e. second order relation between the coupling constant g and a.

NB2 In 1D the correction is consistent with the result obtained by Kirchhoff 1880 within the electrostatic analogy

TONKS-GIRARDEU LIMIT

Hard-core bosons, $g = \infty$, are impenetrable and share many properties with an ideal Fermi gas

- The bosonic ground-state wave function Ψ_B is related to the wave function of ideal fermions Ψ_F as (Girardeau 1960)

$$\Psi_B = |\Psi_F|$$

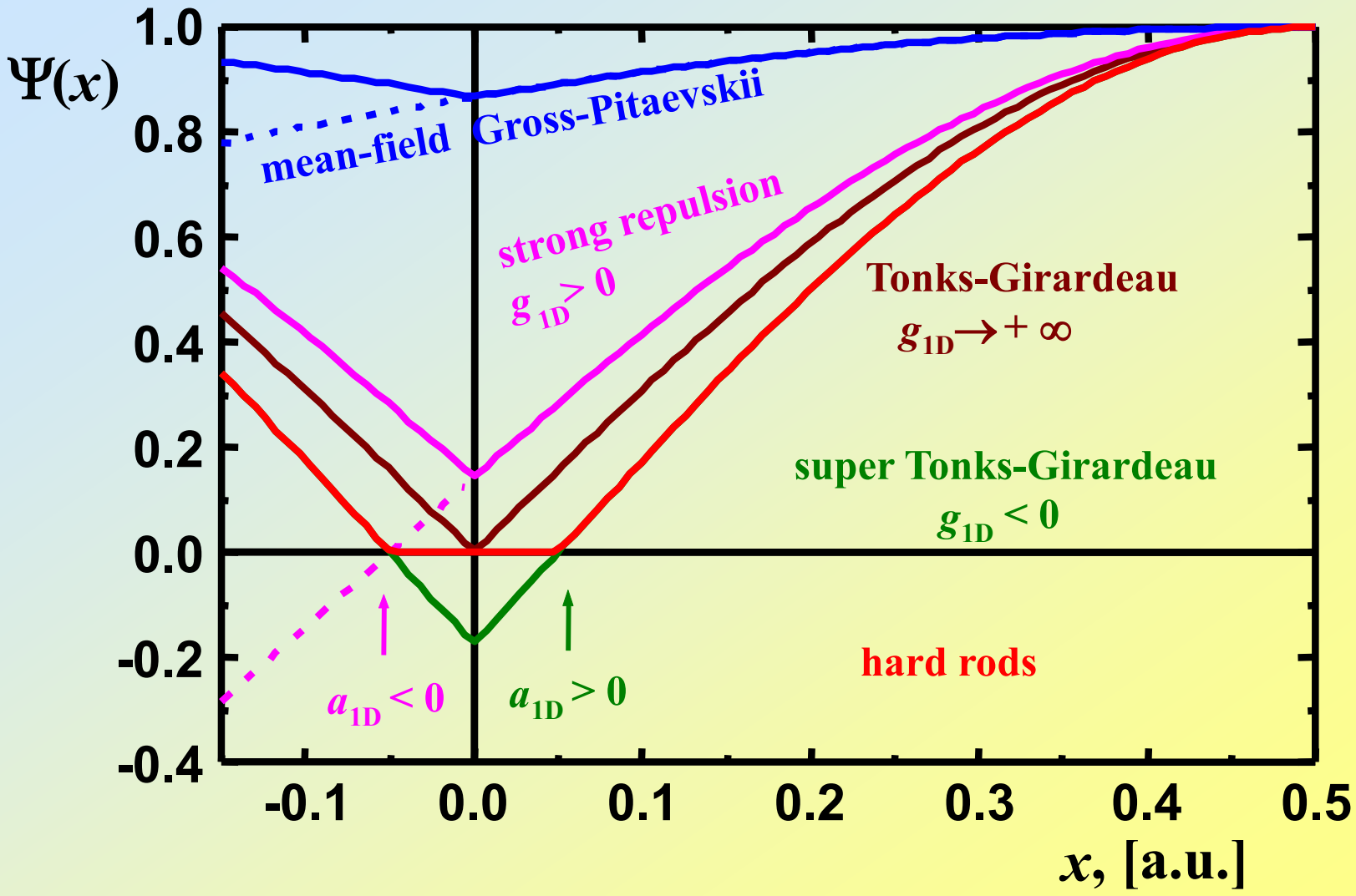
- Local properties are the same.

- Energy per particle is quadratic in density:
$E/N = \pi^2\hbar^2 n^2 \ /(6m)$

- Hard rod of size $a>0$ energy is obtained from the *excluded volume* correction $L \rightarrow L$ - Na : $E/N = \pi^2\hbar^2 n^2/[6m(1 - na)^2]$

- Same correction for $g \rightarrow \infty$ even if the sign of $a \rightarrow$ -0 is different ("*included volume*") $L \rightarrow L + N|a|$: $E/N = \pi^2\hbar^2 n^2/(6m)(1 + 2na)$

TWO-BODY SCATTERING SOLUTION



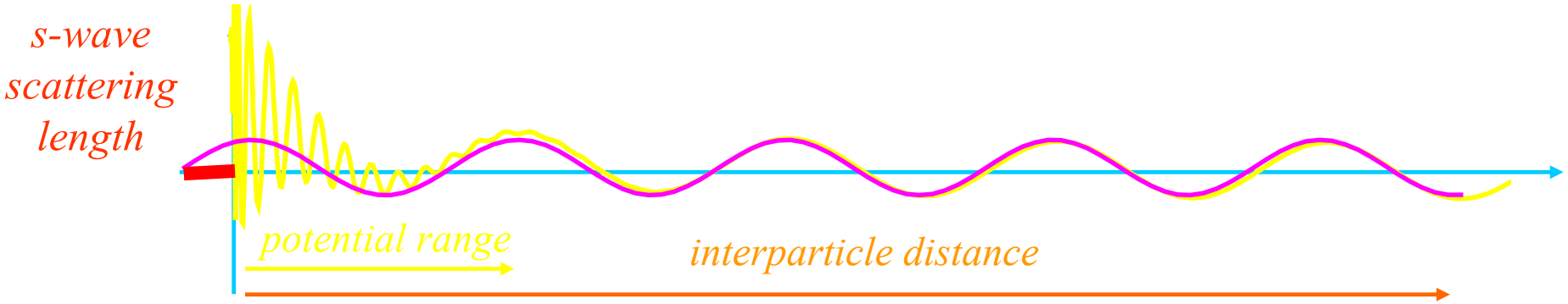
UNIVERSAL REGIME

The *universal regime* at ultralow densities can be understood by considering the properties of two-body scattering problem:

$$-\frac{\hbar^2}{2\mu}\Delta f(r) + V_{int}(r) f(r) = E f(r)$$

When the typical interparticle spacing is large compared to the range of the potential, the exact shape of the potential is no longer important and the interaction potential can be describe by a single parameter:

- the phase shift or
- the *s*-wave scattering length *a*



Scattering length *a* is the position of the first node, closest to zero of the analytic continuation of the scattering solution from the region where the interaction potential is absent

LUTTINGER LIQUID

An effective description of gapless one-dimensional systems

- Is very generic as it applies to any 1D system with linear excitation spectrum, $E(k) = \hbar\, k\, v_s$ where v_s is the speed of sound

- Luttinger parameter, $K = v_F / v_s$, where v_F is the Fermi velocity

- In homogeneous continuous system $v_F = \pi\, \hbar\, n/m$

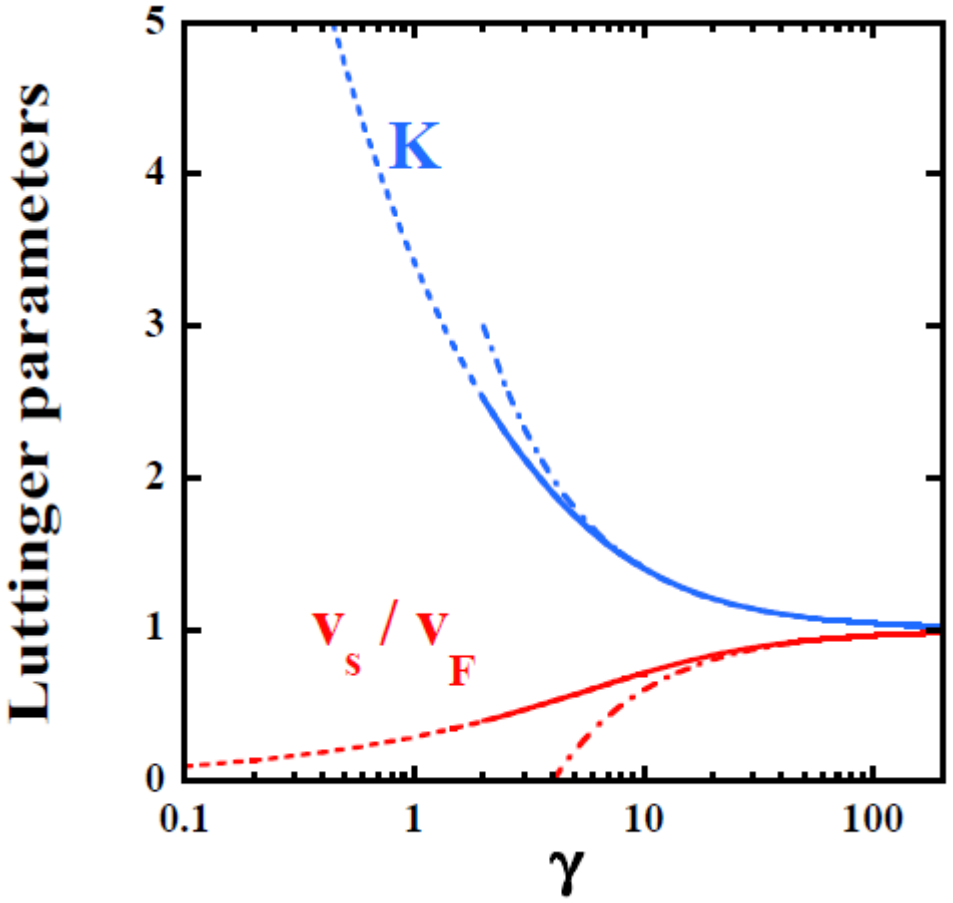
- Provides description of the long-range decay of the correlation functions

- Can be used for prediction of low-temperature thermodynamics

- With renormalization group theory can be used for prediction of pinning, superfluid – Mott insulator transitions, etc

- Is an effective theory, takes speed of sound as an input parameter.

LUTTINGER PARAMETER IN LIEB-LINIGER GAS



Luttinger exponent K versus γ. The dashed lines are the small γ approximations obtained from Bogoliubov theory whereas the dotted-dashed lines correspond to the asymptotic expressions for large γ. Fig. from M. A. Cazalilla J. Phys. B 37, S1 (2004)

MONTE CARLO METHODS

Expectation values (energy, correlation functions, etc) can be expressed as multidimensional integrals and can be efficiently calculated by Monte Carlo methods

- Can be used for any interaction potential (contact interaction, van der Waals, dipolar, etc)
- Energy and correlation functions can be calculated in the ground state of thermodynamic equilibrium
- The results are obtained within some error bars
- The error bars are controllable and can be decreased by making the simulation time larger
- In 1D geometry the Slater determinant of an ideal Fermi gas/ Tonks-Girardeau gas is a Wronskian and can be simplified

VARIATIONAL MONTE CARLO METHOD

- Variational Monte Carlo (VMC) method evaluates multidimensional averages of physical quantities over the N-body trial wave function Ψ_T

$$\langle \hat{A} \rangle = \frac{\int ... \int A(\mathbf{r}_1, ..., \mathbf{r}_N) |\psi_T(\mathbf{r}_1, ..., \mathbf{r}_N)|^2 \, d\mathbf{r}_1 ... d\mathbf{r}_N}{\int ... \int |\psi_T(\mathbf{r}_1, ..., \mathbf{r}_N)|^2 \, d\mathbf{r}_1 ... d\mathbf{r}_N}$$

- Metropolis algorithm can be used to generate set of points $\{\boldsymbol{R}_\mathrm{i}\}$ in $3N$-dimensional space $\boldsymbol{R}=\{\boldsymbol{r}_1,...,\boldsymbol{r}_\mathrm{N}\}$ according to probability distribution $p(\boldsymbol{R}) = |\psi_\mathrm{T}(\boldsymbol{R})|^2$.

- Average of some operator A over $|\psi_\mathrm{T}(\boldsymbol{R})|^2$ is approximated as

$$\langle \hat{A} \rangle \approx \frac{1}{N_{iter}} \sum_{i=1}^{N_{iter}} A(\mathbf{r}_i)$$

-Applied to Hamiltonian, $A = H$, one obtains an upper bound

$$E_0 \leq E_T = \frac{\langle \psi_T | \hat{H} | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}$$

-Variational principle can be used to optimize parameters

DIFFUSION MONTE CARLO METHOD

- Difffusion Monte Carlo (DMC) method is based on solving the Schrodinger equation in imaginary time

$$-\frac{\partial \Psi(\mathbf{R},\tau)}{\partial \tau} = (\hat{H} - E_{offset})\Psi(\mathbf{R},\tau)$$

- Formal solution $\psi(\mathbf{R},\tau) = e^{-(\hat{H}-E_{offset})\tau}\psi(\mathbf{R},\tau=0)$

- Expanding over eigenstates $\psi(\mathbf{R},\tau=0) = \sum_n c_n \phi_n(\mathbf{R})$

- At large times only contribution from the ground state survives:

$$\psi(\mathbf{R},\tau) = \sum_{n=0} e^{-(E_n-E_{offset})\tau} c_n \phi_n(\mathbf{R}) \rightarrow e^{-(E_0-E_{offset})\tau} c_0 \phi_0(\mathbf{R})$$

- Permits to calculate static ground state properties exactly

- Provide correlations in imaginary time, e.g. $S(k,\ \tau)$
  + inverse Laplace transform gives $S(k,\ \omega)$

- Importance sampling uses $\Psi_T(\mathrm{R})\,\Psi(\mathrm{R},\tau)$ instead of $\Psi(\mathrm{R},\tau)$

TRIAL WAVEFUNCTION

We chose the trial wave function in pair-product form:

$$\psi_T(\mathbf{r}_1, \cdots, \mathbf{r}_N) = \prod_{i<j} f_2(|\mathbf{r}_i - \mathbf{r}_j|) \ ,$$

where the Jastrow terms $f_2(r)$ describe correlations and satisfy:

1) at short distances, 2-body scattering problem

   $f_2(x) = \cos(k\,x + \delta), \quad x < R_{\text{match}}$

   with momentum k and phase shift δ chosen in order to satisfy the Bethe-Peiels boundary condition

   $f_2'(x) \ / \ f_2(x) = -1/a$

2) at large distances, phononic tail [Reatto & Chester 1967]

   $f_2(x) = \cos^{1/K}(\pi\ x\ /\ \mathrm{L}), \quad R_{\text{match}} < x < L/2$

   where K is the Luttinger parameter

NB for Tonks-Girardeau gas, K=1, short and long-range parts became the same, $f_2(x) = \cos(k\,x + \delta)$, and trial wave function becomes exact and equal to Slater determinant.

VARIATIONAL ENERGY

The variational energy with the physically sound trial wave function can be pretty good

- Simple ansatz provides accuracy of the order of 1%
- More sophisticated optimization can be much more precise. Carleo tVMC optimization, error of the order of 10^{-4} %

POLARON HAMILTONIAN

The Lieb-Liniger Hamiltonian models one-dimensional Bose gas with short-range interactions

$$H = -\frac{\hbar^2}{2m}\sum_i \frac{d^2}{dx_i^2} + g_{BB}\sum_{i<k}\delta(x_i - x_k) - \frac{\hbar^2}{2m_{imp}}\frac{d^2}{dx_{imp}^2} + g_{BI}\sum_i \delta(x_i - x_{imp})$$

where the coupling constant $g_{BB} = -2\hbar^2/m_B a_{BB}$ describes boson-boson interactions, $g_I = -\hbar^2/\mu_{BI} a_{BI}$ the boson-impurity interactions and $\mu_{BI} = m_B m_I/(m_B + m_I)$ is the reduced mass

- Interaction strength is related to the s-wave scattering lengths a_{BB} and a_{BI}
- Impurity mass, m_{imp}, can be different from the boson mass m_B.

CHARACTERISTIC PARAMETERS

The system properties are governed by the following dimensionless parameters

- gas parameter na_{BB}
- or the Lieb – Liniger parameter $\gamma = -2/na_{BB} = m_B\, g_{BB}\, /(\hbar^2\, n)$

describing the strength of Bose-Bose interactions

- strength of Bose-impurity interactions na_{BI}
- or, analog of the Lieb-Liniger parameter, $\eta = -2/na_{BI} \propto g_{\mathrm{BI}}$

- mass ratio $m_I \,/\, m_B$

DIFFERENT REGIMES 1/2

The following different regimes can be realized in the system

Changing boson-impurity interaction strength

- Repulsive polaron $\eta > 0$
- Attractive polaron $\eta < 0$
- Weakly interacting polaron, $|\eta| < 1$
- Strongly interacting polaron, $|\eta| > 1$
- Hard-core polaron $\eta = \infty$

Changing boson-boson interaction strength

- Repulsive gas $\gamma > 0$, homogeneous system is stable
- Attractive gas $\gamma < 0$, bright soliton is formed
- Tonks-Girardeau / fermionized gas, $\gamma = \infty$

DIFFERENT REGIMES

Changing mass

- light impurity $m_I \ll m_B$
- heavy impurity $m_I \ll m_B$
- mobile impurity, finite m_I
- pinned impurity, $m_I = \infty$

THEORIES

Different method can be used to address the problem of 1D

•***Bethe ansatz*** method (exact) applicable for contact interactions
a)repulsive interactions, Lieb-Liniger uniform gas
b)Attractive interactions, McGuire bright soliton

•can be generalized for an impurity with equal mass $m_I = m_B$ and equal interactions $g_{BB} = g_{BI}$

•Impenetrable bosons / ideal fermions, $g_{BB} = \infty$, plus one impurity, $g_{BB} = \infty$

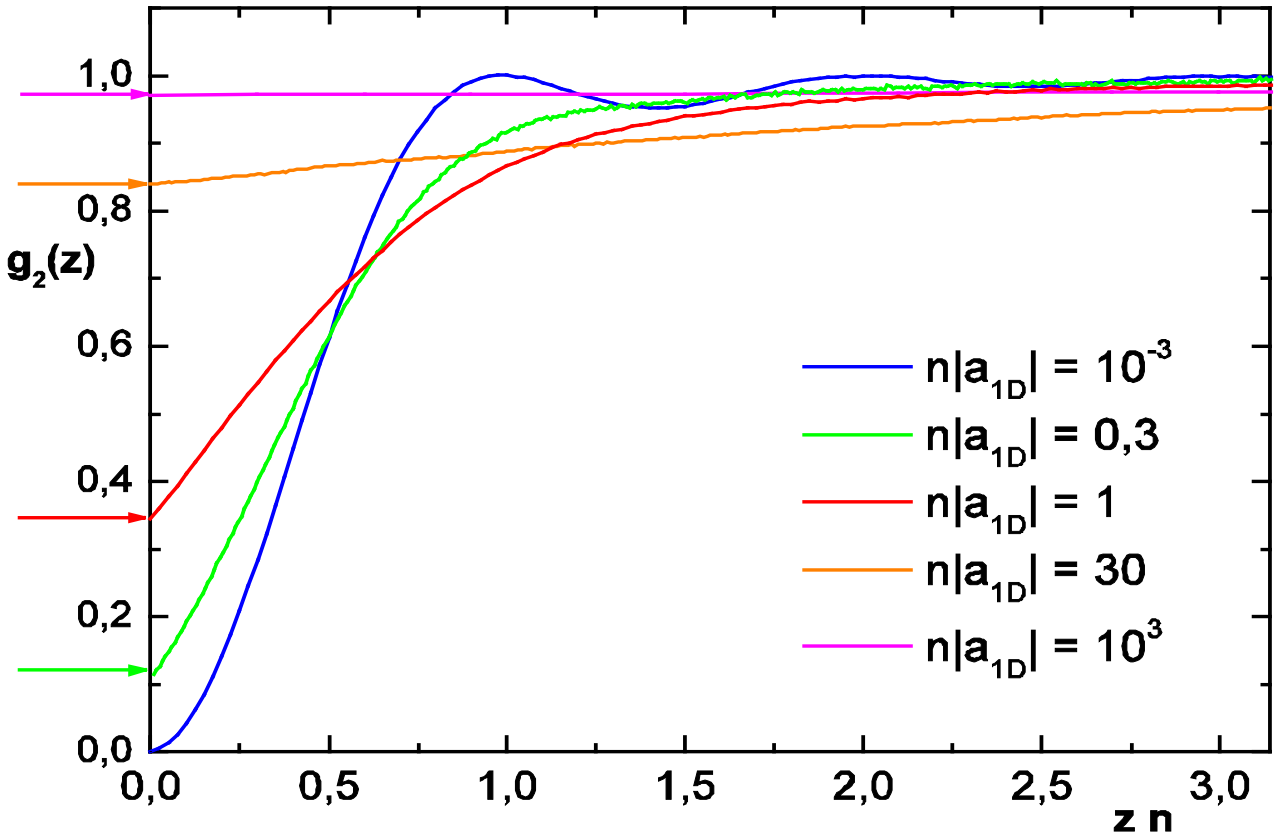
RESULTS

- Pure bosonic system (no impurities)
- Bosons plus single impurity (polaron)
- Bosons plus two impurities (bipolaron)

Results:

Pure bosonic system (no impurities)

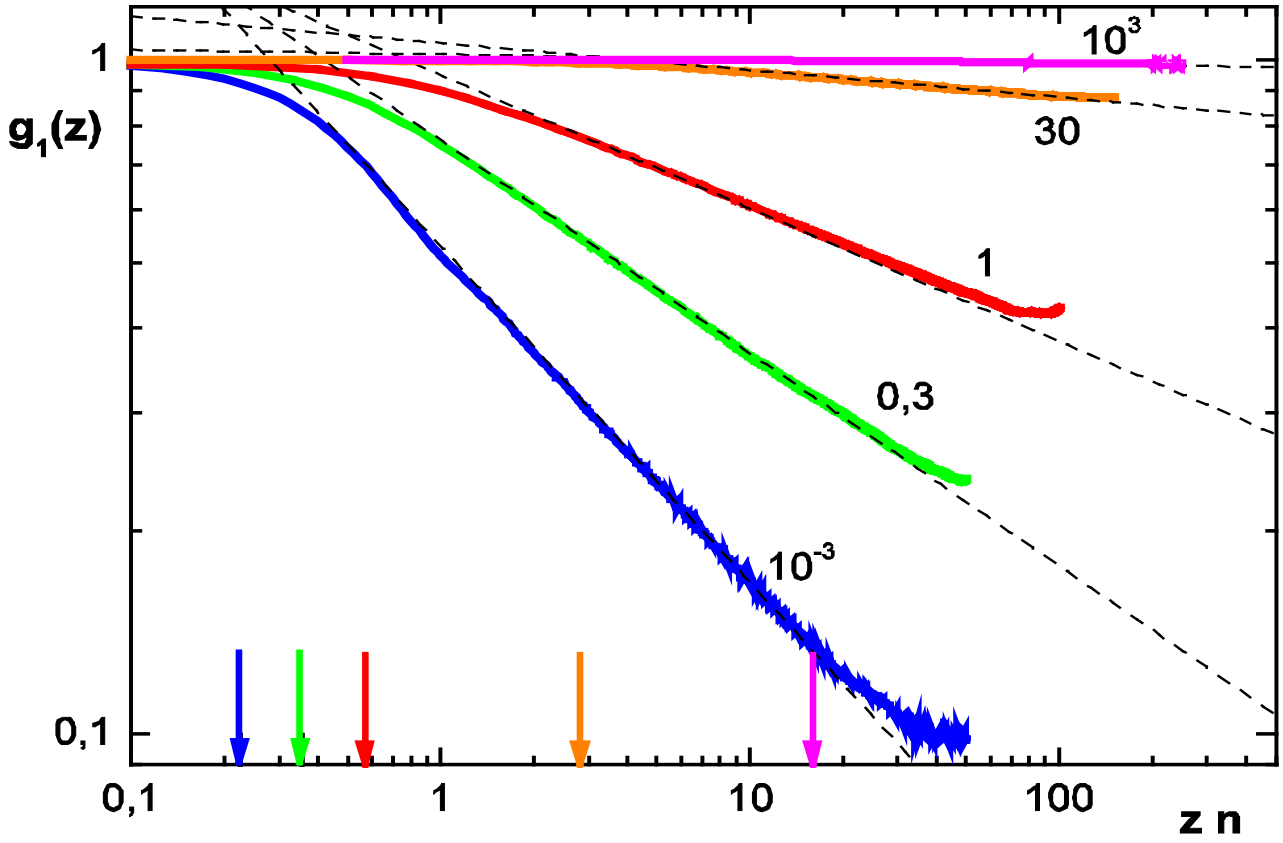
PAIR DISTRIBUTION FUNCTION



Pair distribution function for different values of the gas parameter. Arrows indicate the value of $g_2(0)$ as obtained from the equation of state. At $n|a_{1D}|=10^{-3}$ the $g_2(z)$ function is similar to that of the a Tonks-Girardeau gas

Ref:. GEA & S. Giorgini PRA 68, 031602 (2003)

ONE-BODY DENSITY MATRIX



One-body density matrix $g_1(z)$ (solid lines), power-law fits (dashed lines). The long-range asymptotic value of OBDM gives the condensate fraction i.e. condensate is absent in all cases.

Ref:. GEA & S. Giorgini PRA 68, 031602 (2003)

Results:

Bosonic system with one impurity (polaron)

PINNED IMPURITY IN GROSS-PITAEVSKII THEORY

A massive/pinned impurity, $m_I = \infty$, with weak interactions $|g_i| \ll g_B$ in the mean-field regime $n|a_B| \gg 1$ is described by the Gross-Pitaevskii energy functional

$$E = \int \left(\frac{\hbar^2}{2m} |\nabla \psi|^2 + (\mu - g_i \delta(\mathbf{r}))|\psi|^2 + \frac{g}{2}|\psi|^4 \right) d^3x,$$

where g_i is the boson-impurity coupling constant ψ is the condensate wavefunction, μ the chemical potential of the gas.

For a small perturbation $\psi(\mathbf{r}, t) = \phi_0 + \delta\psi(\mathbf{r}, t)$, linearized equation can be solved in momentum space and has a screened Yukawa form, $\delta\psi_{\mathbf{k}} = -\frac{g_i \phi_0}{\frac{\hbar^2 k^2}{2m} + 2\mu}$

The density profile is $n(x) = n + \frac{\sqrt{2} n \xi}{a_i} \exp\left(-\frac{\sqrt{2}|x|}{\xi} \right)$

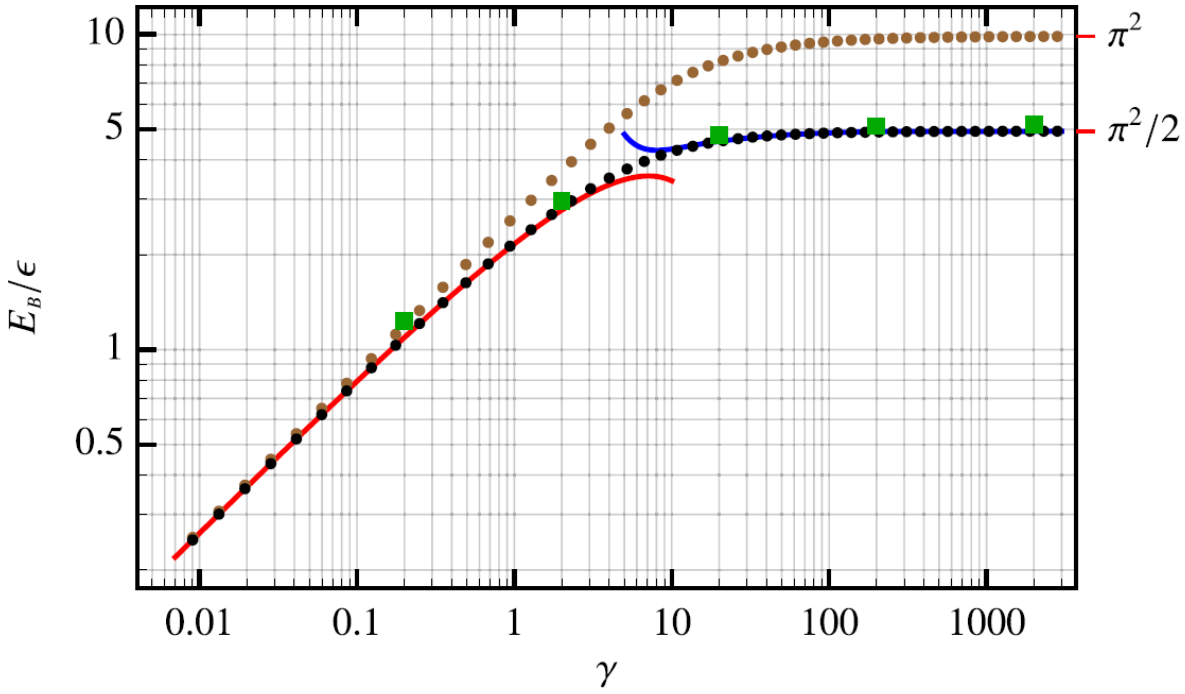
- exponential decay with the typical scale given by the healing length ξ
- effect is symmetric for weak repulsion ($g_i > 0$ or $a_i < 0$) and attraction ($g_i < 0$ or $a_i > 0$)

Ref: GEA & L.P. Pitaevskii PRA **70**, 013608 (2004)

IMPENETRABLE PINNED IMPURITY IN BETHE ANSATZ

Energy of a massive/pinned impurity, $m_I = \infty$, with hard-core interactions $g_i = \infty$ for any value of $n|a_B|$ can be found in Bethe ansatz. The value of the *edge energy* was first considered by M. Gaudin in 1971.

Unfortunately, his results for the thermodynamic limit were rather corresponginds to Lieb II solitonic solution.



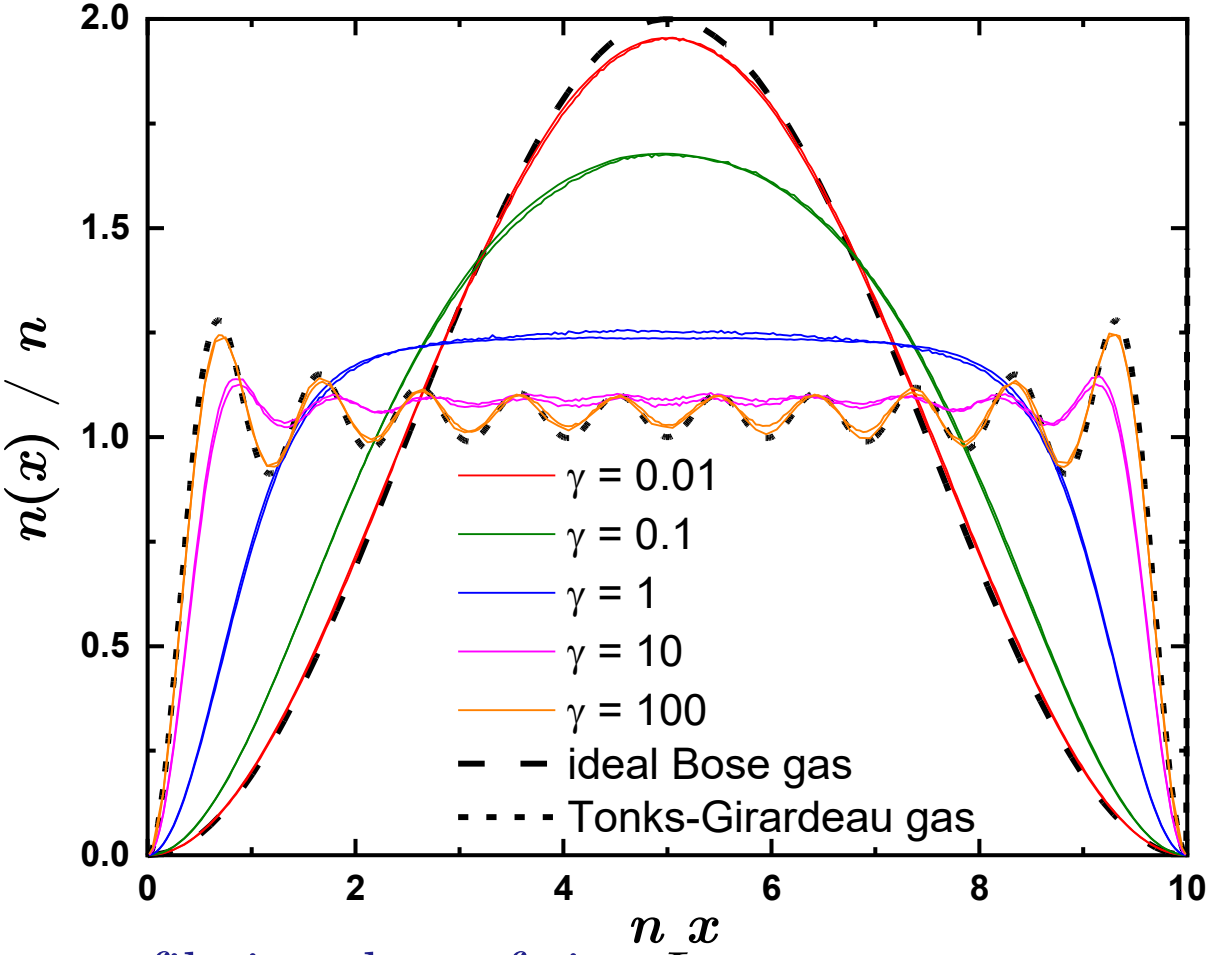
- upper curve Lieb II dark soliton energy [1,2]
- lower curve polaron energy [3]

Units of $\varepsilon = \hbar^2 n^2/(2m)$

NB: factor 2 in TG limit

[1] M. Gaudin, *Boundary energy of a Bose gas in one dimension*, PRA 4, 386 (1971).
[2] Michel Gaudin "Bethe wavefunction" Cambridge University Press (2014)
[3] B.Reichert, GEA, A.Petković & Z.Ristivojevic PRL **123**, 250602 (2019)

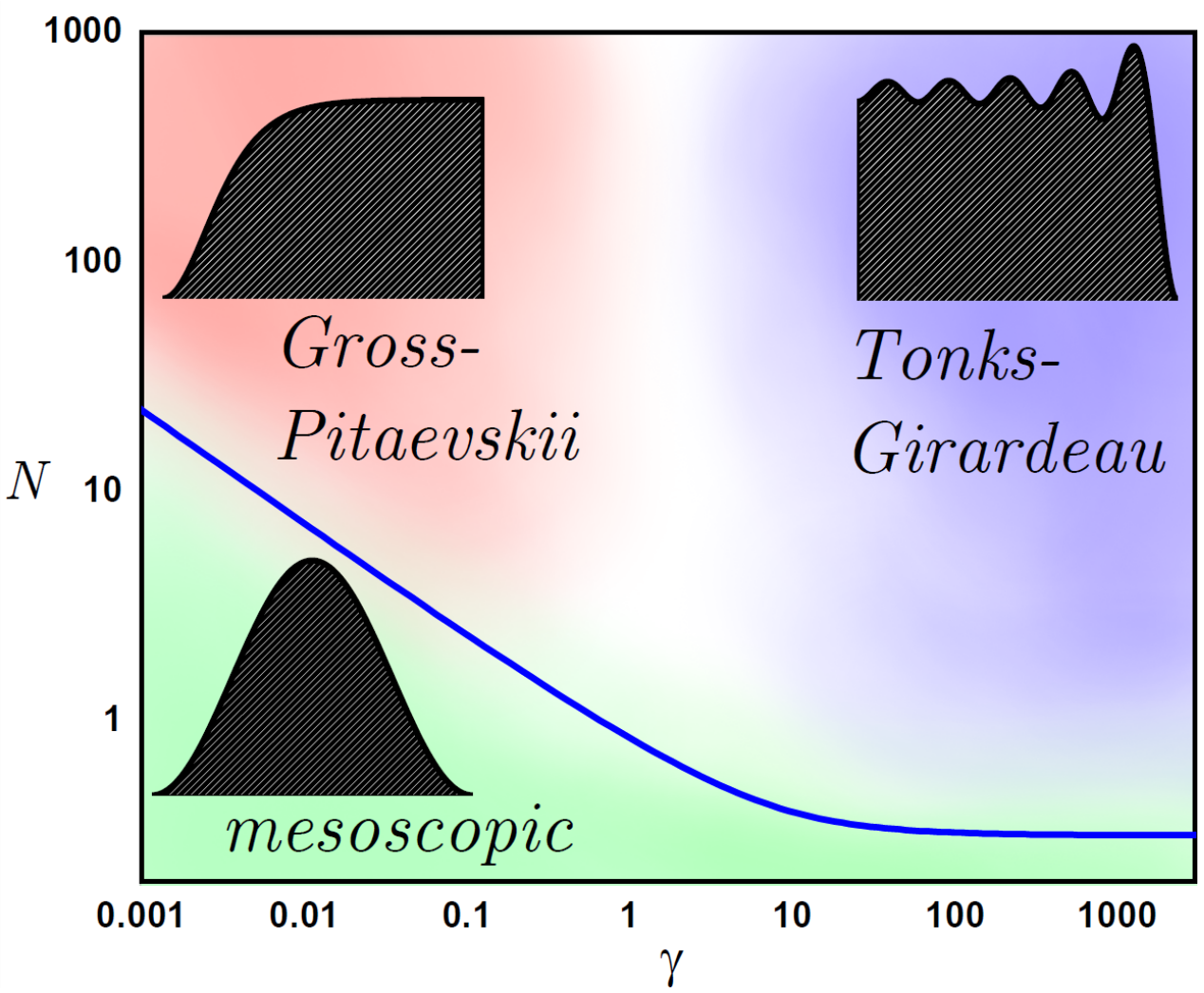
IMPENETRABLE PINNED IMPURITY



Polaron density profile in a box of size L

- $a \gg n^{-1} \gg L$ (i.e. $\gamma \ll 1$, $a \gg L$) : Ideal Bose gas / standing wave
- $L \gg a \gg n^{-1}$ (i.e. $\gamma \ll 1$, $a \ll L$) : GP dark soliton
- $L \gg n^{-1}$ (i.e. $\gamma \gg 1$) : Girardeau-Wright dark soliton

IMPENETRABLE PINNED IMPURITY



Polaron density profile in a box as a function of the interaction strength and number of bosons N in a box.

IMPURITY IN AN IMPENETRABLE GAS

Energy of a mobile $m_I = m$ in impenetrable gas, $g_B = \infty$, for any value of boson-impurity interaction $g_i = \infty$

- solved in homogeneous system by McGuire (1965)
- can be generatlized in trapped case according to the mapping $k_F \to k_F^t = \sqrt{2N}/a_{||}$
- we define $\gamma_t = -2\pi/(k_F^t a_{1D}) = -\sqrt{2/N}\,\pi a_{||}/a_{1D}$.

The resulting energy in terms of γ_t is

$$\frac{E}{\hbar\omega_{||}} = \frac{N^2+1}{2} + \frac{N\gamma_t}{\pi^2}\left[1 - \frac{\gamma_t}{4} + \left(\frac{\gamma_t}{2\pi} + \frac{2\pi}{\gamma_t}\right)\text{arctg}\,\frac{\gamma_t}{2\pi}\right]$$

[1] J. B. McGuire, J. Math. Phys. **6**, 432 (1965).
[2] GEA and I. Brouzos Phys. Rev. A **88**, 021602(R) (2013)

EXPERIMENT IN FLORENCE

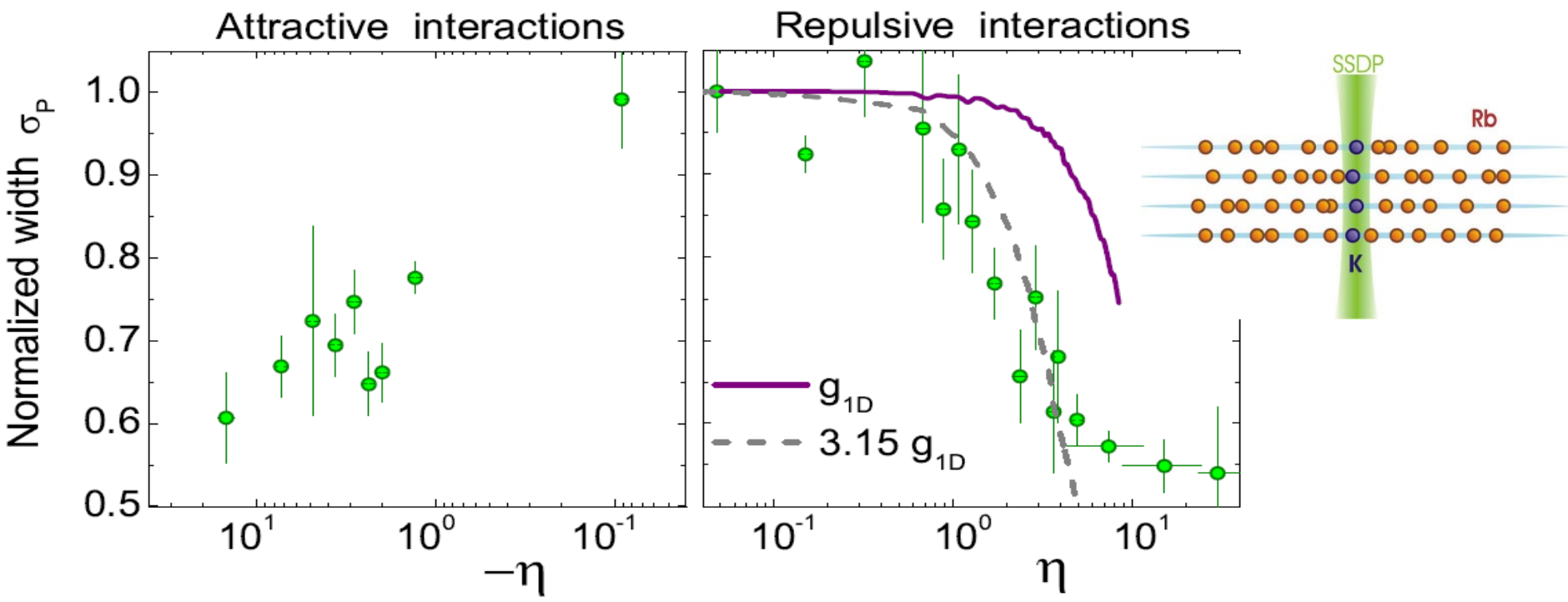
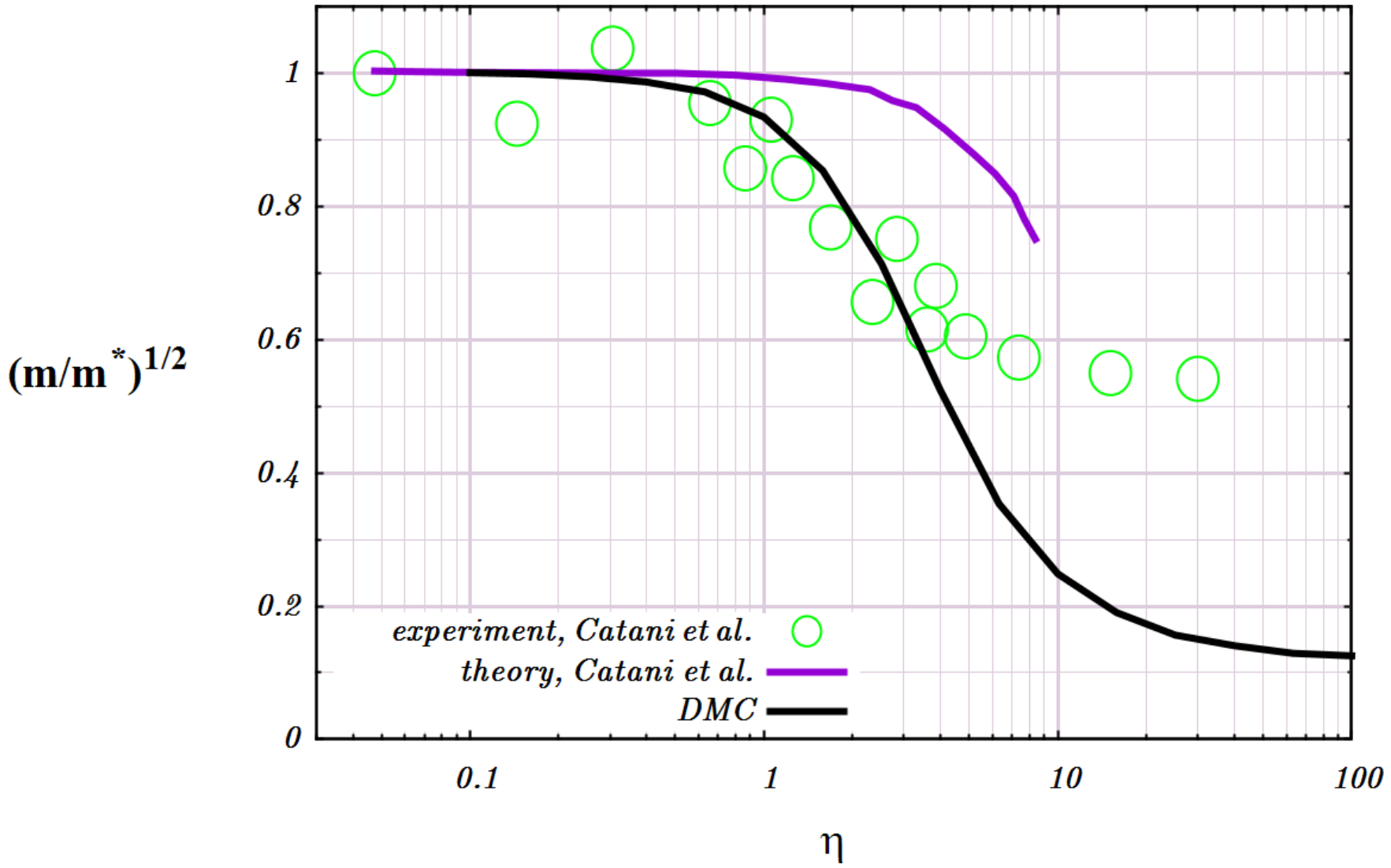


FIG. 4. (Color online) Experiment: impurities' axial size at the first oscillation maximum σ_p, normalized so that $\sigma_p = 1$ for $\eta = 0$, versus the coupling strength parameter $\eta = g_{1D,KRb}/g_{1D,Rb}$, for attractive (left, $\eta < 0$) and repulsive (right, $\eta > 0$) interactions (circles). Theory: $\sqrt{m_K/m_K^*}$

Ref: J. Catani, G. Lamporesi, D. Naik, M. Gring, M. Inguscio, F. Minardi, A. Kantian, T. Giamarchi (2012)

POLARON MASS

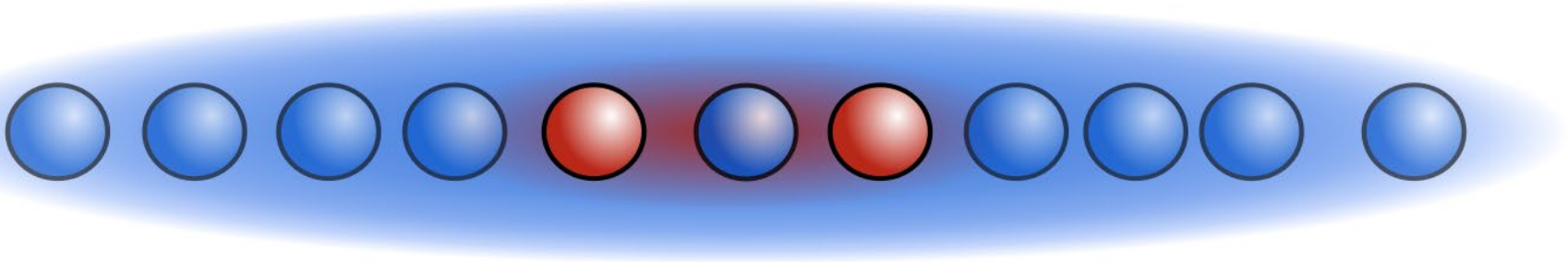


Repulsive polaron mass vs experiment by Catani et al 2012

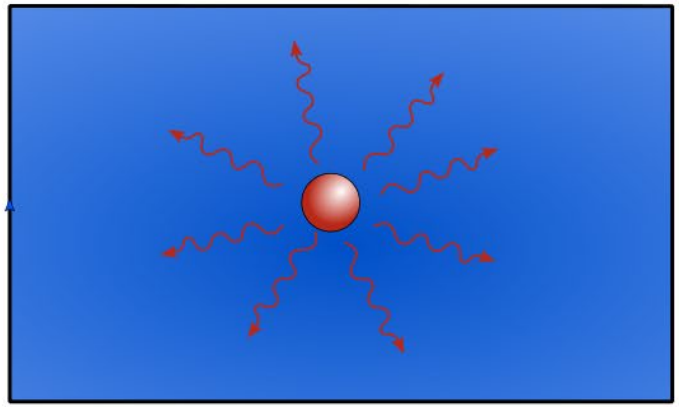
Ref: F.Grusdt, GEA & E.Demler New Journal of Physics 19, 103035 (2017)

PERTURBING GP SOLUTION

a)

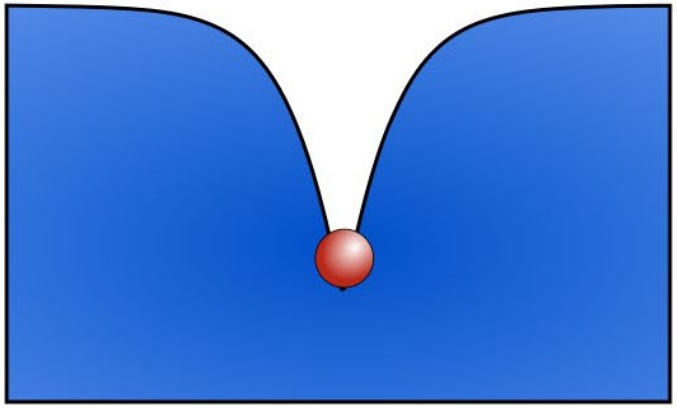


b)



$$\hat{\phi}(x) = \sqrt{n} + \hat{\xi}(x)$$

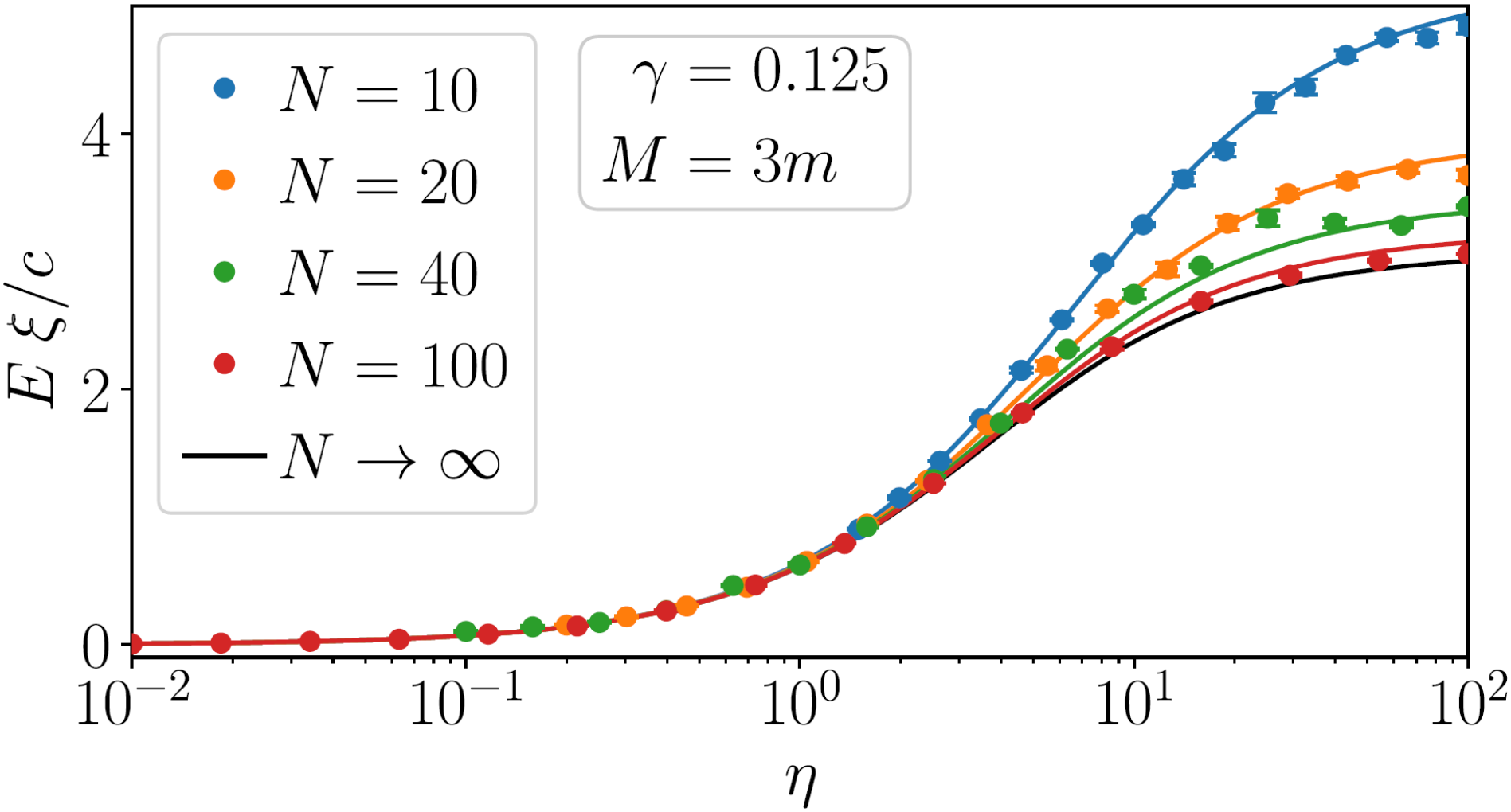
c)



$$\hat{\phi}(x) = \phi(x) + \hat{\xi}(x)$$

Martin Will, GEA, Michael Fleischhauer "Polaron interactions and bipolarons in one-dimensional Bose gases in the strong coupling regime" arXiv:2101.11997

PERTURBING GP SOLUTION



Polaron energy dependence on IB interaction strength in the weakly interacting regime, $\gamma \ll 1$, as a function of the relative interaction strength $\eta = g_{\mathrm{IB}}/g$ for mass ratio of 3

Results:

Bosonic system with two impurities (bipolaron)

BIPOLARON: WEAKLY INTERACTING GAS

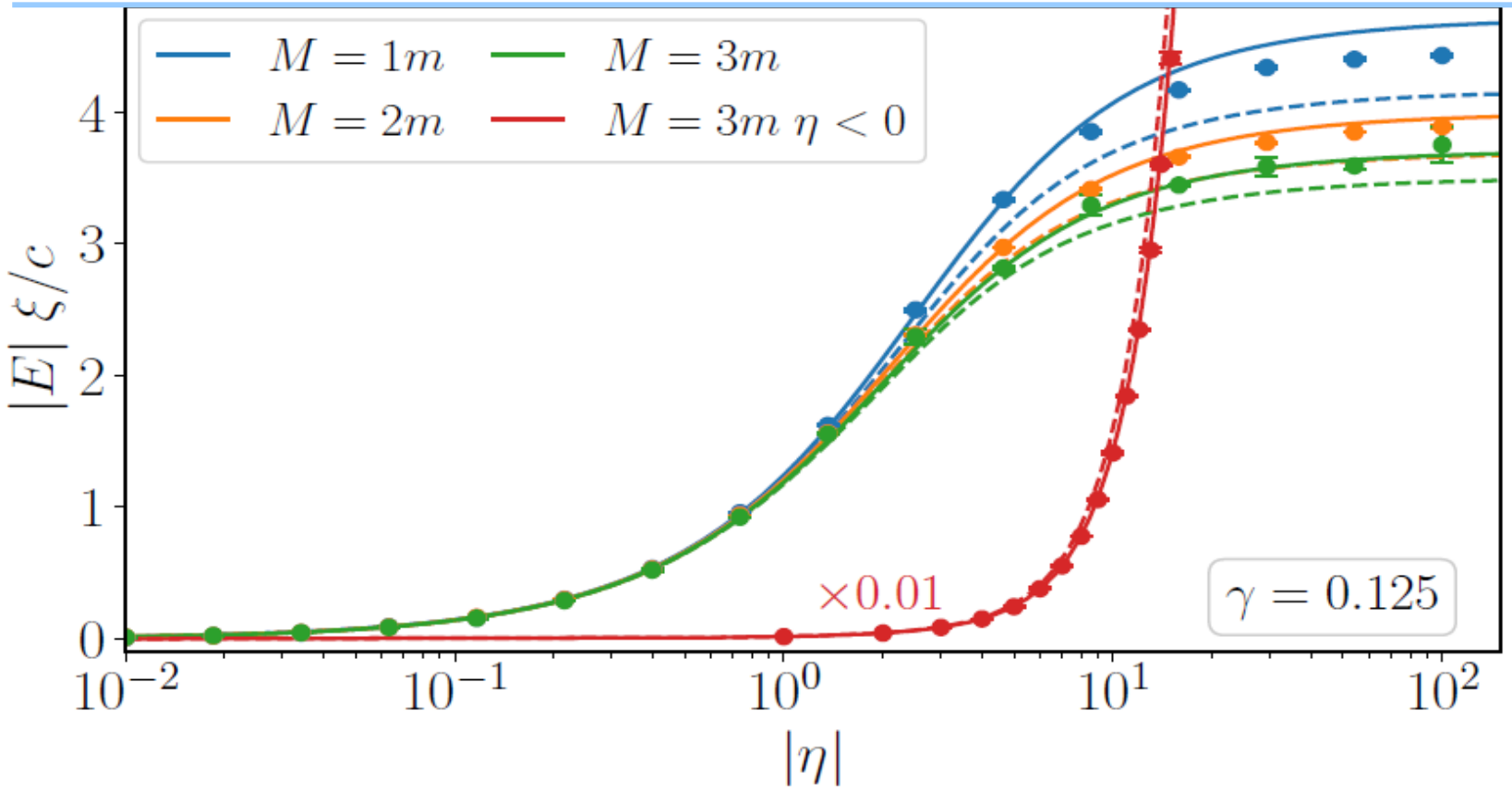


FIG. 4. Comparison of ground state energy of bound bipolaron and QMC (dots) for different mass ratios m/M and weak-to-moderate boson-boson coupling $\gamma = 0.125$. Dashed lines correspond to BO potential $V(r)$, solid lines include first BO correction $V(r)+W(r)$.

BIPOLARON: STRONGLY CORRELATED GAS

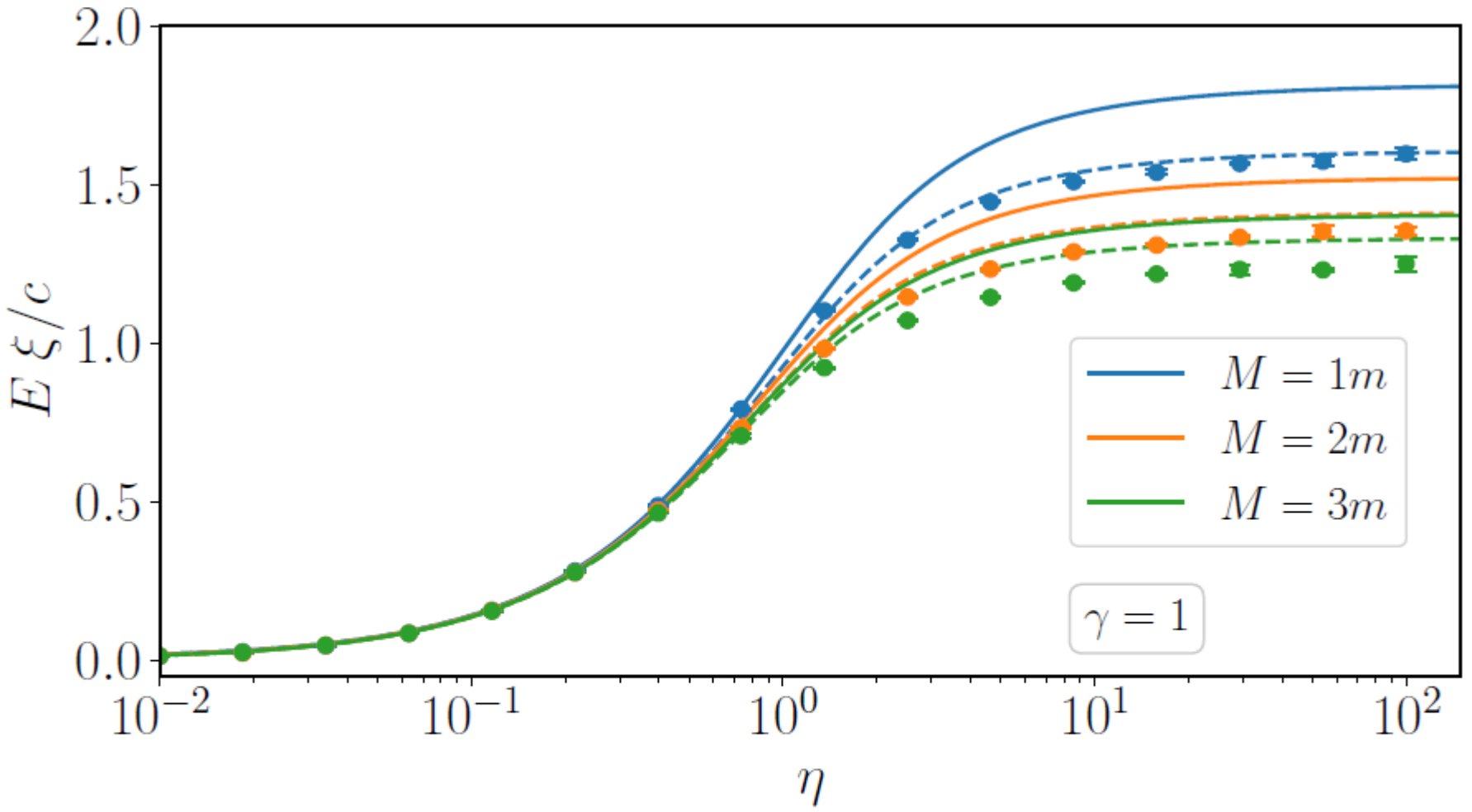


FIG. Comparison of ground state energy of bound bipolaron and QMC for different mass ratios m/M and strong boson-boson coupling $\gamma = 1$.

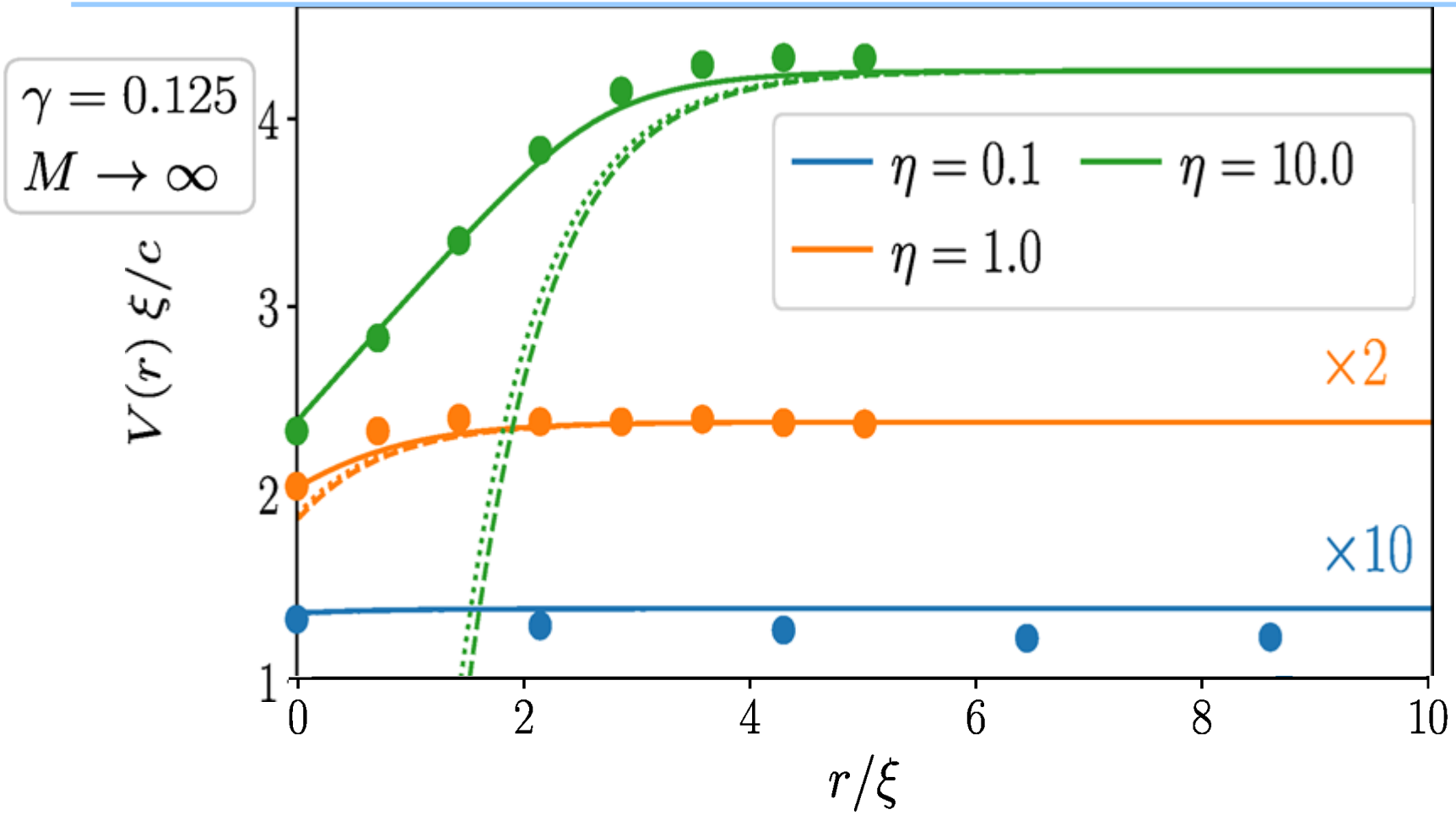
EFFECTIVE INTERACTIONS: HEAVY IMPURITIES

For infinite impurity mass the polaron-polaron interaction potential is calculated as

$$U(x_2 - x_1) = E_2 - E_0$$

E_2: the ground-state energies of the system with two impurities at positions x_1 and x_2
E_0: the ground-state energies of the system with no impurities

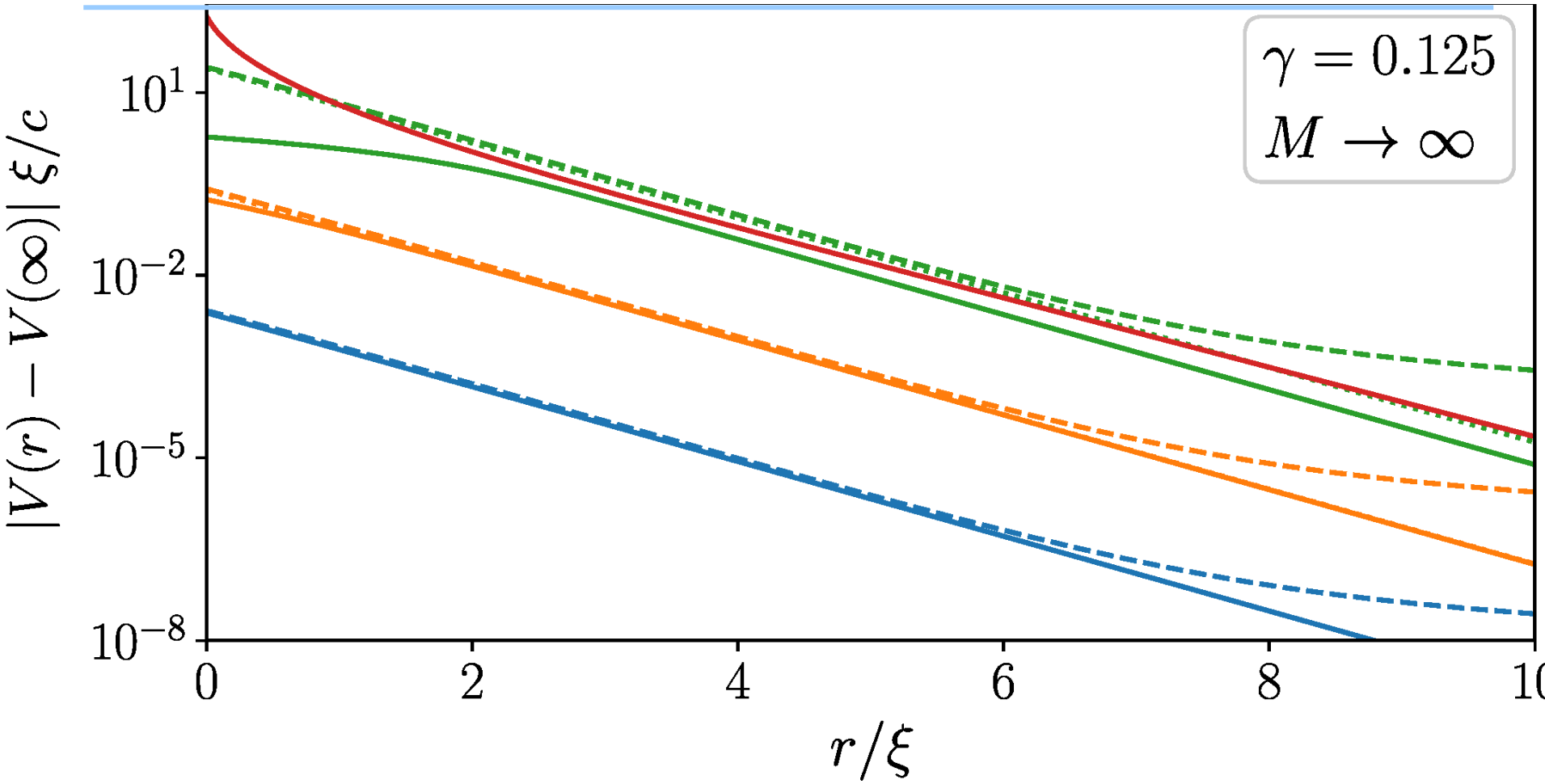
EFFECTIVE INTERACTION: WEAKLY INTERACTING GAS



Effective impurity interaction for $M=\infty$. The solid lines represent the semi analytical approximation and the dots are QMC simulations. The perturbative predictions from [1], are shown as dashed and dotted lines, including and excluding Casimir-type contribution.

[1] B.Reichert, A.Petković & Z.Ristivojevic PRB 99, 205414 (2019)

CASIMIR INTERACTION



The perturbative predictions are shown as dashed and dotted lines, including and excluding Casimir-type contribution. Exponential decay for weak impurity-boson couplings is seen as straight lines. The Casimir effect (absent in the mean-field description) results in the slow $1/r^3$ decay at $r\,/\,\xi > 6$.

EFFECTIVE INTERACTIONS: MOBILE IMPURITIES

- impurity-impurity distribution function is calculated $g_{ii}(X)$
- ground-state wave function $\psi_{ii}(X) = \sqrt{g_{ii}(X)} > 0$ is extracted
- it satisfies the two-impurity Schrödinger equation

$$-\frac{1}{2\mu^*}\psi_{ii}''(X) + V(X)\psi_{ii}(X) = E_{ii}\psi_{ii}(X),$$

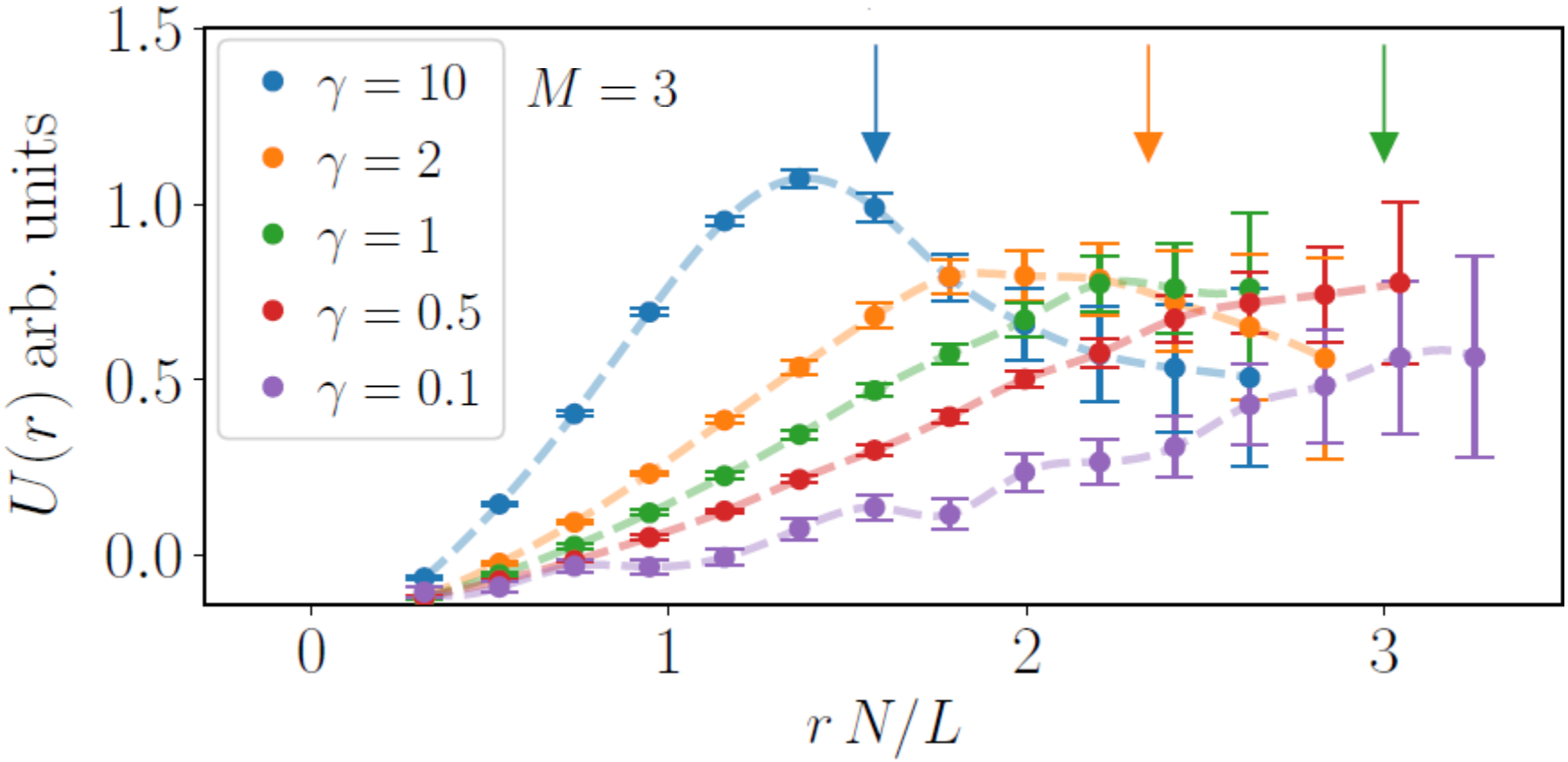
where μ^* is the reduced effective polaron mass. and $E_{ii} = E_2 - E_0$

- The unknown effective interaction potential $V(X)$is obtained as

$$V(X) = E_{ii} + \frac{1}{2\mu^*}\frac{(\sqrt{g_{ii}(X)})''}{\sqrt{g_{ii}(X)}}.$$

- bipolaron binding energy E_{ii} provides a vertical offset in $V(X)$
- reduced effective mass μ^* "stretches" interaction potential vertically

INTERACTIONS: MOBILE IMPENETRABLE IMPURITIES

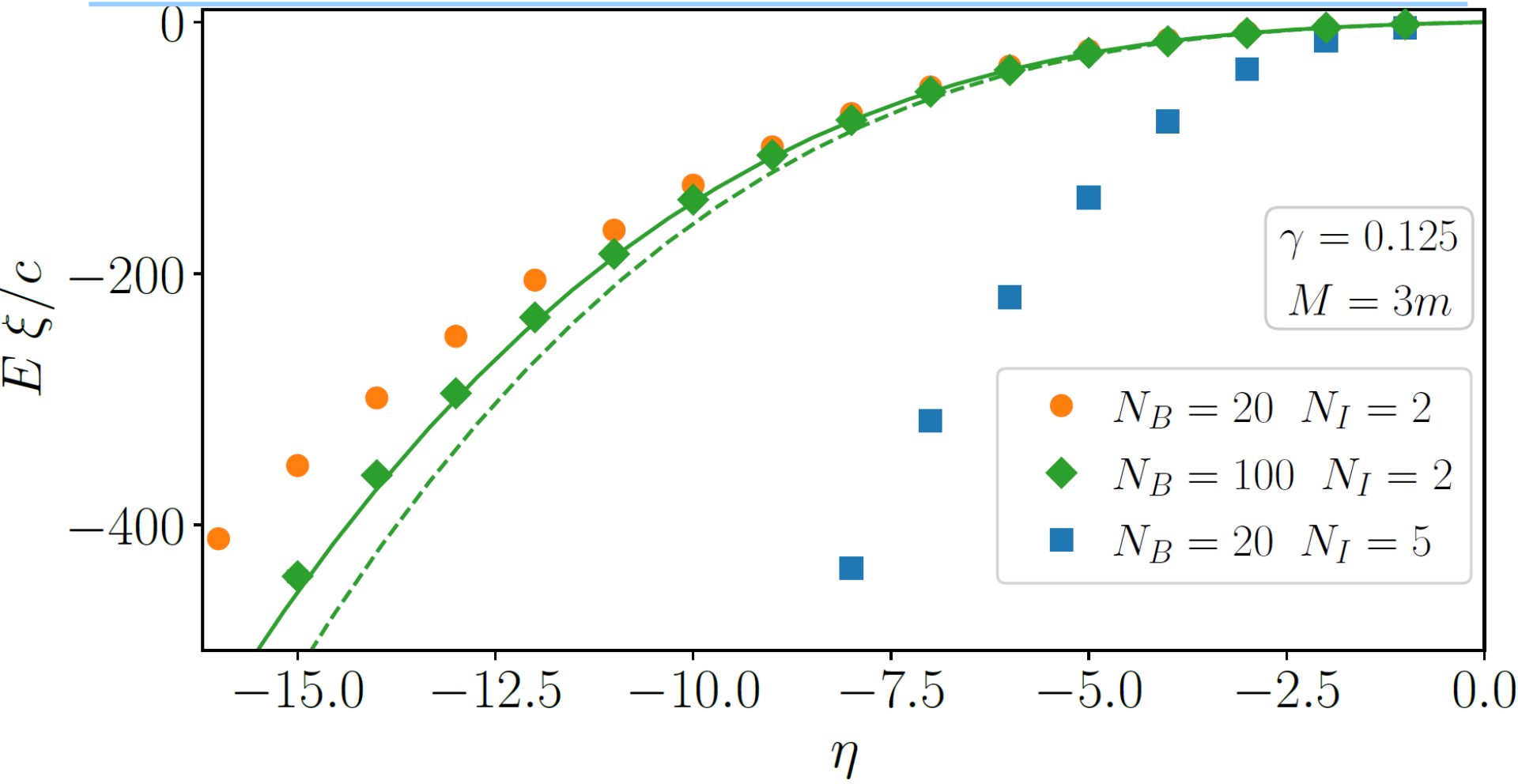


Total interaction potential $U(r)$ from Monte-Carlo simulations for the same mass ratio, but $\eta = \infty$ and different Lieb-Liniger parameters. The arrows point to the analytical estimation of the maxima $r_{\max} = \pi\bar{\xi} = \pi/\sqrt{2m_{\mathrm{r}}\mu}$, where we used the equation of state for μ from Bethe Ansatz

Results:

Bosonic system with many impurities

MULTIPLE-IMPURITY STATE: ENERGY



QMC ground state energy of a system containing N_{B} bosons and N_{I} impurities interacting attractively with each other. The solid (dashed) line is the MF prediction of the bipolaron energy including (excluding) the first order BO correction in the thermodynamic limit.

MULTIPLE-IMPURITY STATE: STABILITY

If direct interaction potential between impurities is neglected, a homogeneous mixture will be always unstable.

Stability criterium for a balanced mixture (N_{B}=N_{I})

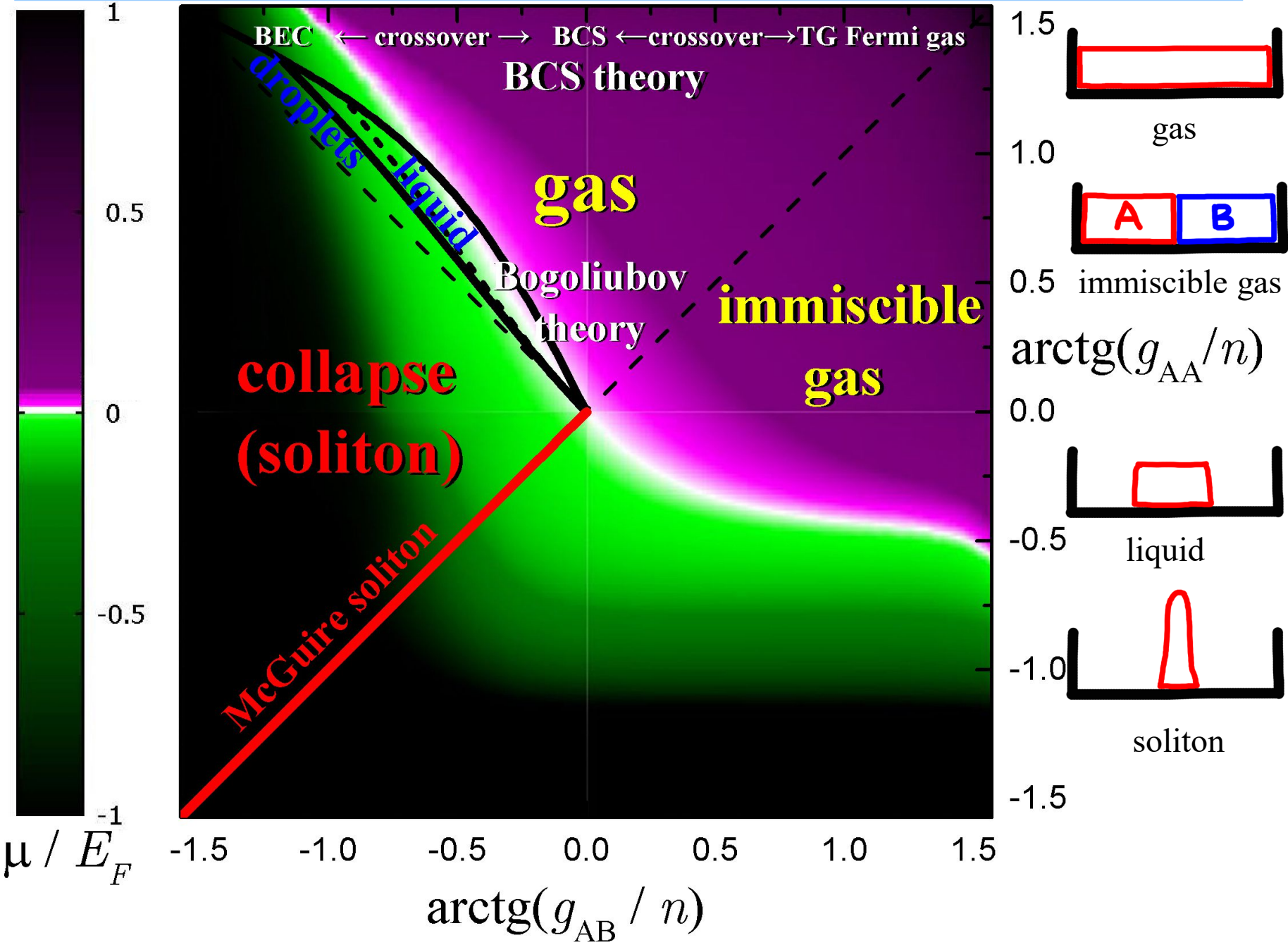
$$g_{\mathrm{BB}}\, g_{\mathrm{II}} > \; g_{\mathrm{BI}}{}^{2}$$

cannot be fulfilled when $g_{\mathrm{II}} = 0$.

Depending on the sign of boson-impurity interaction different instabilities are present

- $g_{\mathrm{BI}}>0$, phase separation
- $g_{\mathrm{BI}}<0$, collapse

BONUS SLIDE* PHASE DIAGRAM OF BOSE-BOSE MIXTURE



CONCLUSIONS

- One-dimensional systems are fantastic!
- Quantum Monte Carlo methods provide useful information
- There is a certain analogy between impenetrable heavy impurity and a dark soliton within Gross-Pitaevskii theory
- McGuire energy generalized for trapped geometry
- Edge energy found within Bethe ansatz theory
- Induced interaction between polarons can be non-monotonous

FUTURE WORK

- Map complete phase diagram in terms of boson-boson, boson-impurity, impurity-impurity interaction and mass ratio
- Regimes of ultrastrong correlations – super Tonks-Girardeau regime for the gas and/or impurity
- Density profiles for impenetrable massive impurity, relation to dark soliton
- Impurities in a bright soliton

MERCI BEAUCOUP POUR VOTRE ATTENTION !