Critical stability

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Ettore Majorama Centre for Scientific Culture

Two-boson correlations in various one-dimensional traps

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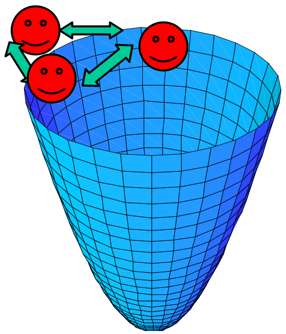
Outline

- Introduction
- Correlation and entanglement measures
- Two bosons in an external trap
  - harmonic confinement: exact results
  - multi-well confinement:
  optimized Configuration Interaction method
- Summary and outlook

N identical particles in a trap



$$H = \sum_{i=1}^{N} [\frac{1}{2m} \vec{p}_i^{\,2} + V(\vec{r}_i) + \sum_{i=1}^{N} U(\vec{r}_i, \vec{r}_j)]$$

trapping potential

interaction potential

Mezoscopic realizations - very promising for Quantum Informatics !

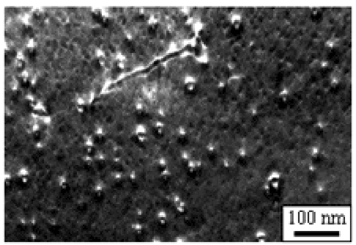
Coulomb interaction $U(\vec{r}_1, \vec{r}_2) = \frac{\lambda}{|\vec{r}_1 - \vec{r}_2|}$

contact interaction $U(\vec{r}_i, \vec{r}_j) = \frac{4\pi\hbar^2 a}{m} \delta(\vec{r} - \vec{r}\,')$

electrons: Quantum Dots

ions: Penning traps

atoms, molecules: quantum gas in optical lattice



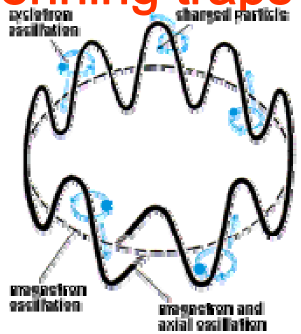
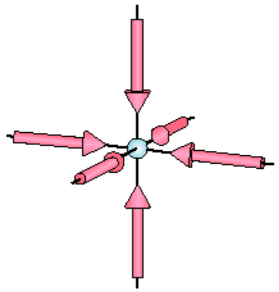
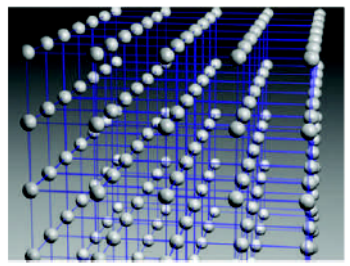


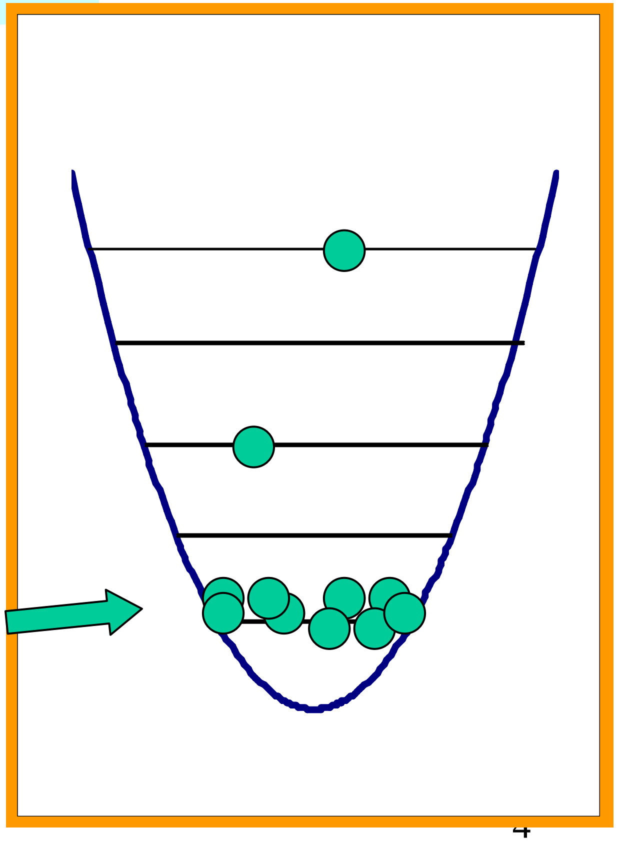
fig. 9





Non-interacting bosons

$$H(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{i=1}^{N} [-\frac{\hbar^2}{2m_i}\Delta_i + V(\vec{r}_i)]$$



$$H\psi_n(\vec{r}) = E_n \psi_n(\vec{r})$$

one-particle states

ff

Interacting bosons

$$H(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)=\sum_{i=1}^{N}[-\frac{\hbar^2}{2m_i}\Delta_i+V(\vec{r}_i)]+\sum_{i=1}^{N}U(\vec{r}_i,\vec{r}_j)$$

One-particle reduced density matrix

$$\rho(\vec{r},\vec{r}\,')=\int d\vec{\xi}_2\ldots d\vec{\xi}_N\ \Psi^*(\vec{r},\vec{\xi}_2,\ldots,\vec{\xi}_N)\Psi(\vec{r}\,',\vec{\xi}_2,\ldots,\vec{\xi}_N) \qquad Tr\,\rho=1$$

Diagonalization:

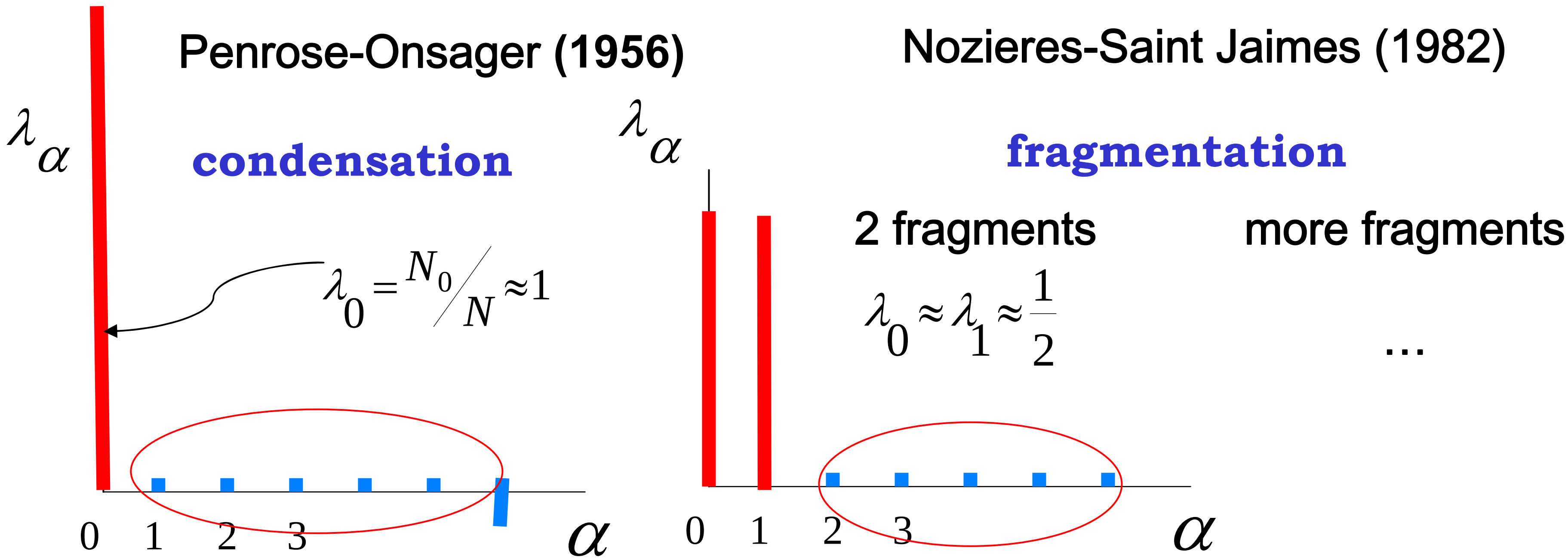
natural orbitals:

$$\rho(\vec{r},\vec{r}\,')=\sum_{\alpha}\lambda_\alpha \nu_\alpha^*(\vec{r})\nu_\alpha(\vec{r}\,') \qquad \sum_{\alpha}\lambda_\alpha=1$$

occupation fractions

Interacting bosons

Distribution of occupancies of natural orbitals:



quasi-1D traps

low T

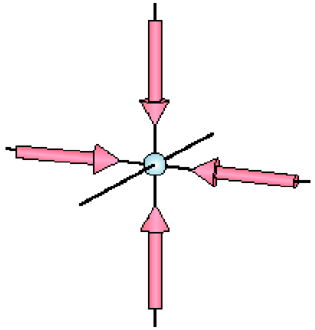
$$g = \frac{2\pi\hbar^2 a}{m}$$

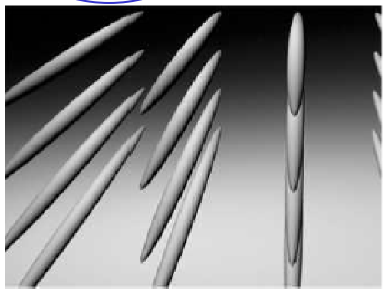
3D

$$H(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{i=1}^{N} [-\frac{\hbar^2}{2m}\Delta_i + V(\vec{r}_i)] + g\sum_{i>j}^{N} \delta(\vec{r}_i - \vec{r}_j)$$

strong transverse confinement

$$\omega_\perp$$





60nm
15μm

1D

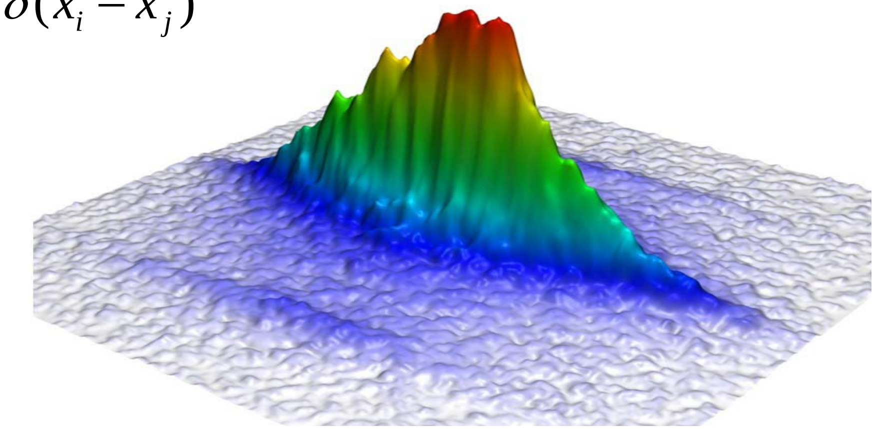
$$H(x_1, x_2, \ldots, x_N) = \sum_{i=1}^{N} [-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2} + V(x_i)] + g_{1D}\sum_{i>j}^{N} \delta(x_i - x_j)$$

M.Olshanii (1998)

$$g_{1D} = \frac{g}{\pi a_\perp^2}\left(1 - C\frac{a}{a_\perp}\right)^{-1} \qquad a_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}}$$

Tonks-Girardeau gas

$$H(x_1, x_2, ..., x_N) = \sum_{i=1}^{N} [-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2} + V(x_i)] + g_{1D}\sum_{i>j}^{N}\delta(x_i - x_j)$$



$g_{1D} \to \infty$

L.Tonks (1936) classical T→0

M.Girardeau (1960) quantum T→0
Bose-Fermi mapping:

$$\psi_B(x_1, x_2, ..., x_N) = |\psi_F(x_1, x_2, ..., x_N)| = \frac{1}{N!}\left|\det\begin{pmatrix} \chi_1(x_1) & \chi_2(x_1) & \dots & \chi_N(x_1) \\ \chi_1(x_2) & \chi_2(x_2) & \dots & \chi_N(x_1) \\ \dots & \dots & \dots & \dots \\ \chi_1(x_N) & \chi_2(x_N) & \dots & \chi_N(x_N) \end{pmatrix}\right|$$

strongly interacting (↑ ψ_B) **non-interacting** (↑ ψ_F)

2 interacting bosons

$$H(x_1, x_2) = \frac{1}{2m}\frac{\partial^2}{\partial x_1^2} + V(x_1) + \frac{1}{2m}\frac{\partial^2}{\partial x_2^2} + V(x_2) + g_{1D}\delta(x_1 - x_1)$$

2-particle wave function

$$\psi(x, y) = \sum_\alpha k_\alpha v_\alpha^*(x) v_\alpha(y)$$

$$\sum_\alpha k_\alpha^2 = 1$$

$$k_\alpha^2 = \lambda_\alpha$$

natural orbitals:

density matrix

$$\rho(x, y) = \sum_\alpha \lambda_\alpha v_\alpha^*(x) v_\alpha(y)$$

occupation fractions

Entanglement & Correlations

Schmidt Number:

$$\psi(x,y) = \sum_{\alpha} k_{\alpha} v_{\alpha}^{*}(x) v_{\alpha}(y)$$

number of nonvanishing terms

Non-entangled particles:

Ghirardi (2004)

distinguishable:	SN=1		
fermions:	SN=2	one determinant	Slater number =1
bosons	SN=1,2	one permanent	„Slater” number =1

Entangled particles:

distribution of Schmidt (Slater) modes provides a measure of entanglement

Correlation measures

Entanglement measures:

von Neumann entropy

$$S = -Tr\rho \log_2 \rho = -\sum k_\alpha^2 \log_2 k_\alpha^2 = -\sum \lambda_\alpha \log_2 \lambda_\alpha$$

linear entropy

$$L = 1 - Tr\rho^2 = 1 - \sum k_\alpha^4 = 1 - \sum \lambda_\alpha^2$$

K coefficient

$$K = \frac{1}{Tr\rho^2} = \frac{1}{1-L}$$

robustness

$$R = (Tr\phi)^2 - 1 = \left(\sum k_\alpha\right)^2 - 1$$

Correlation measures

Kutzelnigg coefficient

$$\tau = \frac{\left\langle \vec{r}_1 \cdot \vec{r}_2 \right\rangle - \left\langle \vec{r} \right\rangle^2}{\left\langle \vec{r}^{\,2} \right\rangle - \left\langle \vec{r} \right\rangle^2} = \frac{\int \vec{r}_1 \cdot \vec{r}_2 \, \phi^2(\vec{r}_1, \vec{r}_2)}{\int \vec{r}^{\,2} n(\vec{r})}$$

$\left\langle \vec{r} \right\rangle = 0$

position measured from the trap center

Correlation measures

Correlation energy $$E_c = E_{mean\ field} - E_{exact}$$

mean field for bosons:

$$\Phi_{GP}(x_1, x_2) = \psi(x_1)\psi(x_2),$$

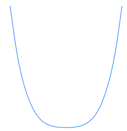
$$E_{GP}[\psi] = 2\int_{-\infty}^{-\infty} \frac{1}{2}\left|\frac{d\psi(x)}{dx}\right|^2 + V(x)|\psi(x)|^2 + \frac{g_{1D}}{2}|\psi(x)|^4 dx.$$

$$\mu\psi(x) = -\frac{1}{2}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) + g_{1D}|\psi(x)|^2\psi(x)$$

Gross-Pitaevski equation

$$\int \left|\psi(\vec{r})\right|^2 d\vec{r} = 1 \quad \longrightarrow \quad \mu \quad \longrightarrow \quad E_{GP} = E_{GP}[\psi]$$

Harmonic trap



$$H(x_1,x_2) = -\frac{1}{2}\frac{\partial^2}{\partial x_1^2} - \frac{1}{2}\frac{\partial^2}{\partial x_2^2} + \frac{1}{2}\left(x_1^2 + x_2^2\right) + \hat{g}_{1D}\delta\left(x_1 - x_1\right)$$

ratio of interaction to confinement energy

$$\hat{g}_{1D} = \sqrt{\frac{m}{\hbar^3\omega}}g_{1D}$$

separation of variables

$$H = H^{CM} + H^{r}$$

$$X = \frac{1}{\sqrt{2}}(x_1 + x_2)$$

$$x = \frac{1}{\sqrt{2}}(x_2 - x_1)$$

$$\psi(x_1,x_2) = \psi^{r}(x)\psi^{CM}(X)$$

CM eq: $H^{CM}\psi^{CM} = E^{CM}\psi^{CM}$

$$H^{CM} = -\frac{1}{2}\frac{\partial^2}{\partial X^2} + \frac{1}{2}X^2$$

$$\psi_n^{CM}(X) \propto H_n(X)e^{-X^2/2}$$

$$E_n^{CM} = n + \frac{1}{2}$$

relative motion eq: $H^r\psi^r = E^r\psi^r$

$$H^{r} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2 + \frac{g_{1D}}{\sqrt{2}}\delta(x)$$

$$\psi_m^r(x) \propto U\left(\frac{1}{4}(1 - E_m^r), \frac{1}{2}, x^2\right)e^{-x^2/2}$$

$$-\frac{2}{\Gamma\left[\left(1 - E_m^r\right)/4\right]} = \frac{g_{1D}}{\sqrt{2}\Gamma\left[\left(3 - 2E_m^r\right)/4\right]}$$

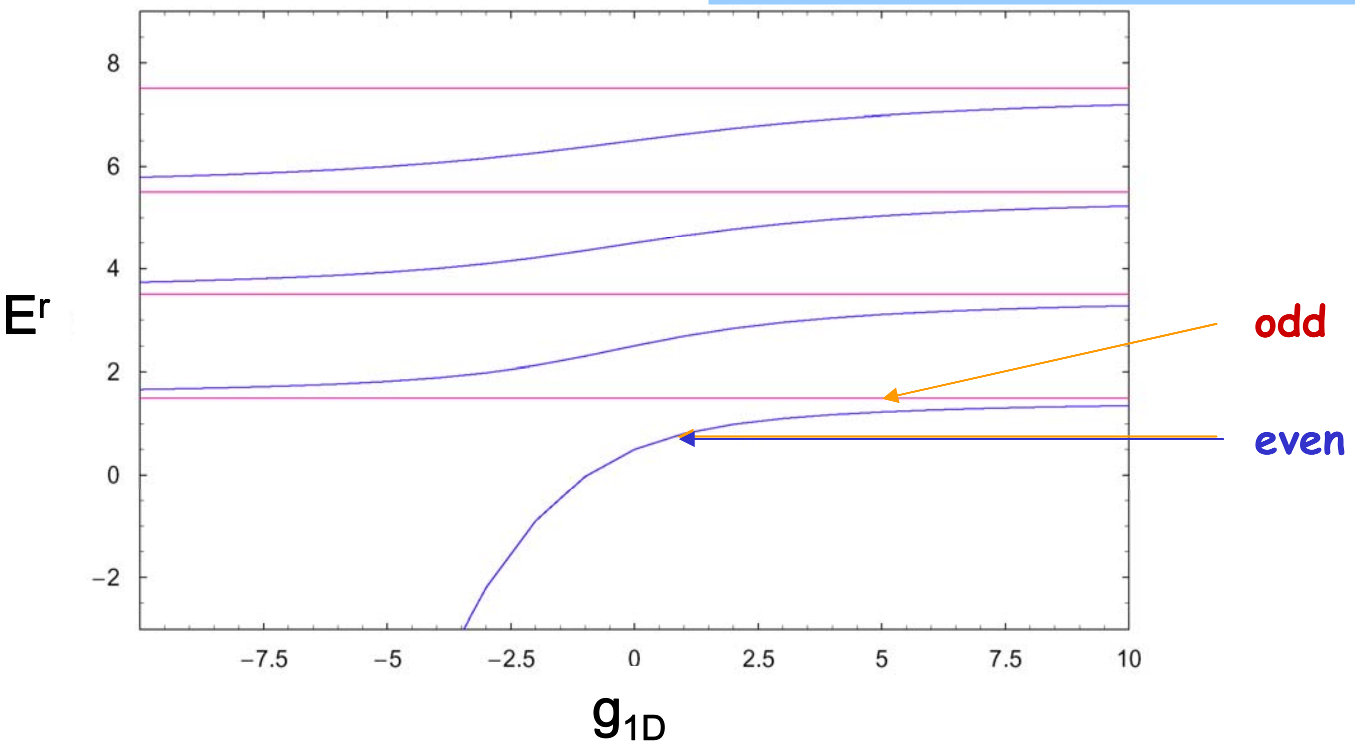
Grobe, Rzazewski,Eberly (1994)

Harmonic trap

Relative motion

$$\psi_m^r(x) \propto U\left(\frac{1}{4}(1-E_m^r), \frac{1}{2}, x^2\right) e^{-x^2/2}$$

$$-\frac{2}{\Gamma\left[(1-E_m^r)/4\right]} = \frac{g_{1D}}{\sqrt{2}\,\Gamma\left[(3-2E_m^r)/4\right]}$$



Harmonic trap

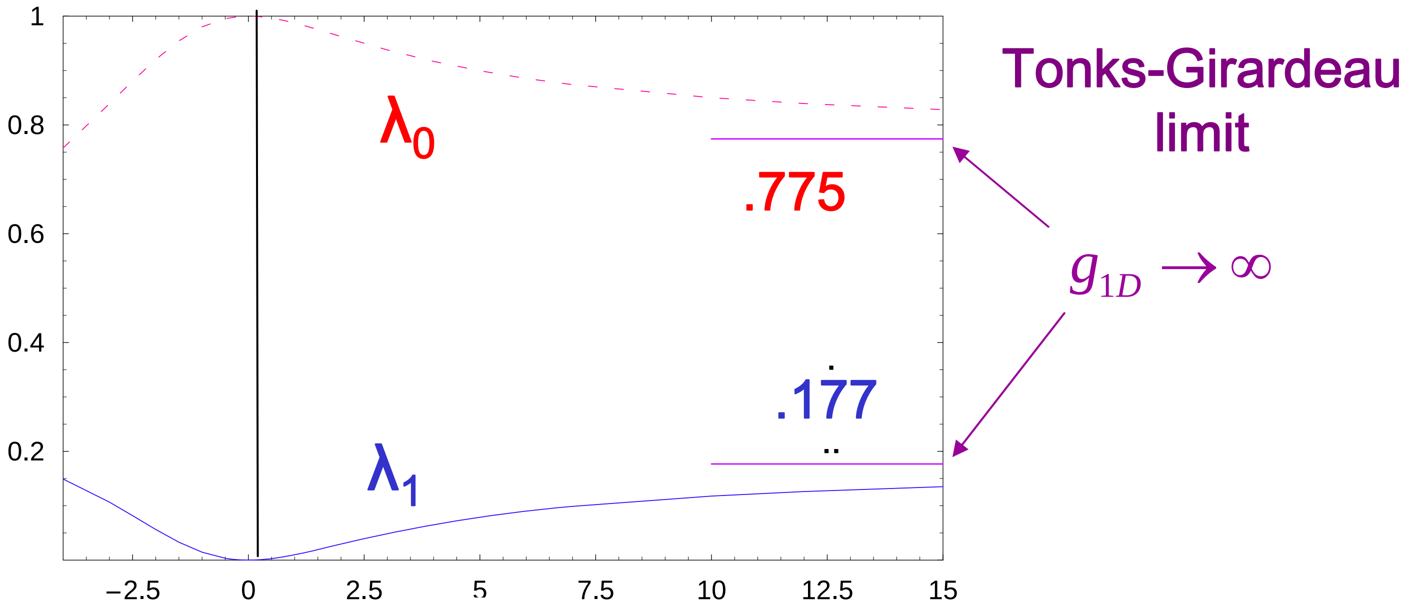
Ground state of the 2-particle system

$$\psi_{GS}(x,y) = \sum_{\alpha} k_{\alpha} v_{\alpha}^{*}(x) v_{\alpha}(y)$$

solved through discretization

$$\lambda_{\alpha} = k_{\alpha}^{2}$$

occupancies of the lowest natural orbitals



attraction

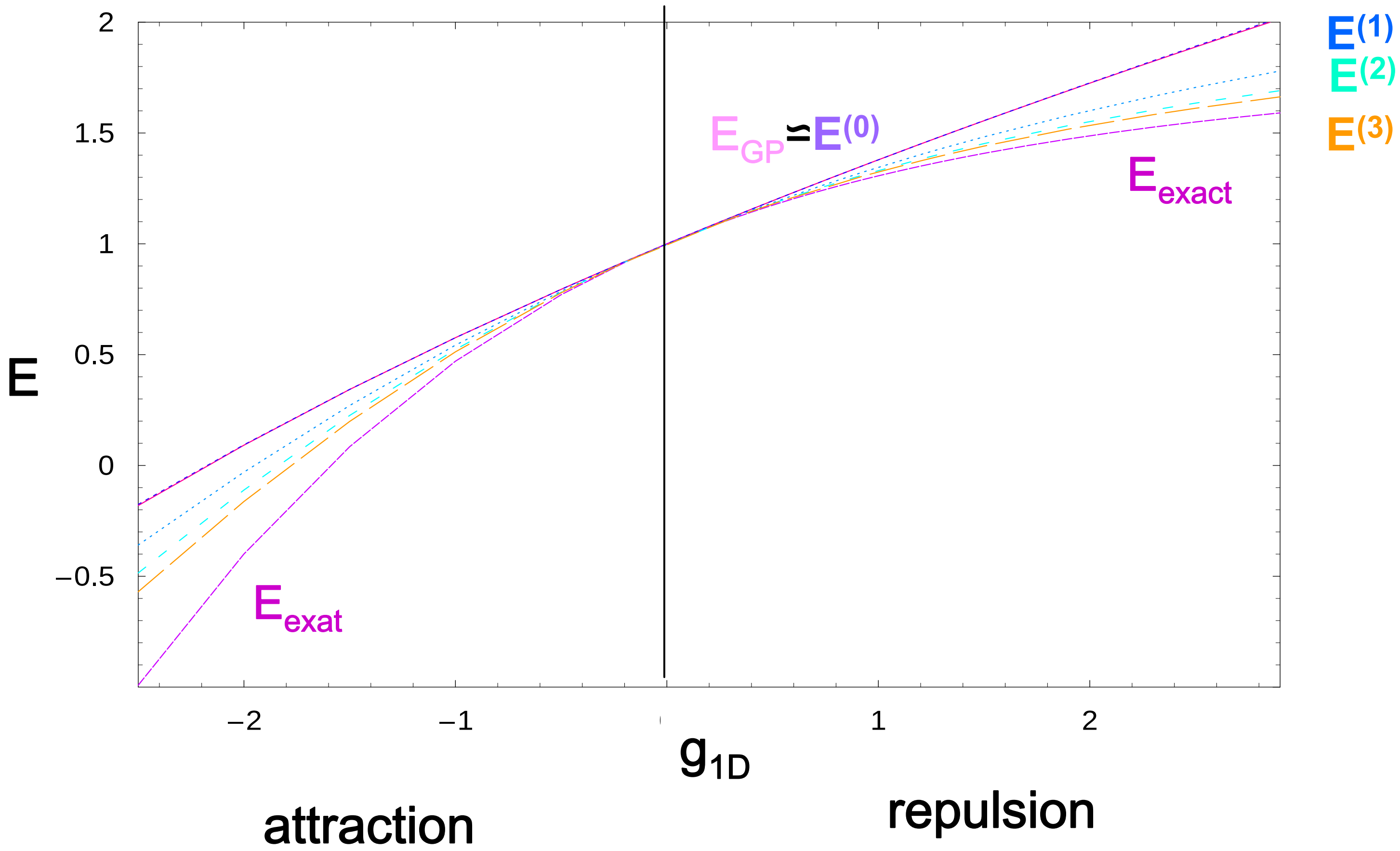
g_{1D} repulsion

Harmonic trap

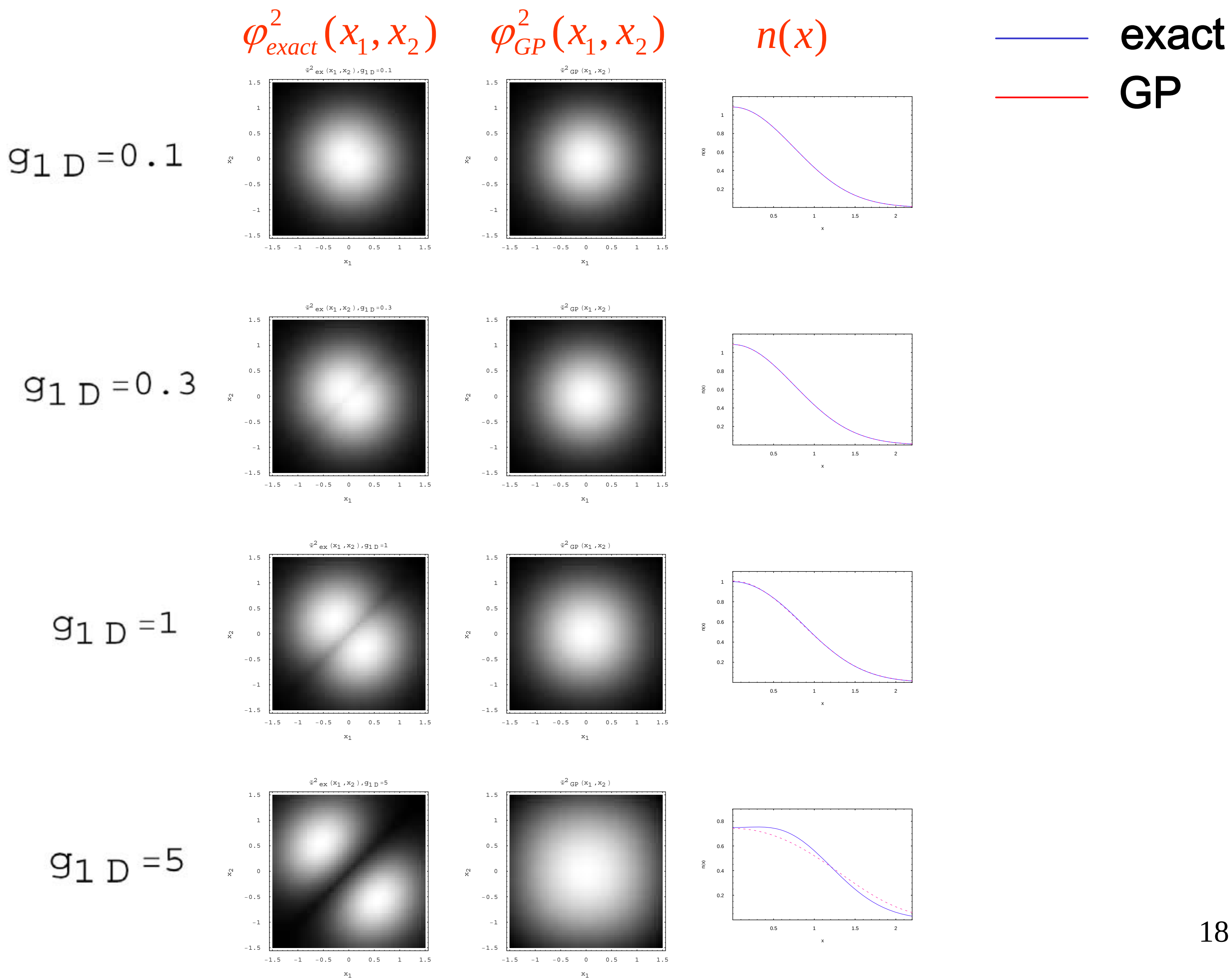
Orbital expansion

$$\psi_N(x,y) = \sum_{\alpha=0}^{N} k_\alpha v_\alpha^*(x) v_\alpha(y)$$

$$E^{(N)} = \langle \Phi^N | H | \Phi^N \rangle / \| \Phi^N \|^2$$

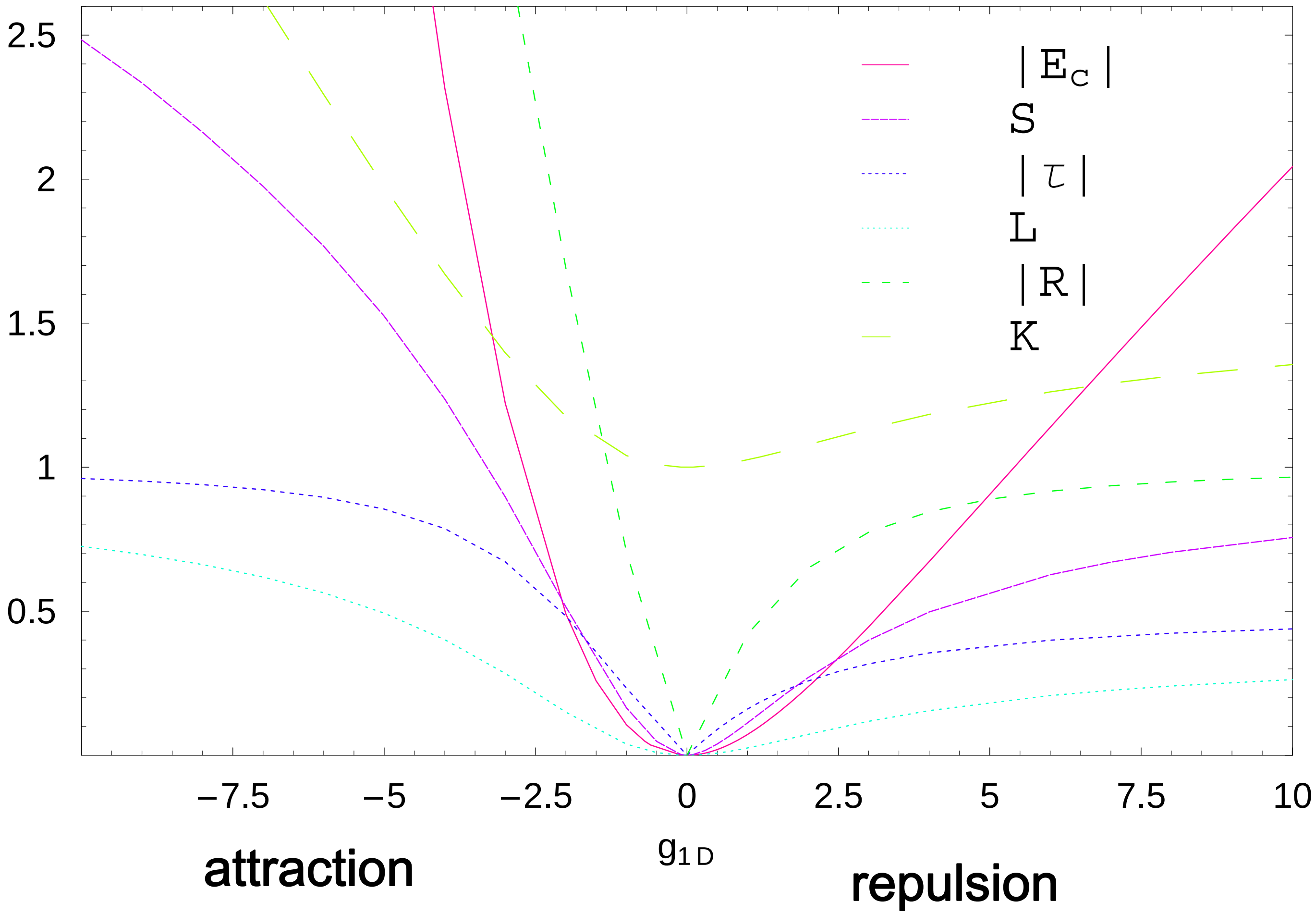


Harmonic trap



Harmonic Trap

Correlation measures



Non-harmonic confinement

$$H(x_1,x_2) = -\frac{1}{2}\frac{\partial^2}{\partial x_1^2} + V(x_1) - \frac{1}{2}\frac{\partial^2}{\partial x_2^2} + V(x_2) + g_{1D}\delta(x_1 - x_2)$$

$$V(x) = wx^2 + z_4 x^4 + z_6 x^6 + \ldots$$

Optimized Configuration Interaction method

Rayleigh-Ritz

$$\phi_D(x_1,x_2) = \sum_{j\geq i}^{D} a_{ij}\psi_{ij}(x_1,x_2).$$

$$\psi_{ij}(x_1,x_2) = \begin{cases} \varphi_j(x_1)\varphi_j(x_2) & \text{for} \quad i=j \\ \frac{1}{\sqrt{2}}[\varphi_i(x_1)\varphi_j(x_2) + \varphi_j(x_1)\varphi_i(x_2)] & \text{for} \quad i\neq j \end{cases}$$

$$\varphi_i^{\Omega}(x) = \left(\frac{\sqrt{\Omega}}{\sqrt{\pi}2^i i!}\right)^{\frac{1}{2}} H_i(\sqrt{\Omega}x)e^{-\frac{\Omega x^2}{2}}.$$

optimization of Ω

Principle of Minimal Sensitivity

$$\frac{\partial TrH}{\partial \Omega} = 0$$

A.O. (1987)
P.K , A.O. (2007)

$$TrH = \sum_{n=0}^{(D+1)(D+2)/2} E_n(\Omega)$$

Non-harmonic confinement

Determining natural orbitals

$$\int \phi(x,x')v(x')dx' = kv(x)$$

through the optimized CI method

$$\phi_D(x_1,x_2) = \sum_{j\geq i}^{D} a_{ij}\psi_{ij}(x_1,x_2).$$

$$v(x) = \sum p_n \varphi_n^{\Omega}(x)$$

$$\sum (A_{mn} - k_n\delta_{mn})p_n = 0,$$

$$A_{mn} = \int \varphi_m^{\Omega}(x_1)\phi_D(x_1,x_2)\varphi_n^{\Omega}(x_2)dx_1dx_2 = \left\{ \begin{array}{lll} a_{nn} & \text{for} & n=m \\ \frac{a_{nm}}{\sqrt{2}} & \text{for} & m>n \\ \frac{a_{mn}}{\sqrt{2}} & \text{for} & n>m \end{array} \right\}$$

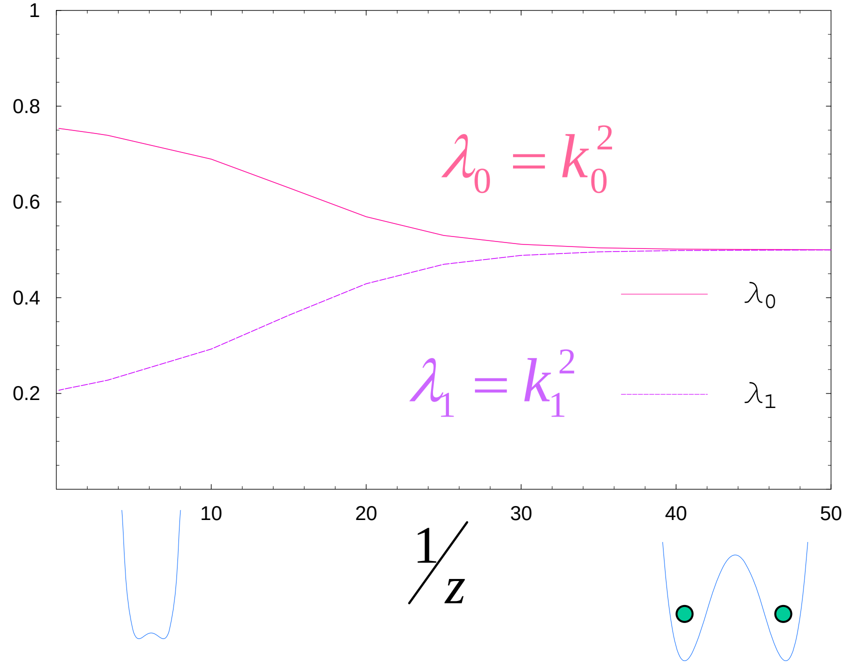
diagonalization of A → k_α → $\lambda_\alpha = k_\alpha^2$

TG limit

Double-well trap

$$V(x) = -\frac{1}{2}x^2 + zx^4$$

occupancies of the lowest natural orbitals



$$k_n \approx 0 : n > 1,$$

$$k_0 \approx \frac{1}{\sqrt{2}}, k_1 \approx -\frac{1}{\sqrt{2}}$$

$$v_0(x) = \frac{1}{\sqrt{2}}[\phi_0(x) + \phi_1(x)]$$

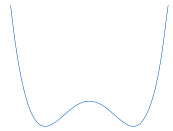
$$v_1(x) = \frac{1}{\sqrt{2}}[\phi_0(x) - \phi_1(x)]$$

$$\langle \phi_1 | \phi_0 \rangle = 0$$

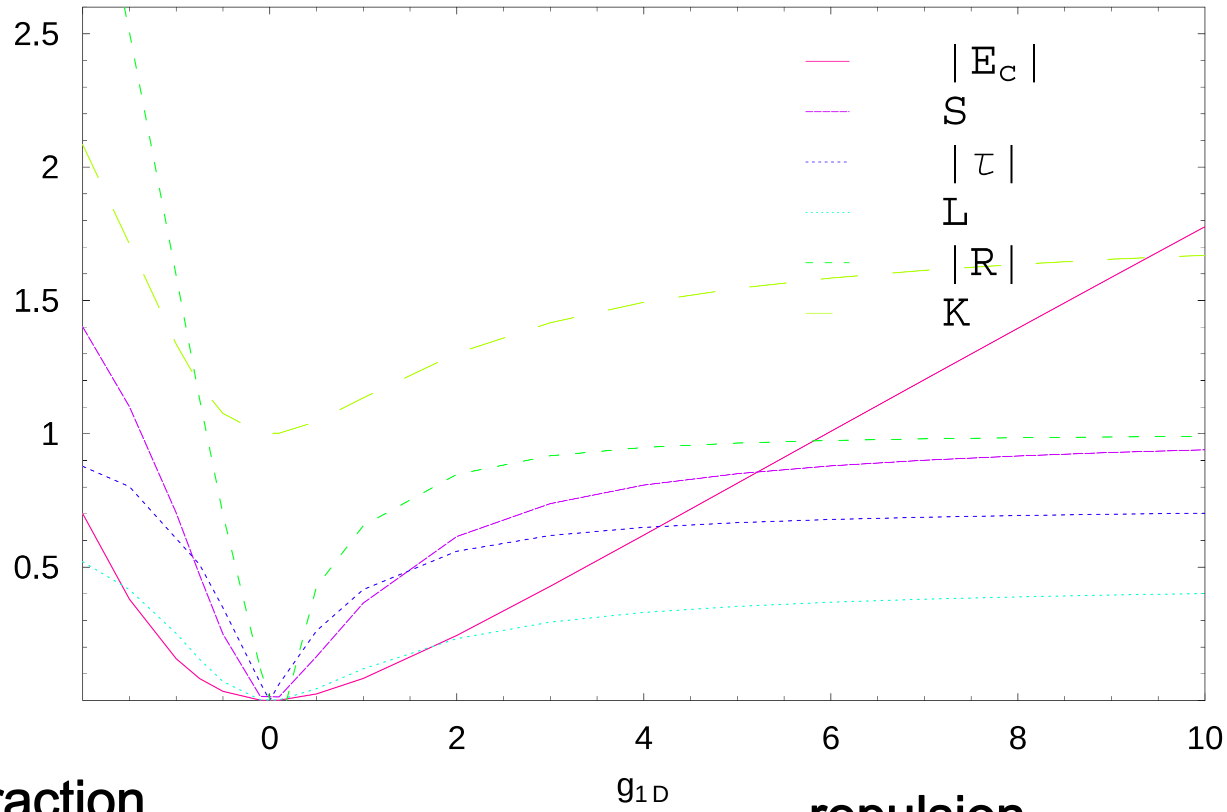
$$\psi(x_1, x_2) \approx \frac{1}{\sqrt{2}}[v_0(x_1)v_0(x_2) - v_1(x_1)v_1(x_2)] = \frac{1}{\sqrt{2}}[\phi_1(x_1)\phi_0(x_2) + \phi_0(x_1)\phi_1(x_2)]$$

Double well trap

$$V(x) = -\frac{1}{2}x^2 + \frac{1}{10}x^4$$



Correlation measures



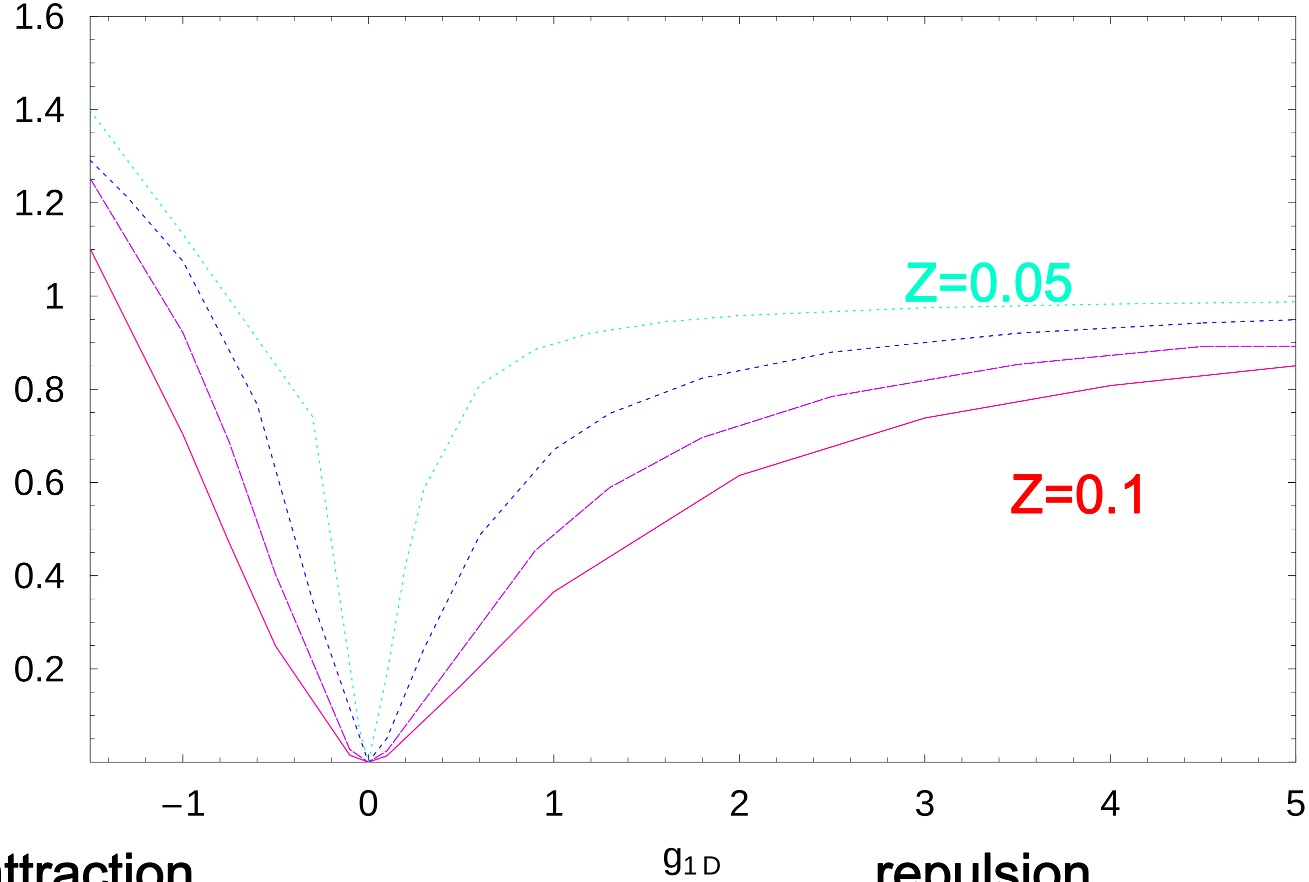
attraction

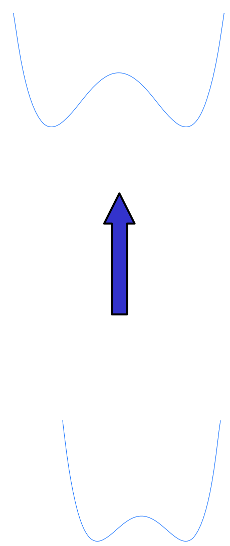
repulsion

Double-well trap

Von Neumann entropy

$$V(x) = -\frac{1}{2}x^2 + zx^4$$





attraction repulsion

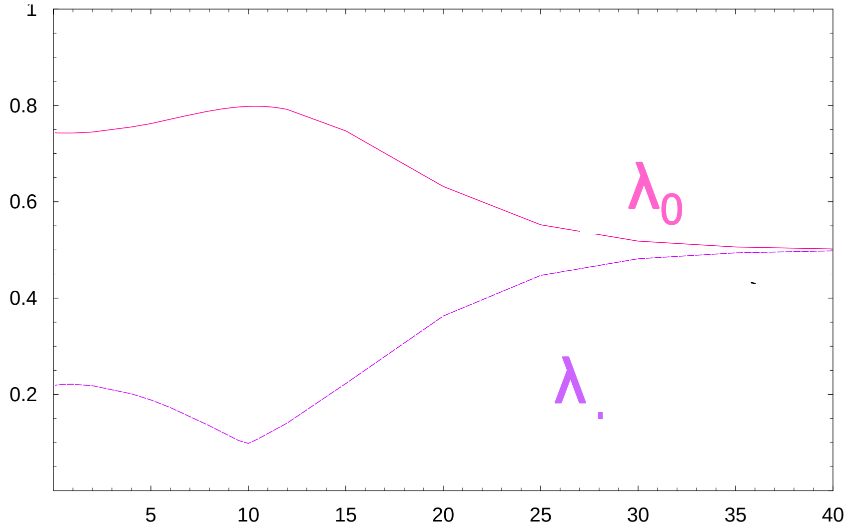
the deeper the wells, the smaler g_{1D} for which the TG behavior is achieved

TG limit

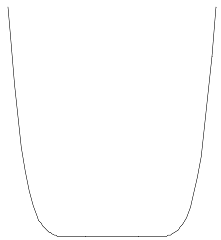
Triple-well trap

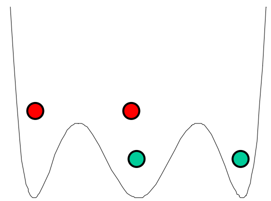
$$V_3(x,a) = \frac{1}{2}x^2 - ax^4 + \frac{a^2}{2}x^6,$$

occupancies of the lowest natural orbitals



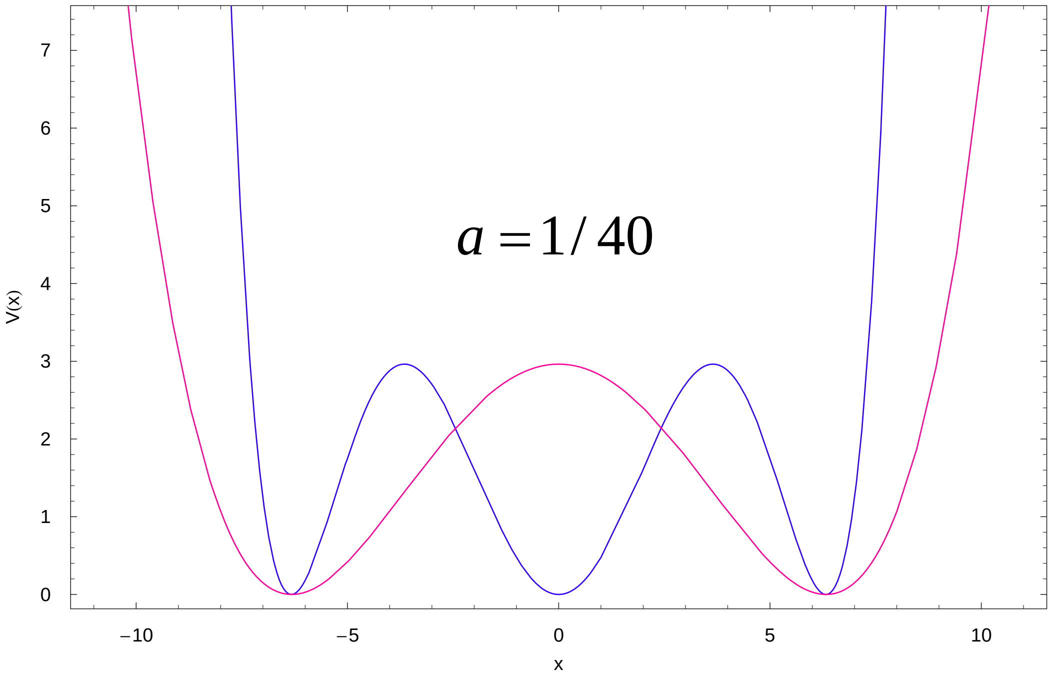
$1/a$





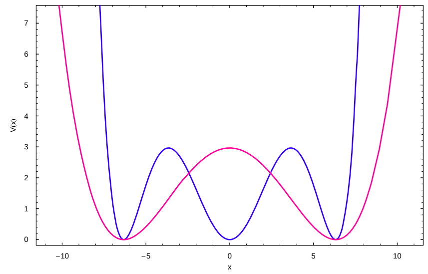
Comparison of 2- and 3-well case

$$V(x,a) = \frac{2}{27a}(x^2 a - 1)^2 \qquad V_3(x,a) = \frac{1}{2}x^2 - ax^4 + \frac{a^2}{2}x^6,$$

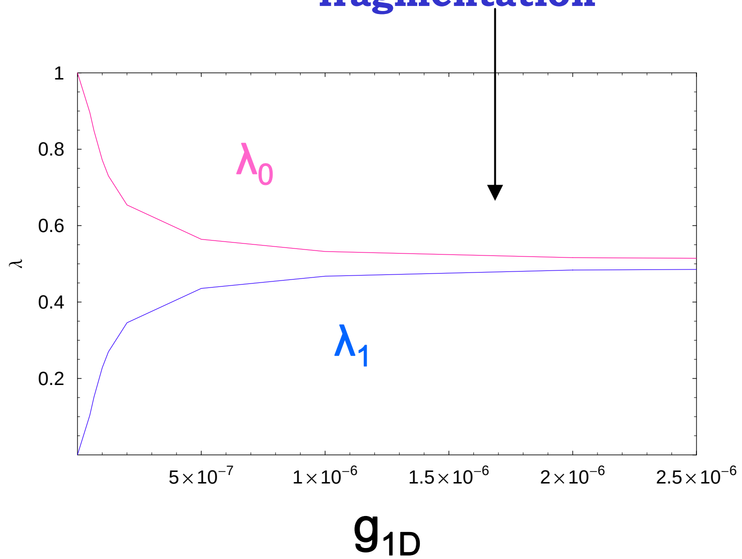


a↘ the barriers higher and wider

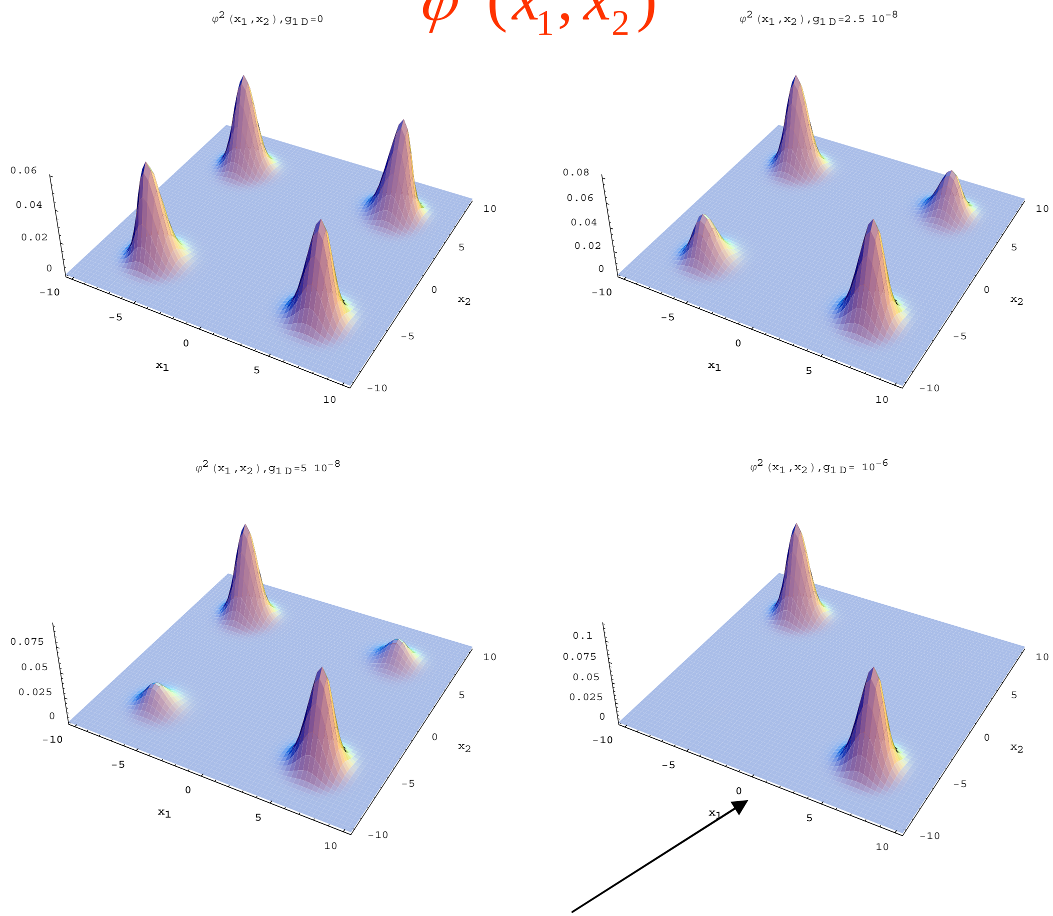
Double-well



fragmentation

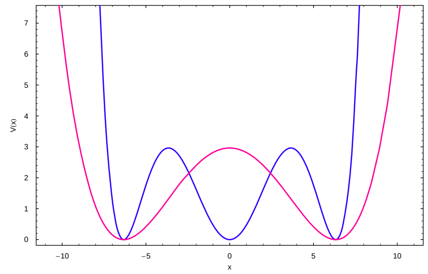


$\varphi^2(x_1, x_2)$



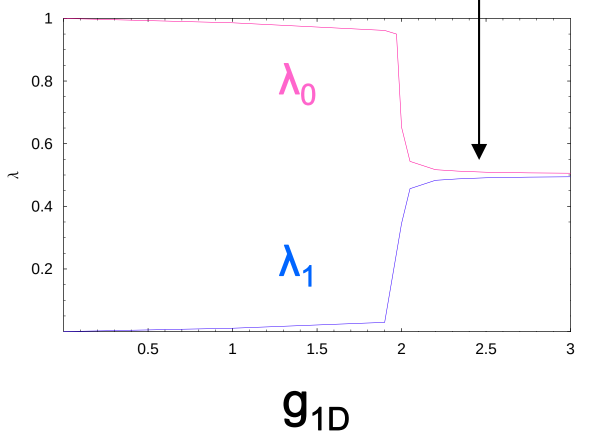
fragmentation

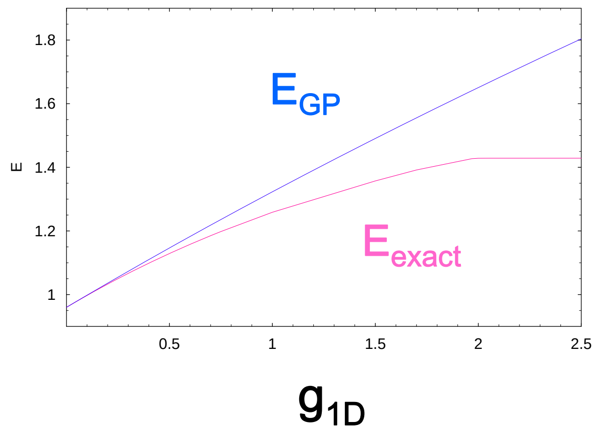
Triple-well

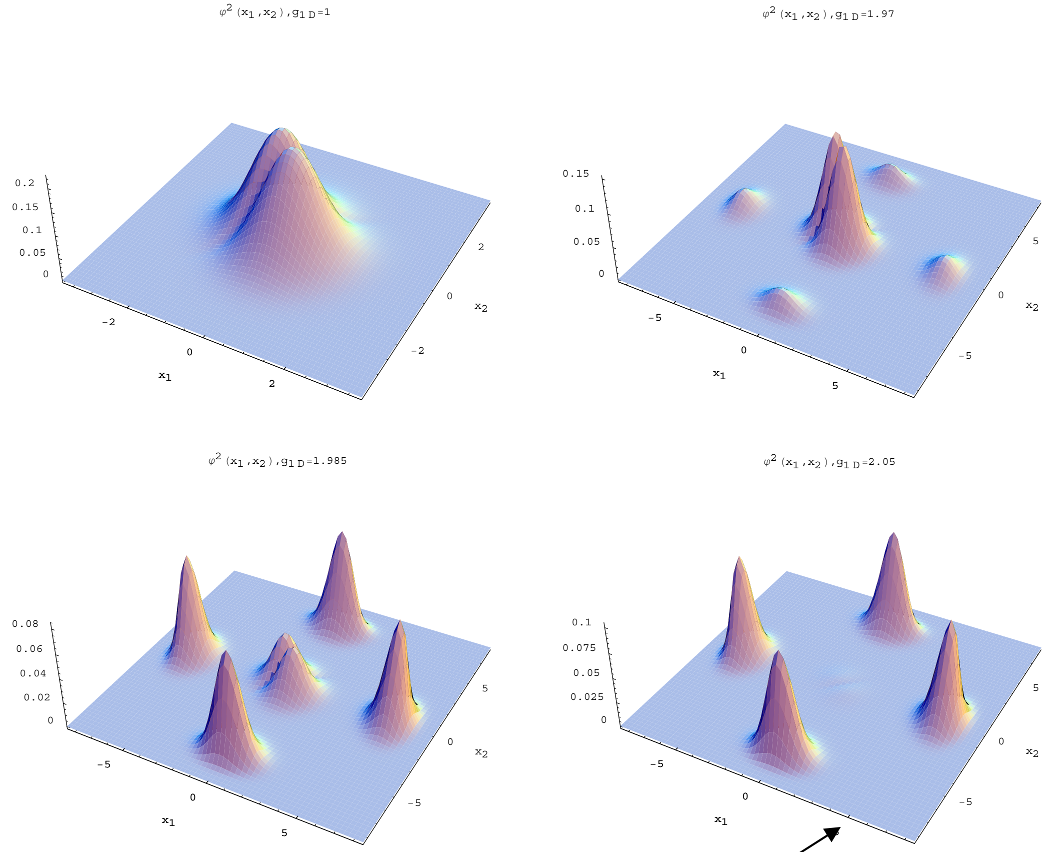


$\varphi^2(x_1, x_2)$

fragmentation







fragmentation

Summary

Ground-state properties of 2-boson systems in function of the contact interaction strength g_{1D} and the confining potential shape

HO confinement

- evolution is smooth in the entire range of g_{1D} : from the attractive to the repulsive case
- various entanglement measures reveal comparable behavior in function of g_{1D}
- correlation energy shows a behavior different from other correlation measures
- mean field (GP) approach applicable only if the interparticle interaction is very weak

DOUBLE- AND TRIPLE- WELL confinement

- occupancies of natural orbitals, strongly depend on the number of potential wells
- behavior of entanglement measures is similar as in the HO confinement case
- fragmentation in non-convex confining potentials depends on the barriers height
- the value of g_{1D}, for which the Tonks-Girardeau regime is approximately achieved depends on the number of potential wells and on their depth: the deeper the barriers, the quickest fermionization

Outlook

Optimized Configuration Interaction method shows high efficiency in determining the Schmidt eigenspectrum of confined few-particle systems

Work in progress : application of the optimized CI method to

- **excited states**
- **resonances**
- **other interaction potentials: 1/r, $1/r^3$,…**
- **N>2 bosons**
- **N>2 fermions - QDs**